Lecture Notes on

Mathematical Ecology and Pattern Formation

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1 Introduction

Ecology is a subdiscipline of biology. It can be defined by (according to Wikipedia): *Ecology is the scientific study of the relation of living organisms with each other and their surroundings.* A formalization in mathematical language has taken place for subfields, most importantly that of *population ecology*, dealing with the effects of births and deaths on the development of populations, i.e. groups of individuals of the *same species,* sharing a living environment (*habitat*). A realistic description of the dynamics of a population might involve the interaction of the population with the environment and with other populations, but also the internal structure (e.g. age or size structure) of the population, or its spatial distribution in the environment. For the purpose of modeling the spatial distribution, we shall consider large ensembles of what we call *particles*. This expression is borrowed from physics. Here, a particle will be any object able to move individually, and which is small compared to the length scales we are interested in. This leads to the idealization of *point particles*. Depending on the situation these can be molecules, cells, or even multicellular organisms. Under the assumption of (partially) random motion of the individual particles, we shall derive mathematical models for the movement of large particle ensembles.

What is a *pattern?* In a scientific context this term usually has a more general meaning than in colloquial English. It stands for any form of recognizable *order*. This last expression in turn has a probabilistic defintion

which distinguishes it from its opposite, *chaos*. We only state an example: If, in the room of a teenager, the probability to find clothes in the closet is at least marginally higher than the probability to find them in any other place, this already constitutes a form of order, although the average parent might not agree with this defintion.

In this course we shall be interested in understanding mechanisms for the creation of patterns, and our motivation will be taken from biology. Some of the most fascinating and still poorly understood pattern formation mechanisms occur in the development of embryos. The wider term *morphogenesis*, i.e. the creation of different forms and shapes, is often used in this context. Meta-theories often state the existence of *morphogenes* as the carriers of structural information. Pattern formation is then described as a process, where many morphogenes of different types interact with each other and with the environment, influencing their creation, annihilation, and movement.

2 Time discrete, spatially homogeneous, single species population dynamics

In this section models for the time evolution of the number of individuals in a population will be considered. We neglect the interaction with other species (see Section 4) and possibly varying properties of individuals within the same population, which would be considered in structured population models (see Section 5). As a third assumption we consider populations with no or small overlap between generations, justifying a time discrete description. Typical models assume that the size N_{k+1} of the population in generation $(k+1)$ only depends on the size of the population in the kth generation, i.e. there is a recursion of the form

$$N_{k+1} = f(N_k)\,. \tag{1}$$

The simplest assumption is that of a constant birth rate r: $f(N) = rN$. In this case the recursion can be solved easily: $N_k = N_0 r^k$, i.e. for $r > 1$ the population grows exponentially, and for $r < 1$ it dies out. For most situations this model is too simple, of course.

2.1 A historical example: the Fibonacci numbers

As a historical remark we describe what can be considered as one of the first contributions to Mathematical Biology. In the year 1202 *Leonardo di*

Pisa (later also called *Fibonacci*) published a book on arithmetic, where he proposed a simple model for the proliferation of rabbits. The modeling assumption is that rabbits reach adulthood after one month and that one month later each couple (female + male) has two babies (again male + female) and the same every month thereafter (attention: wrong explanation in [6]).

Neglecting death of rabbits, these assumptions lead to the recursion

$$N_{k+1} = N_k + N_{k-1}$$

for the number N_k of couples in the kth generation. In contrast to (1) this is a *two-stage recursion*, where the population size is determined by two previous generations. Starting with a pair of newborn rabbits, i.e. $N_0 = 1$, no new rabbits are born after the first month, i.e. $N_1 = 1$. From the second month on the recursion can be used, producing the so called *Fibonacci sequence*

$$1, 1, 2, 3, 5, 8, 13, \ldots$$

In the following an explicit formula for its terms will be derived. The first observation is that the Fibonacci recursion

$$u_{k+1} = u_k + u_{k-1}\,, \qquad k \geq 1 \tag{2}$$

constitutes an (infinite) system of homogeneous linear equations. Therefore the set of all solutions is a vector space. Since u_0 and u_1 can be chosen arbitrarily and determine the sequence uniquely, this vector space is two-dimensional. A basis $\{\{a_k\}, \{b_k\}\}$ can be determined by

$$\begin{aligned} a_0 &= 1\,, \quad a_1 = 0\,, \quad a_{k+1} = a_k + a_{k-1}\,, \quad k \geq 1\,, \\ b_0 &= 0\,, \quad b_1 = 1\,, \quad b_{k+1} = b_k + b_{k-1}\,, \quad k \geq 1\,, \end{aligned}$$

leading to $a_k = N_{k-2}$ und $b_k = N_{k-1}$ für $k \geq 2$. Every solution of the recursion can be written as

$$u_k = u_0 a_k + u_1 b_k\,, \quad k \geq 0\,.$$

Without an explicit formula for a_k und b_k, this is not very helpful, however. We shall derive an explicitly computable basis. Motivated by the general solution of the linear one-step recursion above, we make the ansatz $u_k = \lambda^k$. This leads to the quadratic equation

$$\lambda^2 = \lambda + 1\,,$$

with the solutions

$$\lambda_{1,2} = \frac{1 \pm \sqrt{5}}{2}\,,$$

(where λ_1 is the *golden ratio* or *sectio aurea*). Thus, an explicit basis for the set of solutions is given by $\{\{\lambda_1^k\}, \{\lambda_2^k\}\}$, and every solution has the form

$$u_k = c\lambda_1^k + d\lambda_2^k$$

with suitable constants c and d. In particular, the Fibonacci sequence can be written as

$$N_k = \frac{1}{2}\left(1 + \frac{1}{\sqrt{5}}\right)\lambda_1^k + \frac{1}{2}\left(1 - \frac{1}{\sqrt{5}}\right)\lambda_2^k\,.$$

For the behavior after many generations it is important to note that $|\lambda_1| > 1$ and $|\lambda_2| < 1$. For large values of k this implies

$$N_k \approx \frac{1}{2}\left(1 + \frac{1}{\sqrt{5}}\right)\lambda_1^k\,,$$

i.e. the Fibonacci sequence is approximately equal to a solution of the one-step recursion $u_{k+1} = \lambda_1 u_k$.

2.2 The logistic map – chaos

We return to population models in the form of one-step recursions (1) and note that the linear model $f(N) = rN$ cannot describe populations which neither die out nor grow above all bounds. In a limited environment it seems reasonable to assume that the growth rate depends on the size of the population, getting smaller for larger populations. In the simplest model of this kind, the constant growth rate r is replaced by $r(1 - N_k/N_{max})$, producing the *logistic map* $f(N) = rN(1 - N/N_{max})$ as the right hand side of (1):

$$N_{k+1} = rN_k\left(1 - \frac{N_k}{N_{max}}\right)\,.$$

Obviously, N_{max} is the largest sensible value of the population size, since otherwise the population size would be predicted to be negative in the following generation. We therefore require that f maps the interval $[0, N_{max}]$ into itself. This leads to the restriction $r \leq 4$ for the growth rate of small populations. The scaling $u_k := N_k/N_{max}$ produces the simplified recursion

$$u_{k+1} = ru_k(1 - u_k)\,, \tag{3}$$

which will keep us busy for the rest of this section. In contrast to what we did so far, (3) is *nonlinear,* and explicit formulas for general solutions cannot be expected. We shall try instead to derive *qualitative* statements on the long time behavior of solutions. Our basic assumptions will be

$$0 < r \leq 4\,, \qquad 0 \leq u_0 \leq 1\,,$$

guaranteeing, that $0 \leq u_k \leq 1$ holds for all $k \geq 0$. It will turn out that the long time behavior of typical solutions strongly depends on the value of the parameter r. Easily understandable is the situation for $r < 1$. Since obviously $u_{k+1} \leq r u_k$, complete induction easily shows $u_k \leq r^k u_0$, implying that all solutions converge to zero as $k \to \infty$, and the population dies out.

This is a good point to start introducing some terminology from the theory of *dynamical systems.* The recursion (3) with the restriction $0 < r \leq 4$ is an example for a dynamical system on the *state space* $[0, 1]$. This means that every initial state u_0 in the state space leads to a time dynamics remaining in the state space. With $u_0 = 0$ the recursion produces the constant solution $u_k = 0$, $k \geq 0$. For this reason, 0 is called a *stationary point.* Stationary points can be determined as solutions $\overline{u}$ of the equation $\overline{u} = r\overline{u}(1 - \overline{u})$.

The important question of *stability* of stationary points arises, dealing with the dynamics, when the initial state is chosen close to the stationary point. A stationary point is called stable, if the dynamics remains close to the stationary point, whenever starting close enough to it. More precisely (but harder to understand):

Definition 1 *The stationary point $\overline{u}$ is called* **stable,** *if for every $\varepsilon > 0$ there exists $\delta > 0$, such that for all u_0 in the state space satisfying $|u_0 - \overline{u}| < \delta$, $|u_k - \overline{u}| < \varepsilon$, $k \geq 0$, follows. Otherwise, the stationary point is called* **unstable**.

In a stricter version it is required that every sequence starting close enough to the stationary point converges to it:

Definition 2 *The stationary point $\overline{u}$ is called* **asymptotically stable,** *if there exists $\delta > 0$, such that for all u_0 in the state space satisfying $|u_0 - \overline{u}| < \delta$, $\lim_{k\to\infty} u_k = \overline{u}$ holds.*

Our observations above show that for $r < 1$ the stationary point $\overline{u} = 0$ is asymptotically stable.

Consider a general one-stage recursion

$$u_{k+1} = f(u_k) \tag{4}$$

with a stationary point $\overline{u} = f(\overline{u})$. Since stability is a local property, it seems reasonable to use the linear approximation of f around $\overline{u}$. With $v_k = u_k - \overline{u}$, this leads to the approximative recursion

$$v_{k+1} = f'(\overline{u})v_k \,.$$

This is called the *linearization* of (4) at $u = \overline{u}$. The explicit solution $v_k = f'(\overline{u})^k v_0$ of the linearized recursion makes the following result plausible:

Theorem 1 *Let $f : [a,b] \to [a,b]$ be twice continuously differentiable. The stationary point $\overline{u}$ of the recursion (4) is asymptotically stable, if $|f'(\overline{u})| < 1$, and unstable, if $|f'(\overline{u})| > 1$.*

Proof: With the definition $v_k = u_k - \overline{u}$, Taylor expansion gives

$$v_{k+1} = f(u_k) - f(\overline{u}) = f'(\overline{u})v_k + f''(\tilde{u}_k)v_k^2/2\,, \tag{5}$$

with $\tilde{u}_k \in [a,b]$. As a consequence of the continuity on the closed interval $[a,b]$ of the second order derivative, $|f''(\tilde{u}_k)| \leq M$ holds and, thus

$$|v_{k+1}| \leq |v_k| \left(|f'(\overline{u})| + |v_k|M/2\right) \,.$$

In the case $|f'(\overline{u})| < 1$, we choose $\delta := (1 - |f'(\overline{u})|)/M$ and $r := (1 + |f'(\overline{u})|)/2 < 1$. Complete induction easily shows that $|v_0| \leq \delta$ implies the estimate $|v_k| \leq r^k\delta \to 0$ für $k \to \infty$, proving the first statement of the theorem.

For $|f'(\overline{u})| > 1$, we deduce from (5) that

$$|v_{k+1}| \geq |v_k|(|f'(\overline{u})| - |v_k|M/2)$$

holds. With $|v_k| \leq \varepsilon := (|f'(\overline{u})| - 1)/M$ and $r := (1 + |f'(\overline{u})|)/2 > 1$, we get

$$|v_{k+1}| \geq r|v_k|\,,$$

implying that for arbitrarily small $|v_0|$, $|v_k| > \varepsilon$ holds after a finite number of steps, which is equivalent with instability of $\overline{u}$. ∎

Remark 1 *In the critical case $|f'(\overline{u})| = 1$ anything is possible, as the examples $u_{k+1} = u_k(1 \pm u_k)$ and $u_{k+1} = u_k$ with $[a,b] = [0,1]$ and $\overline{u} = 0$ show.*

Let us return to the specific recursion (3). Theorem 1 shows that for increasing values of the parameter r, the stationary point $\overline{u}_1 = 0$ looses its stability at $r = 1$.

Definition 3 *For a parameter dependent dynamical system a* **bifurcation point** *is a point in parameter space, such that in arbitrarily small neighborhoods the dynamical system possesses qualitatively different long time behavior.*

Apparently $r = 1$ is a bifurcation point for (3). The behavior in its neighborhood can be understood by considering the second stationary point $\overline{u}_2 = 1 - 1/r$, which belongs to the state space for $r \geq 1$. At the bifurcation point both stationary points coincide. The identity $f'(\overline{u}_2) = 2 - r$ shows that $\overline{u}_2$ is asymptotically stable for $1 < r < 3$. At the bifurcation point $r = 1$, an *exchange of stability* between the stationary points $\overline{u}_1 = 0$ and $\overline{u}_2 = 1 - 1/r$ occurs.

At the second bifurcation point $r = 3$ the stationary point $\overline{u}_2$ also looses its stability. The behavior of the dynamical system for $r > 3$ can be understood by analyzing the sequences $z_k := u_{2k}$, $k \geq 0$, satisfying the recursion

$$z_{k+1} = ru_{2k-1}(1 - u_{2k-1}) = r^2 z_k(1 - z_k)(1 - rz_k(1 - z_k)) \,. \tag{6}$$

Besides $\overline{u}_1 = 0$ and $\overline{u}_2 = 1 - 1/r$, it possesses (for $r > 3$) the additional stationary points

$$\overline{z}_{3,4} = \frac{1}{2r}\left(1 + r \pm \sqrt{(r+1)(r-3)}\right) .$$

It is easily checked that $\overline{z}_3 = f(\overline{z}_4)$ and $\overline{z}_4 = f(\overline{z}_3)$, i.e. the points $\overline{z}_3$ and $\overline{z}_4$ constitute a *periodic orbit with period 2* of the original recursion (3). Note that at the bifurcation point $r = 3$ the periodic orbit grows out of the stationary point $\overline{u}_2$: $\overline{u}_2 = \overline{z}_3 = \overline{z}_4 = 2/3$ for $r = 3$.

The results described in the following are not as easy to check. It can be shown that $\overline{z}_3$ and $\overline{z}_4$ are asymptotically stable stationary points of (6) for $r > 3$, as long as r remains close enough to the value 3. This implies *asymptotic stability of the periodic orbit* of the recursion (3), where the meaning of this statement should be clear without an exact definition. This stability is lost at another bifurcation point $r = r_4$. The bifurcation is similar to the one at $r = 3$: From each of the stationary points $\overline{z}_3$ and $\overline{z}_4$ of the twice iterated map $f \circ f$, two new stationary points of the four times iterated map $f \circ f \circ f \circ f$ are created, which together constitute a stable periodic orbit with period 4 of (3). This kind of bifurcation event is called *period doubling*. For increasing values of r a sequence of period doublings occurs at the bifurcation points $r_4 < r_8 < r_{16} < \ldots$ This sequence converges to $r_c < 4$. Typical sequences created by (3) with $r > r_c$ do not exhibit any

recognizable order. This fact was a sensational finding (of the 1970s) and has been called *deterministic chaos.* An explicit example for a sequence with chaotic behavior is

$$u_k = \sin^2(2^k)\,,$$

a solution of (3) with $r = 4$.

3 Time continuous, spatially homogeneous, single species population dynamics

Verzweigungen

Eindimensionale Dynamik ist also recht langweilig. Lösungen konvergieren entweder gegen stationäre Punkte oder verabschieden sich Richtung $\pm\infty$. Nun wollen wir allerdings unsere Fragestellung verallgemeinern und Familien von dynamischen Systemen betrachten, indem wir die rechte Seite der Differentialgleichung von *Parametern* abhängig machen. Beginnen wir mit eindimensionalen Sytemen, die von einem skalaren Parameter $r \in \mathbb{R}$ abhängen, d.h. wir betrachten Differentialgleichungen der Form

$$\dot{y} = f(y, r) \qquad \text{mit } f \in C^\infty(\mathbb{R}^2)\,.$$

Die rechte Seite soll also nicht nur vom Zustand y, sondern auch vom Parameter r auf glatte Art und Weise abhängen. Unser Interesse gilt Situationen, in denen Änderungen des Parameterwertes zu *qualitativen* Änderungen in der Dynamik führen, d.h. zu Änderungen in der Anzahl, der Anordnung bzw. der Stabilität stationärer Punkte. Wir sagen, dass am Parameterwert $r = r_0$ eine *Verzweigung* auftritt, wenn r_0 Parameterbereiche mit qualitativ unterschiedlicher Dynamik trennt.

Zunächst beschreiben wir Situationen, in denen Verzweigungen ausgeschlossen sind.

Theorem 2 *Sei $B \subset \mathbb{R}$ eine beschränkte offene Teilmenge des Phasenraumes und $r_0 \in \mathbb{R}$ ein Parameterwert. Seien alle in B liegenden stationären Punkte $(\overline{y})$ des dynamischen Systems $\dot{y} = f(y, r_0)$ hyperbolisch ($f(\overline{y}, r_0) = 0$, $\partial f/\partial y(\overline{y}, r_0) \neq 0$) und es gäbe keine stationären Punkte auf ∂B. Dann gibt es endlich viele davon, und es existiert ein $\varepsilon > 0$ sodass für $|r - r_0| < \varepsilon$ das dynamische System $\dot{y} = f(y, r)$ gleich viele stationäre Punkte hat, die auch alle hyperbolisch sind und die dieselben Stabilitätseigenschaften wie die entsprechenden stationären Punkte von $\dot{y} = f(y, r_0)$ besitzen.*

Proof: Nach dem Hauptsatz über implizite Funktionen sind hyperbolische stationäre Punkte isoliert. Gäbe es unendlich viele in der beschränkten Menge B, dann müssten sie einen Häufungspunkt besitzen. Der wäre wegen der Stetigkeit von f dann auch ein stationärer Punkt, der allerdings nicht isoliert ist und daher nicht hyperbolisch sein könnte.

Aus dem Hauptsatz für implizite Funktionen folgt auch, dass für jeden stationären Punkt $\overline{y}$ und für r nahe genug bei r_0 eine Lösung $\tilde{y}$ der Gleichung $f(\tilde{y}, r) = 0$ existiert, für die $\partial f/\partial y(\tilde{y}, r) \neq 0$ gilt, d.h. dass $\tilde{y}$ ein hyperbolischer stationärer Punkt von $\dot{y} = f(y, r)$ ist. Der Hauptsatz über implizite Funktionen sagt weiters, dass der stationäre Punkt $\tilde{y}$ in einer Umgebung von $\overline{y}$ eindeutig ist. Teilt man also B in kleine Umgebungen der stationären Punkte von $\dot{y} = f(y, r_0)$ und den Rest, dann folgt aus der Vorzeichenbeständigkeit stetiger Funktionen, dass für r nahe bei r_0 im Rest keine stationären Punkte von $\dot{y} = f(y, r)$ existieren, und dass es in jeder der Umgebungen genau einen hyperbolischen stationären Punkt gibt, der dieselben Stabilitätseigenschaften wie der entsprechende stationäre Punkt von $\dot{y} = f(y, r_0)$ besitzt. ∎

Die Dynamik von eindimensionalen Systemen, die nur hyperbolische stationäre Punkte besitzen, wird also durch kleine Störungen qualitativ nicht verändert. Man nennt diese Eigenschaft *Strukturstabilität.* Man sagt auch, die Eigenschaft eines dynamischen Systems, nur hyperbolische stationäre Punkte zu besitzen, ist *generisch.* Um Verzweigungen zu studieren, müssen wir also für den kritischen Parameterwert r_0 die Existenz mindestens eines nichthyperbolischen stationären Punktes $\overline{y}$ annehmen. Im Folgenden werden wir o.B.d.A. immer $\overline{y} = r_0 = 0$ setzen.

Die Falte

Nehmen wir also an, dass für $r = 0$ an der Stelle $y = 0$ ein nichthyperbolischer stationärer Punkt auftritt. Die Taylorentwicklung der rechten Seite bezüglich y und r hat dann die Gestalt

$$f(y, r) = a_{01}r + a_{20}y^2 + a_{11}ry + a_{02}r^2 + O(y^3 + r^3)\,. \tag{7}$$

Ein einfaches Beispiel ist die Familie von dynamischen Systemen

$$\dot{y} = r + y^2\,. \tag{8}$$

Die Verzweigung, die hier bei $r = 0$ auftritt, kann man so beschreiben: Für $r < 0$ gibt es zwei hyperbolische stationäre Punkte, und zwar den instabilen Punkt $y = \sqrt{-r}$ und den asymptotisch stabilen Punkt $y = -\sqrt{-r}$. Die

beiden verschmelzen für $r = 0$, und für positive r gibt es keinen stationären Punkt.

Diese Verzweigung wird in der Literatur *Falte* oder auch *saddle-node*-Verzweigung genannt. Warum gleich 2 Namen für ein einfaches spezielles Beispiel? Nun, das Beispiel ist nicht so speziell, wie es den Anschein hat. Kehren wir zurück zu der allgemeinen Taylorentwicklung (7) und betrachten wir die generische Situation, dass die ersten beiden Koeffizienten a_{01} und a_{20} verschieden von Null sind. Ich behaupte, dass dann durch eine Neudefinition des Parameters und eine Transformation im Zustandsraum das dynamische System mit der rechten Seite (7) in der Form (8) geschrieben werden kann. Im Folgenden wird diese Behauptung zwar nicht vollständig bewiesen aber hoffentlich glaubwürdig gemacht.

Als ersten Schritt ersetzen wir y durch $\frac{y}{a_{20}}$ und r durch $\frac{r}{a_{01}a_{20}}$. Das bringt das dynamische System mit der rechten Seite (7) in die Form

$$\dot{y} = r + y^2 + a_{11}ry + a_{02}r^2 + O(y^3 + r^3)\,,$$

wobei die Koeffizienten umbenannt wurden. Der Anfang des Taylorpolynoms hat also schon die Form (8). Ein heuristisches Argument wäre nun, dass $a_{11}ry$, $a_{02}r^2$ und $O(r^3)$ klein sind im Vergleich zu r und dass $O(y^3)$ klein ist im Vergleich zu y^2 und alle diese Terme daher vernachlässigt werden können. Das stimmt insofern, als durch 'identitätsnahe' Transformationen von r und y alle außer den ersten beiden Termen auf der rechten Seite eliminiert werden können. Wir werden nur die Elimination der beiden quadratischen Terme demonstrieren. Wir setzen

$$r = R + bR^2\,, \qquad y = Y + cY^2\,. \tag{9}$$

Man muss ein bisschen rechnen, bis man das transformierte System ermittelt hat:

$$\dot{Y} = R + Y^2 + (a_{11} - 2c)RY + (a_{02} + b)R^2 + O(Y^3 + R^3)\,.$$

Durch die Wahl $b = -a_{02}$ und $c = a_{11}/2$ produziert man (8) bis auf einen Rest dritter Ordnung. Ersetzt man die quadratischen Polynome auf den rechten Seiten in (9) durch vollständige Taylorentwicklungen, dann lässt sich exakt die Form (8) erzeugen (siehe, z.B., [3]).

Das bedeutet, dass in jedem dynamischen System mit einer rechten Seite der Form (7) bei $r = 0$ eine Falte auftritt, wenn die beiden Koeffizienten a_{01} und a_{20} nicht verschwinden. Die Gleichung (8) nennt man eine *Normalform* der Falte. Wir werden in Zukunft auch Normalformen anderer Verzweigungen analysieren, ohne jedes Mal die Transformation auf Normalform zu diskutieren.

Die transkritische Verzweigung

Die Falte ist *die* generische Verzweigung in eindimensionalen dynamischen Systemen. Andere Arten von Verzweigungen können dann auftreten, wenn das System spezielle Eigenschaften hat, die auch bei Variation von Parametern erhalten bleiben. Eine typische Eigenschaft dieser Art ist es, dass es einen ausgezeichneten stationären Punkt gibt, der immer erhalten bleibt, also z.B. $\overline{y} = 0$. In diesem Fall müssen in der allgemeinen Taylorentwicklung (7) die Koeffizienten a_{01} und a_{02} verschwinden. Nimmt man, abgesehen davon, generisches Verhalten an, dann gilt $a_{20}, a_{11} \neq 0$. Eine entsprechende Normalform ist

$$\dot{y} = ry - y^2 \,.$$

Die dadurch gegebene *transkritische Verzweigung* hat die folgenden Eigenschaften: Sowohl für $r < 0$ als auch für $r > 0$ gibt es die beiden stationären Punkte $y = 0$ und $y = r$. Für $r < 0$ ist $y = 0$ asymptotisch stabil und $y = r$ instabil; für $r > 0$ ist es umgekehrt. Bei der Verzweigung findet also ein *Stabilitätsaustausch* statt.

Der 'Spruce Budworm'

Der spruce budworm ist ein nordamerikanischer Baumschädling, der immer wieder eine große Gefahr für Nadelwälder darstellt. Wir wollen die Entwicklung einer budworm-Population durch ein dynamisches System beschreiben. Sei $N(\tau)$ ein Maß für die Größe der Population zum Zeitpunkt τ. Die Gleichung

$$\frac{dN}{d\tau} = RN\left(1 - \frac{N}{K}\right) - \frac{BN^2}{A^2 + N^2}$$

ist ein typisches Modell der *Populationsdynamik*. Der Faktor $R(1 - N/K)$ im ersten Term ist die Differenz zwischen Geburten- und Sterberate. Für sehr kleine Populationen ist diese Differenz durch die positive Konstante R gegeben. Für wachsende Populationen wird sie aufgrund von Nahrungsmangel und Konkurrenz kleiner, bis sie schließlich negativ wird, wenn die Population den kritischen Wert K überschreitet. Der zweite Term beschreibt Verluste durch natürliche Feinde. Im Fall des spruce budworms sind das Vögel. Die Vögel fressen die budworms mit einer maximalen Rate B. Die Abhängigkeit der Rate von der Größe der Population hat die folgende Interpretation: Ist die Population kleiner als der Schwellwert A, dann ist es für die Vögel zu mühsam, nach den budworms zu suchen. Sie ernähren sich

dann hauptsächlich von Anderem und lassen die budworms in Ruhe. Über dem Schwellwert A werden die budworms als Vogelfutter attraktiv, und sie werden fast mit der maximalen Rate B gefressen.

Bevor das Modell als dynamisches System analysiert wird, möchten wir uns mit Fragen der *Dimensionsanalyse* beschäftigen. Will man konkret mit dem Modell rechnen (d.h. Zahlen einsetzen), muss man zunächst *Einheiten* fixieren. Diese können auf zwei *Grundeinheiten* zurückgeführt werden, eine Einheit für die Zeit, z.B. die Sekunde (abgekürzt durch 'sec'), und eine Einheit für die Populationsgröße, abgekürzt durch 'pop' (z.B. 1pop = 1000 budworms). In der folgenden Tabelle sind die Einheiten der Unbekannten N, der unabhängigen Variable τ und der vier Parameter R, K, A, und B mit Hilfe von pop und sec ausgedrückt.

Größe	Einheit
N	pop
τ	sec
R	sec^{-1}
K	pop
A	pop
B	$\mathrm{pop}\,\mathrm{sec}^{-1}$

Diese Wahl der Grundeinheiten ist willkürlich und unter Umständen für das konkrete Modell nicht sehr sinnvoll. Eine andere Möglichkeit der Einheitenwahl ist die Verwendung von *intrinsischen Referenzgrößen* als Einheiten für die abhängigen und unabhängigen Variablen N und τ. Intrinsische Referenzgrößen sind Enheiten, die sich aus den Parametern des Problems berechnen lassen. Für die Populationsgröße haben wir reiche Auswahl: K, A und B/R haben alle dieselbe Dimension wie N. Für die Zeit gibt es die Möglichkeiten $1/R$, K/B und A/B. Wir treffen unsere Wahl, indem wir uns auf einen der modellierten Effekte konzentrieren, und zwar auf den Einfluss der natürlichen Feinde. Daher verwenden wir die Parameter A und B bei der *Skalierung:*

$$t := \frac{\tau}{A/B}\,, \qquad y(t) := \frac{N(tA/B)}{A}\,.$$

Die neuen Variablen y und t sind dimensionslos. Die Gleichung für y lautet

$$\dot{y} = ry\left(1 - \frac{y}{k}\right) - \frac{y^2}{1+y^2}$$

mit den beiden *dimensionslosen Parametern* $r = RA/B$ und $k = K/A$. Ein wesentlicher Effekt der Verwendung intrinsischer Referenzgrßen für die

Skalierung ist die Reduktion der Anzahl der Parameter von vier auf zwei. Das ist eine große Erleichterung der Analyse aller möglichen qualitativen Eigenschaften des Modells.

Neben dem trivialen stationären Punkt $y = 0$ (der immer instabil ist, d.h. die budworms sterben nicht aus) gibt es noch andere stationäre Zustände, die durch die Gleichung

$$r\left(1 - \frac{y}{k}\right) = \frac{y}{1 + y^2}$$

bestimmt werden. Kurvendiskussion und/oder graphische Darstellung zeigen, dass diese Gleichung je nach den Werten von r und k 1–3 positive Lösungen hat. Faltenverzweigungen treten immer dann auf, wenn die Gerade auf der linken Seite die Kurve auf der rechten Seite berührt. Aus dieser Bedingung ergibt sich ein Zusammenhang zwischen den Schnittpunkten und den Parameterwerten:

$$r = \frac{2y^3}{(1 + y^2)^2}\,, \qquad k = \frac{2y^3}{y^2 - 1} \qquad \text{mit } y > 1\,.$$

Das kann man als Parameterdarstellung (mit Parameter y) einer Kurve in der r-k-Ebene interpretieren. Diese Kurve hat am Punkt $(r_0, k_0) = (3\sqrt{3}/8, 3\sqrt{3})$ (für den Parameterwert $y_0 = \sqrt{3}$) eine Spitze. Zwischen den beiden Ästen der Kurve gibt es drei stationäre Punkte, und außerhalb einen. Dieser eine ist immer stabil. Wenn es drei stationäre Punkte gibt, dann sind zwei davon stabil mit einem instabilen dazwischen.

Nach diesen Resultaten ist folgendes Szenario möglich: Sei r fest und zwischen $1/2$ und $3\sqrt{3}/8$; k wachse langsam (z.B. dadurch, dass die Nadelbäume wachsen). Das gibt eine waagrechte Linie in der r-k-Ebene, die die Verzweigungskurve zweimal schneidet. Bevor sie das tut, gibt es ein stabiles Gleichgewicht mit kleinen Werten der budworm-Population. Beim ersten Überqueren der Verzweigungskurve entstehen ein großes stabiles und ein instabiles Gleichgewicht. Das kleine Gleichgewicht bleibt dabei stabil und die Population daher auf niedrigem Niveau. Beim zweiten Überqueren der Kurve passiert allerdings etwas Dramatisches: Das kleine Gleichgewicht verschmilzt mit dem instabilen, und beide verschwinden. Nun ist nur mehr das große Gleichgewicht übrig, und es kommt zu einem sprunghaften Anstieg der Population.

Dieses qualitative Verhalten kann man vollständig erklären, indem man eine kleine Umgebung des kritischen Punktes (r_0, k_0) im Parameterbereich analysiert. Eine Normalform für die dort auftretende *cusp-Verzweigung*

(cusp = Spitze) ist gegeben durch

$$\dot{y} = r + ky + y^3 \,.$$

Die cusp-Verzeigung ist die generische Verzweigung, wenn man (wie bei der Heugabel) annimmt, dass auch die zweite Ableitung nach y am Verzweigungspunkt verschwindet, wenn aber (im Gegensatz zur Heugabel) keine Symmetrie gefordert wird. Für die cusp-Verzweigung sind zwei Parameter notwendig. Ein Fachausdruck dafür ist *Verzweigung der Kodimension 2* zum Unterschied der bisher behandelten Verzweigungen, die die Kodimension 1 hatten.

4 Continuous models for interacting species

This section is concerned with the interaction of two species. Three prototypical interaction mechanisms are:

- **Predator-prey interaction:** The presence of the prey species leads to increased fertility of the predator species, whose presence in term leads to an increased death rate of the prey.
- **Competition:** Two species competing for resources reduce each others growth rate.
- **Symbiosis:** Two species improve the environment for each other and increase each others growth rate.

4.1 Predator-prey interaction

One of the classical models of Mathematical Ecology is the *Lotka-Volterra model* for predator-prey interaction. Denoting by $N(\tau)$ the size of the prey density and by $P(\tau)$ the size of the predator density, it reads

$$\begin{aligned} \frac{dN}{d\tau} &= aN - bNP \,, \\ \frac{dP}{d\tau} &= cNP - dP \,, \end{aligned}$$

with positive constants a, b, c, d. We nondimensionalize by $N = ud/c$, $P = va/b$, $\tau = t/a$:

$$\begin{aligned} \frac{du}{dt} &= u(1 - v) \,, \\ \frac{dv}{dt} &= \alpha v(u - 1) \,, \end{aligned}$$

with the dimensionless parameter $\alpha = d/a$. There are two steady states, $(u, v) = (0, 0)$ and $(u, v) = (1, 1)$. Linearization leads to a system where the matrix of coefficients is the Jacobian of the right hand side:

$$J(u, v) = \begin{pmatrix} 1 - v & -u \\ \alpha v & \alpha(u - 1) \end{pmatrix} .$$

By

$$J(0, 0) = \begin{pmatrix} 1 & 0 \\ 0 & -\alpha \end{pmatrix} , \qquad J(1, 1) = \begin{pmatrix} 0 & -1 \\ \alpha & 0 \end{pmatrix} ,$$

the origin is a saddle. Saddles being hyperbolic, this property carries over to the nonlinear problem. By the special form of the equations, even the property that the coordinate axes are the stable and unstable manifolds, is still true for the nonlinear system. The point $(1, 1)$ is a center (i.e. encircled by a family of periodic solutions) of the linearised problem. Centers are not hyperbolic, however, and the stability of $(1, 1)$ cannot be deduced from the linearisation.

4.2 Competition

4.3 Symbiosis

5 Structured populations

Two types of structured population models will be considered:

- Populations with a variable genetic trait,
- Age structure.

5.1 Selection

Let $x \in \mathbb{R}$ denote a genetic trait and let $n(t, x)$ be the population density at time t with respect to the trait. We consider a trait dependent reproduction rate and a death rate proportional to the total population size (as in the logistic model). A nondimensionalized model then has the form

$$\partial_t n(t, x) = b(x)n(t, x) - N(t)n(t, x) , \qquad N(t) = \int_{\mathbf{R}} n(t, x)dx , \qquad (10)$$

with the reproduction rate $b(x) > 0$. The support of the initial data is assumed to be a bounded interval: $n(t=0) = n_0 \in C(\mathbb{R})$, with

$$n_0(x) > 0 \quad \text{for } x_{min} < x < x_{max}\,, \qquad n_0(x) = 0 \quad \text{for } x \notin (x_{min}, x_{max})\,. \tag{11}$$

For steady states $\overline{n}(x)$ ($\overline{N} = \int_{\mathbb{R}} \overline{n}\, dx$), $\overline{n}(x) \neq 0$ is only possible for x such that $b(x) = \overline{N}$. At least formally, this allows for a family of steady states: $\overline{n}(x) = b(y)\delta(x-y)$ ($\overline{N} = b(y)$) for any $y \in \mathbb{R}$ (with the Delta distribution δ). Convergence to the steady state with the largest possible value of b can be expected, i.e. selection of the most favorable trait. In order to prove such a result, we assume

$$b \in C(\mathbb{R})\,, \quad b(x) \geq \underline{b} > 0 \quad \text{for } x \in (x_{min}, x_{max})\,, \qquad b(\overline{x}) = \max_{[x_{min}, x_{max}]} b\,, \tag{12}$$

for a unique $\overline{x}$. For fixed x, (10) is a simple ordinary differential equation with the solution

$$n(t,x) = n_0(x) \exp\left(b(x)t - \int_0^t N(s)ds \right)\,. \tag{13}$$

Integration with respect to x gives

$$N(t) \exp\left(\int_0^t N(s)ds \right) = \int_{\mathbb{R}} n_0(x) e^{b(x)t} dx\,,$$

and integration with respect to t:

$$\exp\left(\int_0^t N(s)ds \right) = \int_{\mathbb{R}} \frac{n_0(x)}{b(x)} \left(e^{b(x)t} - 1 \right) dx + 1\,.$$

Now we apply the logarithm and differentiate:

$$N(t) = \int_{\mathbb{R}} n_0(x) e^{b(x)t} dx \left(\int_{\mathbb{R}} \frac{n_0(x)}{b(x)} \left(e^{b(x)t} - 1 \right) dx + 1 \right)^{-1}$$

By our assumptions,

$$N(t) \leq b(\overline{x}) \int_{\mathbb{R}} \frac{n_0(x)}{b(x)} e^{b(x)t} dx \left(\int_{\mathbb{R}} \frac{n_0(x)}{b(x)} \left(e^{b(x)t} - 1 \right) dx + 1 \right)^{-1} \overrightarrow{t \to \infty}\, b(\overline{x})\,.$$

On the other hand, let $I_\varepsilon = \{x \in [x_{min}, x_{max}] : b(x) \geq b(\overline{x}) - \varepsilon\}$. Then

$$N(t) \geq \int_{I_\varepsilon} n_0(x) e^{b(x)t} dx \left(\int_{\mathbb{R}} \frac{n_0(x)}{b(x)} \left(e^{b(x)t} - 1 \right) dx + 1 \right)^{-1} \geq (b(\overline{x}) - \varepsilon) A_\varepsilon(t)\,,$$

with

$$A_\varepsilon(t) = \int_{I_\varepsilon} \frac{n_0(x)}{b(x)} e^{b(x)t} dx \left(\int_{\mathbb{R}} \frac{n_0(x)}{b(x)} \left(e^{b(x)t} - 1 \right) dx + 1 \right)^{-1} \overrightarrow{t \to \infty}\, 1\,.$$

Theorem 3 *Let (11) and (12) hold. Then the solution n of the initial value problem for (10) satisfies*

$$\lim_{t\to\infty} N(t) = b(\overline{x})\,, \qquad \lim_{t\to\infty} n(t,x) = b(\overline{x})\delta(x-\overline{x})\,,$$

where the latter has to be understood in the distributional sense.

Proof: The limit for $N(t)$ has already been proven above.

The next step is to prove that the family I_ε introduced above contracts to the point $\overline{x}$. Let $x_\varepsilon \in I_\varepsilon$, $\varepsilon > 0$. Since I_ε is uniformly (in ε) bounded, for every sequence $\varepsilon_k \to 0$, as $k \to \infty$, there exists a subsequence, again denoted by ε_k, such that $x_{\varepsilon_k} \to \hat{x} \in [x_{min}, x_{max}]$. By the continuity of b, $b(x_{\varepsilon_k}) \to b(\hat{x})$, but also $b(\overline{x}) - \varepsilon_k \le b(x_{\varepsilon_k}) \le b(\overline{x})$. So $b(\hat{x}) = b(\overline{x})$ and, since the maximum is unique, $\hat{x} = \overline{x}$. As a consequence, $\lim_{\varepsilon\to 0} x_\varepsilon = \overline{x}$.

For $x \notin I_\varepsilon$, the exponent in the solution formula (13) can be estimated by

$$b(x)t - \int_0^t N(s)ds \le t\left(-\varepsilon + \frac{1}{t}\int_0^t (b(\overline{x}) - N(s))ds\right)$$

For fixed $\varepsilon > 0$, this provides a bound for n, which is uniform in x and converges to zero as $t \to \infty$, since

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t (b(\overline{x}) - N(s))ds = 0$$

by the convergence of $N(t)$.

Combining these results leads to

$$\lim_{t\to\infty} \int_{\mathbf{R}} n(t,x)\varphi(x)dx = b(\overline{x})\varphi(\overline{x})$$

for every $\varphi \in C(\mathbb{R})$, which completes the proof. ∎

5.2 Age structured populations

We shall analyse the *renewal equation*, the simplest model for the growth of age structured populations. For more details see [8].

The variable $x \ge 0$ will denote the age of an individual and $n(t,x)$ the density of individuals with respect to age at time $t \ge 0$. Individuals having ages between x_1 and $x_2 > x_1 > 0$ at time zero, have the ages between $x_1 + t$

and $x_2 + t$ at time $t > 0$. Neglecting death, the number of these individuals is the same at times zero and t:

$$\int_{x_1}^{x_2} n(0,x)dx = \int_{x_1+t}^{x_2+t} n(t,x)dx\,.$$

The derivative of this equation with respect to t can be written as

$$\int_{x_1+t}^{x_2+t} (\partial_t n + \partial_x n)dx = 0\,,$$

which only holds for arbitrary x_1, x_2, if the partial differential equation

$$\partial_t n + \partial_x n = 0\,, \qquad x > 0\,,\, t > 0\,, \tag{14}$$

is satisfied. A model for birth has to prescribe the production of individuals with age $x = 0$:

$$n(t,0) = \int_0^\infty B(y)n(t,y)dy\,, \qquad t > 0\,, \tag{15}$$

where $B(y) \geq 0$ is an age dependent birth rate. The model is completed by prescribing an initial age distribution:

$$n(0,x) = n_0(x)\,, \qquad x > 0\,. \tag{16}$$

We shall be interested in the long time behaviour of solutions of (14)–(16) under the assumptions

$$B \geq 0\,, \qquad B \in L^\infty(\mathbb{R}^+) \cap L^1(\mathbb{R}^+)\,, \qquad \int_0^\infty B(x)dx > 1\,. \tag{17}$$

A reasonable guess concerning the long time behavior is $n(t,x) \approx e^{\lambda_0 t}N(x)$ as $t \to \infty$, leading to the eigenvalue problem

$$\begin{aligned} &\lambda_0 N + N' = 0\,, \quad N(0) = \int_0^\infty B(y)N(y)dy\,, \\ &\text{Normalisation:} \quad \int_0^\infty N(y)dy = 1\,. \end{aligned} \tag{18}$$

Under the assumptions (17) a unique positive eigenvalue λ_0 and a positive eigenfunction N exist, such that

$$N(x) = \lambda_0 e^{-\lambda x}\,, \qquad \int_0^\infty B(y)e^{-\lambda_0 y}dy = 1\,.$$

For the purpose of proving a result on the long time behavior, we introduce the normalised density $\tilde{n}(t,x) = e^{-\lambda_0 t} n(t,x)$, satisfying

$$\partial_t \tilde{n} + \partial_x \tilde{n} + \lambda_0 \tilde{n} = 0\,, \qquad x > 0\,,\, t > 0\,, \tag{19}$$

$$\tilde{n}(t,0) = \int_0^\infty B(y)\tilde{n}(t,y)dy\,, \qquad t > 0\,, \tag{20}$$

$$\tilde{n}(0,x) = n_0(x)\,, \qquad x > 0\,. \tag{21}$$

One interesting fact concerning this problem is that it permits a conservation law. Since the operator $A\tilde{n} = -\partial_x \tilde{n} - \lambda_0 \tilde{n}$, subject to the boundary condition (20) has a zero eigenvalue, the same is true for the adjoint A^*. Eigenfunctions φ corresponding to the eigenvalue zero (left eigenfunctions of A) satisfy

$$\begin{aligned} &\lambda_0 \varphi - \varphi' = \varphi(0) B(x)\,, \\ &\text{Normalisation:} \quad \int_0^\infty N(y)\varphi(y)dy = 1\,, \end{aligned} \tag{22}$$

which can be solved explicitly:

$$\varphi(x) = \int_x^\infty e^{\lambda_0(x-y)} B(y)dy \left(\lambda_0 \int_0^\infty y e^{-\lambda_0 y} B(y)dy\right)^{-1}.$$

The properties $\varphi \geq 0$, $\varphi \in L^\infty(\mathbb{R}^+)$ are immediate from (17). For the following, we need assumptions on the initial data: There exists a constant $C_0 \geq 0$ such that

$$0 \leq n_0(x) \leq C_0 N(x)\,. \tag{23}$$

A straightforward computation proves:

Lemma 1 *Let (17) and (23) hold. Then the solution of (19)–(21) satisfies*

$$\int_0^\infty \tilde{n}(t,x)\varphi(x)dx = m := \int_0^\infty n_0(x)\varphi(x)dx\,, \qquad t > 0\,.$$

By this result it is reasonable to expect that $\tilde{n}(t,x) \to mN(x)$ as $t \to \infty$. This will be proven by means of the Lyapunov function

$$H(t) = \int_0^\infty \frac{\varphi(x)}{N(x)} (\tilde{n}(t,x) - mN(x))^2 dx\,.$$

We compute

$$\frac{dH}{dt} = -\varphi(0) \int_0^\infty \frac{B(x)}{N(x)} (\tilde{n}(t,x) - \hat{m}(t)N(x))^2 dx\,, \tag{24}$$

with

$$\hat{m}(t) = \frac{1}{N(0)} \int_0^\infty \tilde{n}(t,x) B(x) dx \,.$$

The result (24) shows that H is a Lyapunov function. Integration with respect to t gives

$$\varphi(0) \int_0^\infty \int_0^\infty \frac{B(x)}{N(x)} (\tilde{n}(t,x) - \hat{m}(t) N(x))^2 dx\, dt \le H(0) \,,$$

which gives hope that $\tilde{n}(t,x) - \hat{m}(t)N(x) \to 0$ as $t \to \infty$. Actually, with some additional work, convergence to equilibrium can be deduced from this [8]. With an additional assumption on the data, it is possible to prove exponential convergence. We assume that there exists a positive constant μ_0 such that

$$\varphi(0) B(x) \ge \mu_0 \varphi(x) \,. \tag{25}$$

If this holds, the right hand side of (24) can be estimated from above by

$$-\mu_0 \int_0^\infty \frac{\varphi(x)}{N(x)} (\tilde{n}(t,x) - \hat{m}(t)N(x))^2 dx = -\mu_0 \left(H(t) + (\hat{m}(t) - m)^2 \right) .$$

As a consequence $\dot{H} \le -\mu_0 H$, and the Gronwall lemma implies exponential decay of $\tilde{n} - mN$ in $L^2(\mathbb{R}^+, \varphi/N\, dx)$.

The assumption (25) is somewhat restrictive. For example, it does not allow $B(x) = 0$ for $x < x_0$. However, it is always satisfied for $B(x)$ decreasing.

Death can easily be included in the model replacing (14) by

$$\partial_t n + \partial_x n + d(x) n = 0 \,, \qquad x > 0 \,, t > 0 \,, \tag{26}$$

subject to the boundary and initial conditions (15), (16), wit h the age dependent death rate $d(x)$. We now make the assumptions

$$B, d \ge 0 \,, \qquad B \in L^\infty(\mathbb{R}^+) \,, \qquad d(x) \to \infty \quad \text{as } x \to \infty \,.$$

The eigenvalue problem

$$\begin{aligned} &\lambda_0 N + N' + dN = 0 \,, \quad N(0) = \int_0^\infty B(y) N(y) dy \,, \\ &\int_0^\infty N(y) dy = 1 \,, \end{aligned} \tag{27}$$

now has a unique solution satisfying

$$N(x) = N(0) \exp\left(-\lambda_0 x - \int_0^x d(\xi) d\xi\right),$$
$$1 = \int_0^\infty B(y) \exp\left(-\lambda_0 y - \int_0^y d(\xi) d\xi\right) dy,$$

where $N(0)$ has to be chosen such that the normalisation condition in (27) is satisfied. Now λ_0 can have both signs since, by the conditions on the data, $N(x)$ will always be integrable.

6 Random motion of particles

Biological particles usually live in a complex nonhomogeneous environment influencing their movement. As a consequence, for an observer this movement looks like having a random component. We therefore accept a random nature of this movement as a postulate for a mathematical description. Another postulate, which makes life much easier (although it is not justified in general), is that regarding the random component of motion the particles are independent in the probabilistic sense.

We start by considering a discrete one-dimensional random motion. Let $x_j = j\Delta x$, $j \in \mathbb{Z}$, denote the possible positions of particles, and assume that at the discrete points $t_n = n\Delta t$, $n \in \mathbb{Z}$, in time particles perform jumps of the length Δx to the left or to the right. Let us assume further that the probability of jumping to the left is q, and the probability of jumping to the right is $1-q$ (with $0 \le q \le 1$, of course). Now we introduce the nonnegative quantities p_j^n, $j, n \in \mathbb{Z}$, which can be interpreted either as the probability that one particle is at the position x_j at time t_n or as the expected number of particles out of a large ensemble at position x_j at time t_n or (if the latter is divided by Δx) as the expected number density of particles at position x_j at time t_n. Then, obviously the values at time t_{n+1} can be computed in terms of the values at time t_n:

$$p_j^{n+1} = q p_{j+1}^n + (1-q) p_{j-1}^n \tag{28}$$

Eventually we are looking for continuous descriptions both in time and in position. Therefore we shall interpret p_j^n as approximation for $p(x_j, t_n)$ where p is a function of two real valued arguments. With this interpretation in mind we rewrite the above equation as

$$\frac{p_j^{n+1} - p_j^n}{\Delta t} - \frac{q\Delta x}{\Delta t} \frac{p_{j+1}^n - p_j^n}{\Delta x} + \frac{(1-q)\Delta x}{\Delta t} \frac{p_j^n - p_{j-1}^n}{\Delta x} = 0.$$

Our aim is to pass to the limit $\Delta x, \Delta t \to 0$. Obviously the result depends on the relative size of Δx and Δt. We have three main options: Either the grid speed $s := \Delta x/\Delta t$ tends to zero, to infinity, or we keep it fixed at a positive finite value. The most interesting result occurs in the latter case, which we call the *significant limit*:

$$\partial_t p + \partial_x(vp) = 0\,, \qquad \text{with } v = s(1-2q)\,. \tag{29}$$

Actually, the other two cases can be recovered by letting $s \to 0$ or $s \to \infty$.

Equation (29) is a one-dimensional *convection equation*. Solutions are travelling waves $p(x,t) = f(x-vt)$ with velocity v. With the interpretation of p as time dependent density of particles along the line, the integrated version of (29),

$$\frac{d}{dt}\int_a^b p(x,t)dx + vp(b,t) - vp(a,t) = 0\,,$$

gives the rate of change of the number of particles contained in the interval (a,b). The term $j(x,t) = vp(x,t)$ can then be interpreted as the *flux* of particles through the point x at time t, and v is the mean velocity of particles.

It is interesting to note that equation (29) could have been derived without any probabilistic effects. The assumption that all particles always move to the right or always to the left, i.e., $q = 0$ or $q = 1$, still leads to (29) with $v = \pm s$. More generally, the same value of v, and therefore the same macroscopic equation (29) can be obtained by different choices of the grid speed s and of the probability q. This shows that the properties of the microscopic movement cannot be completely recovered from macroscopic observations.

In the symmetric situation $q = 1/2$, the mean velocity vanishes, and (29) becomes trivial. This unsatisfactory situation can be clarified by returning to the discrete equation (28) and by rewriting it in a different way:

$$\frac{p_j^{n+1} - p_j^n}{\Delta t} - \frac{(\Delta x)^2}{2\Delta t}\,\frac{p_{j+1}^n - 2p_j^n + p_{j-1}^n}{(\Delta x)^2} = 0\,.$$

This shows that for $q = 1/2$, the significant limit is achieved, when $D = (\Delta x)^2/(2\Delta t)$ is kept fixed as $\Delta x, \Delta t \to 0$:

$$\partial_t p - D\partial_x^2 p = 0\,. \tag{30}$$

This is the one-dimensional *diffusion equation* with diffusivity D. Integration as above shows that the diffusive flux is given by *Fick's law* $j = -D\partial_x p$.

As for the convection equation we want to demonstrate that the diffusion equation can also be obtained as macroscopic model for different microscopic dynamics as long as they do not have a directional bias. Instead of a *position jump process* as considered above, we now describe a *velocity jump process*. Consider particles, which move along the line with velocity $s > 0$ or $-s$. At discrete points $t_n = n\Delta t$ in time they change to the other velocity with probability q. We denote the expected density of particles moving to the right at time t_n (after the velocity jump) by $r^n(x)$, and the expected density of particles moving to the left at time t_n by $l^n(x)$. Then the densities at time t_{n+1} before the velocity jump are given by

$$\hat{r}^{n+1}(x) = r^n(x - s\Delta t)\,, \qquad \hat{l}^{n+1}(x) = l^n(x + s\Delta t)\,.$$

After the velocity jump at time t_{n+1} we obtain

$$r^{n+1}(x) = (1-q)\hat{r}^{n+1}(x) + q\hat{l}^{n+1}(x)\,, \qquad l^{n+1}(x) = (1-q)\hat{l}^{n+1}(x) + q\hat{r}^{n+1}(x)\,,$$

which can be rewritten as

$$\begin{aligned}
\frac{r^{n+1}(x) - r^n(x)}{\Delta t} + s\frac{r^n(x) - r^n(x - s\Delta t)}{s\Delta t} &= \frac{q}{\Delta t}(l^n(x + s\Delta t) - r^n(x - s\Delta t))\,,\\
\frac{l^{n+1}(x) - l^n(x)}{\Delta t} - s\frac{l^n(x + s\Delta t) - l^n(x)}{s\Delta t} &= \frac{q}{\Delta t}(r^n(x - s\Delta t) - l^n(x + s\Delta t))\,.
\end{aligned}$$

A significant limit is obtained with the scaling assumption that $\tau := \Delta t/q$ remains fixed as $\Delta t \to 0$:

$$\partial_t r + s\partial_x r = \frac{l - r}{\tau}\,, \qquad \partial_t l - s\partial_x l = \frac{r - l}{\tau}\,.$$

This is the simplest example of a *kinetic transport equation*, describing an ensemble of particles not only by its positional distribution but also its distribution with respect to velocity. Kinetic transport equations are often called *mesoscopic models*. In a *macroscopic scaling*, x is replaced by x/ε and t is replaced by t/ε^2, where ε is a small positive dimensionless parameter. This leads to the rescaled version

$$\varepsilon^2\partial_t r + \varepsilon s\partial_x r = \frac{l - r}{\tau}\,, \qquad \varepsilon^2\partial_t l - \varepsilon s\partial_x l = \frac{r - l}{\tau}\,. \tag{31}$$

For carrying out the macroscopic limit $\varepsilon \to 0$, we replace the system by the first equation an the sum of the equations. After dividing by ε and, respectively, by ε^2, we obtain

$$\varepsilon\partial_t r + s\partial_x r = \frac{l - r}{\varepsilon\tau}\,, \qquad \partial_t p + s\partial_x \frac{r - l}{\varepsilon} = 0\,, \tag{32}$$

where $p = r + l$ is the total (or macroscopic) density. In the limit $\varepsilon \to 0$, (31) gives $r = l$, and the first equation in (32) shows that the flux $s(r-l)/\varepsilon$ converges to $-s^2\tau\partial_x r = -D\partial_x p$ with $D = s^2\tau/2$, such that we again obtain the diffusion equation (30).

So far we have seen that the macroscopic limit of a biased random motion is a convection equation, and for an unbiased motion it is a diffusion equation. Actually, both effects can be combined in the macroscopic equation by an appropriate scaling assumption. We shall also generalize the position jump process by allowing a dependence of the jump probability on position and time:

$$p_j^{n+1} = q_{j+1}^n p_{j+1}^n + (1 - q_{j-1}^n) p_{j-1}^n \,.$$

As in the derivation of the diffusion equation we assume that $D = (\Delta x)^2/(2\Delta t)$ is fixed and that the jump probabilities are close to $1/2$:

$$q_j^n = \frac{1}{2} - \frac{v(x_j, t_n)\Delta t}{2\Delta x} \,,$$

where $v(x,t)$ is a given velocity function. The analogous computations as in the derivation of the diffusion equation now lead to the one-dimensional *convection-diffusion equation*

$$\partial_t p + \partial_x(vp - D\partial_x p) = 0 \,. \tag{33}$$

Everything we did so far can be extended to higher dimensions with the result

$$\partial_t p + \nabla \cdot (vp - D\nabla p) = 0 \,, \tag{34}$$

where now the density $p(x,t)$ depends on position $x \in \mathbb{R}^d$, with $d = 2$ or $d = 3$, and on time $t \in \mathbb{R}$. The gradient with respect to x is denoted by ∇ and the divergence by $\nabla\cdot$. The velocity $v(x,t)$and the flux $vp - D\nabla p$ are vector fields. The interpretation of the flux vector is the following: Its component in the direction ν is the number of particles per time and per unit area moving through an area element orthogonal to ν. This can be seen by integrating (34) over a bounded position domain $\Omega \subset \mathbb{R}^d$ and using the divergence theorem:

$$\frac{d}{dt}\int_\Omega p\, dx + \int_{\partial\Omega} (vp - D\nabla p)\cdot \nu \, d\sigma = 0 \,, \tag{35}$$

where ν denotes the unit outward normal vector along the boundary $\partial\Omega$, and $d\sigma$ is the line element for $d = 2$ and the surface element for $d = 3$.

So far we only described the movement of particles. Equation (34) is a conservation law. No particles are created or destroyed. As the final step in this modelling section, we also allow for this possibility. We denote by $f(x,t)$ the number of particles created or destroyed (depending on the sign of f) per unit time and unit volume. Then the right hand side of (35) has to be replaced by the integral of f over Ω, and the differential version (34) becomes the *reaction-convection-diffusion equation*

$$\partial_t p + \nabla \cdot (vp - D\nabla p) = f\,. \tag{36}$$

Why reaction? In a typical situation our particles are molecules whose creation or destruction is the result of a chemical reaction. Another interpretation of f in the following will be as a birth/death term.

In the following, systems of equations of the form (36) for different species of particles will be considered, when x varies in a domain $\Omega \subset \mathbb{R}^d$. Typically we shall either assume that Ω is bounded with zero flux boundary conditions

$$(vp - D\nabla p) \cdot \nu = 0 \quad \text{along } \partial\Omega\,,$$

or, as an idealization, that $\Omega = \mathbb{R}^d$. In the latter case it is usually assumed that $f(x,t) \to 0$ as $|x| \to \infty$, and that either the total number of particles is bounded, i.e., $\int_{\mathbb{R}^d} p\,dx < \infty$, or that $p(x,t)$ converges to a constant value as $|x| \to \infty$.

For given v and f, the formulation of a well posed problem for the unknown p is completed by prescribing initial conditions $p(x,0) = p_I(x)$ for $x \in \Omega$, with given initial data p_I. Well posedness means that the initial-boundary value problem has a unique solution continuously dependent on the data v, f, and p_I.

7 Stability of homogeneous steady states

In this section we consider reaction and diffusion of one species of particles in a stationary homogeneous environment, i.e., equations of the form

$$\partial_t p - D\Delta p = f(p)\,, \tag{37}$$

where $\Delta = \nabla\cdot\nabla$ is the Laplace operator and the stationarity and homogeneity of the environment is reflected by the fact that the reaction rate f does not explictly depend on t or x. A *homogeneous steady state* is a constant solution p_0 of (37), implying that p_0 is a zero of f. If (37) is considered on the position domain Ω, then a homogeneous steady state satisfies zero flux

boundary conditions ($\nu \cdot \nabla p = 0$ on $\partial\Omega$) for bounded Ω and, obviously, the condition $p(x,t) \to p_0$ for $|x| \to \infty$ for $\Omega = \mathbb{R}^d$. We shall consider these two situations.

The stability of p_0 is examined by introducing the perturbation $u(x,t) = p(x,t) - p_0$ where p is a solution of (37) close to p_0, i.e., u is small. Substitution in (37), Taylor expanding f around $p = p_0$ ($u = 0$), and keeping only the linear term gives the *linearized equation*

$$\partial_t u - D\Delta u = f'(p_0)u\,,$$

with zero flux boundary conditions for Ω bounded, and with $u \to 0$ as $|x| \to \infty$ for $\Omega = \mathbb{R}^d$.

For bounded Ω, the linearized problem can be solved by separation of variables leading to a representation of solutions in the form

$$u(x,t) = \sum_{k=0}^{\infty} u_k \varphi_k(x) \exp([D\lambda_k + f'(p_0)]t)\,,$$

where $\varphi_0 = 1, \varphi_1, \ldots$ are the eigenfunctions of the Laplace operator subject to zero flux boundary conditions and $\lambda_0 = 0, \lambda_1, \ldots$ are the corresponding eigenvalues, i.e.,

$$\Delta\varphi_k = \lambda_k \varphi_k\,, \qquad \nu \cdot \nabla\varphi_k = 0 \text{ on } \partial\Omega\,,$$

for $k = 0, 1, \ldots$ Different solutions are distinguished by the choice of the constants $u_0, u_1, \ldots$ The computation

$$\int_\Omega \varphi_l \Delta\varphi_k \, dx = -\int_\Omega \nabla\varphi_k \cdot \nabla\varphi_l \, dx$$

implies that the Laplace operator with zero flux boundary conditions is symmetric with respect to the scalar product defined by pointwise multiplication and subsequent integration. This has the consequence that all eigenvalues are real and that $\{\varphi_k,\ k \geq 0\}$ can be chosen as an orthonormal sequence. The above formula also implies that the eigenvalues are nonpositive. Actually it can be shown that $\lambda_k \to -\infty$ as $k \to \infty$. W.l.o.g. we assume the eigenvalues to be ordered: $\lambda_0 \geq \lambda_1 \geq \ldots$

A steady state solution is called *stable* if, when starting with an initial condition close to the steady state the solution remains close to the steady state for all times, it is called *asymptotically stable* if, furthermore, such solutions converge to the steady state as time tends to infinity.

The steady state $u = 0$ of the linearized problem is stable iff $f'(p_0) \leq 0$, it is asymptotically stable iff $f'(p_0) < 0$. In these cases we say that the

steady state p_0 of the original nonlinear equation is *linearized (asymptotically) stable*. It can be shown that linearized asymptotic stability implies asymptotic stability and that linearized instability implies instability.

In the case $\Omega = \mathbb{R}^d$, we solve the linearized equation by the *Fourier transform*. The Fourier transform with respect to the position variables is defined by

$$\widehat{u}(k,t) := \int_{\mathbb{R}^d} u(x,t) e^{-ik\cdot x} dx\,.$$

Its inverse is given by

$$u(x,t) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \widehat{u}(k,t) e^{ik\cdot x} dk\,.$$

The latter equation is certainly true for smooth u decaying sufficiently fast as $|x| \to \infty$. The usefulness of the Fourier transform for our purposes is a consequence of the identity

$$\widehat{\nabla u} = ik\widehat{u}\,,$$

implying $\widehat{\Delta u} = -|k|^2\widehat{u}$. Application of the Fourier transform to the linearized equation results in the ordinary differential equation

$$\partial_t \widehat{u} = (f'(p_0) - D|k|^2)\widehat{u}\,,$$

and, thus, in the general solution

$$u(x,t) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \widehat{u_I}(k) e^{(f'(p_0)-D|k|^2)t} e^{ik\cdot x} dk\,,$$

where $\widehat{u_I}$ is the Fourier transform of $u(t=0)$. Obviously the condition for (asymptotic) stability is the same as in the case of a bounded domain.

8 The KPP-Fisher equation

8.1 Bounded domains: the transcritical bifurcation

In the previous section, the stability of homogeneous steady states was examined. Now we extend our interest to situations, where the stability properties of a steady state change in dependence of a parameter, i.e. *bifurcations*. We consider the simplest nonlinear model of population dynamics.

The dynamics of a spatially homogeneous population with density $p(t)$, living in an environment with limit resources, can be described by the ordinary differential equation

$$\frac{dp}{dt} = \alpha \left(1 - \frac{p}{\overline{p}}\right) p = \alpha p - \beta p^2 \,,$$

where the right hand side is called *logistic growth* with the growth rate α of small populations and the critical density p_0 above which the growth rate is negative. By an appropriate nondimensionalization, the second parameter can be eliminated:

$$\frac{dp}{dt} = ap - p^2 \,,$$

where a is a dimensionless parameter. Although biologically irrelevant, it is instructive to observe what happens when a takes both positive and negative values. A bifurcation then occurs at $a = 0$ where the trivial steady state $p = 0$ changes its stability properties from stable for $a < 0$ to unstable for $a > 0$. The stability properties of the second steady state $p = a$ are just opposite. We say that the nontrivial steady state *bifurcates* from the trivial steady state at $a = 0$. There an *exchange of stability* between the two steady states occurs. This situation is called a *transcritical bifurcation*.

Actually, exactly the same happens, if we allow a spatially nonhomogeneous diffusing population $p(x,t)$ on a bounded domain with zero flux boundary conditions:

$$\begin{aligned} &\partial_t p = \Delta p + ap - p^2 \,, \quad \text{for } x \in \Omega \subset \mathbb{R}^d \,, \\ &\nu \cdot \nabla p = 0 \,, \quad \text{on } \partial\Omega \,. \end{aligned}$$

A transcritical bifurcation with the homogeneous steady states $p = 0$ and $p = a$.

A more interesting situation occurs under different boundary conditions. Consider a situation where Ω does not represent a container. The individuals can leave the domain. However, the environment is hostile to them outside of Ω, such that they cannot survive there. This can be modelled by the (*Dirichlet*) boundary conditions $p = 0$ on $\partial\Omega$. For computational simplicity we consider a one-dimensional situation:

$$\begin{aligned} &\partial_t p = \partial_x^2 p + ap - p^2 \,, \quad \text{for } 0 < x < \pi \,, \\ &p(0,t) = p(\pi,t) = 0 \,. \end{aligned} \tag{38}$$

The length π of the domain has been achieved by the nondimensionalization. The Dirichlet boundary conditions still permit the trivial steady state $p = 0$, but eliminate the other homogeneous steady state. Linearization at $p = 0$ leads to the eigenvalues $\lambda_j = a - j^2$, $j = 1, 2, \ldots$, and the according eigenfunctions $\varphi_j(x) = \sin(jx)$. So the trivial steady state is stable even for positive $a < 1$. Diffusion subject to Dirichlet boundary conditions has a stabilizing effect. At $a = 1$, the largest eigenvalue λ_1 changes sign.

We shall demonstrate by an asymptotic analysis for values of a close to 1 that again a transcritical bifurcation occurs. We choose a parameter ε taking small positive and negative values and set $a = 1 + \varepsilon$. For the solution we make the ansatz

$$p(x,t) = \varepsilon p_0(x, |\varepsilon|t) + \varepsilon^2 p_1(x, |\varepsilon|t) + O(\varepsilon^3)\,,$$

which takes into account that we expect solutions close to the trivial steady state varying slowly. Substitution in (38) and comparing coefficients of equal powers of ε leads to

$$\begin{aligned} &0 = \partial_x^2 p_0 + p_0\,, \quad p_0(0,\tau) = p_0(\pi,\tau) = 0\,,\\ &\sigma\partial_\tau p_0 = \partial_x^2 p_1 + p_1 + p_0 - p_0^2\,, \quad p_1(0,\tau) = p_1(\pi,\tau) = 0\,, \end{aligned} \tag{39}$$

where we have set $\tau = |\varepsilon|t$ and $\sigma = \operatorname{sign}\varepsilon$. The first line is a linear problem for p_0 with the solution $p_0(x,\tau) = A(\tau)\sin x$, where $A(\tau)$ can be chosen arbitrarily. The second line can be seen as an inhomogeneous version of the same linear problem, now with the unknown p_1, if p_0 is considered as known.

Now the idea is the following: Since the kernel of the linear problem is nontrivial, we expect the inhomogeneous problem to require a solvability condition on the inhomogeneity. This solvability condition will provide the missing information for determining the leading term p_0 completely.

Actually, the solvability condition is obtained by multiplication with $\sin x$ and integration with respect to x from 0 to π. Doing this with (39) after substitution of the general solution for p_0 gives an ordinary differential equation for the as yet unknown coefficient $A(\tau)$:

$$\frac{dA}{d\tau} = \sigma\left(A - \frac{8}{3\pi}A^2\right)\,.$$

We deduce the existence of a second steady state which is close to $(a-1)\frac{3\pi}{8}\sin x$ for a close to 1, and which is unstable for $a < 1$ and stable for $a > 1$. Thus, a transcritical bifurcation occurs with a bifurcating nonhomogeneous steady state. The bifurcating solution is biologically relevant only for $a > 1$, since it is negative for $a < 1$.

8.2 Unbounded domains: traveling waves

$$\partial_t p = \partial_x^2 p + ap - p^2\,, \quad \text{for } x \in \mathbb{R}\,,$$

with $a > 0$. Traveling wave: $p(x,t) = p_{TW}(\xi)$, $\xi = x - st$:

$$-sp'_{TW} = p''_{TW} + p_{TW}(a - p_{TW})\,. \tag{40}$$

Invasion: $s > 0$ and

$$p_{TW}(-\infty) = a\,, \qquad p_{TW}(\infty) = 0\,. \tag{41}$$

Theorem 4 *Let $s \geq s_0 := 2\sqrt{a}$. Then (40), (41) has a positive, strictly monotone solution, which is unique up to a shift in ξ.*

Proof: The steady states $(0,0)$ and $(a,0)$ in the (p_{TW}, p'_{TW})-plane are asymptotically stable and a saddle, respectively. One side of the unstable manifold of $(a,0)$ points into the triangle

$$0 > p'_{TW} > -\frac{s}{2} p_{TW}\,, \qquad p_{TW} < a\,,$$

which is positively invariant. Therefore, this part of the unstable mainfold has to converge to $(0,0)$ as $\xi \to \infty$. The second part of the unstable manifold is monotonically increasing and, thus, cannot provide a solution. ∎

Remark 2 *1) The condition $s \geq s_0$ is necessary since, for $s < s_0$, the origin $(0,0)$ is a stable spiral. In this case a traveling wave solution might still exist, but it cannot remain positive.*
2) For $s > s_0$, there exists a constant $p_0 > 0$ such that

$$p_{TW}(\xi) \approx p_0 \exp\left(\frac{\sqrt{s^2 - s_0^2} - s}{2}\xi\right)\,, \qquad \text{as } \xi \to \infty\,. \tag{42}$$

Linearized stability for $\kappa := \frac{s^2}{4} - a > 0$ (i.e. $s > s_0$): $u \approx p - p_{TW}$, and (ξ, t) instead of (x,t):

$$\partial_t u = \partial_\xi^2 u + s\partial_\xi u + (a - 2p_{TW})u\,. \tag{43}$$

Because of the shift invariance and the range of wave speeds, neutral stability would be the best possible result. However, not even this is true for general perturbations. We shall therefore restrict to perturbations decaying faster

than the wave as $\xi \to \infty$. Multiplication by u and integration with respect to ξ gives

$$\frac{1}{2}\frac{d}{dt}\int_{-\infty}^{\infty} u^2 d\xi = -\int_{-\infty}^{\infty} (\partial_\xi u)^2 d\xi + \int_{-\infty}^{\infty} (a - 2p_{TW}) u^2 d\xi \,, \tag{44}$$

which shows the main difficulty already, since the coefficient $(a - 2p_{TW})$ has the unfavorable sign for $\xi \to \infty$. Fast decay of the perturbation will be inforced by requiring $u(\cdot, t) \in L^2\left((1 + W^2)d\xi\right)$, with

$$W(\xi) = e^{s\xi/2} \,.$$

Note that, by (42), $p_{TW} \notin L^2\left((1 + W^2)d\xi\right)$. A straightforward computation shows

$$\partial_t(uW) = \partial_\xi^2(uW) - (\kappa + 2p_{TW})uW \,,$$

with the positive coefficient $(\kappa + 2p_{TW})$. Multiplication by uW and integration with respect to ξ gives

$$\frac{1}{2}\frac{d}{dt}\int_{-\infty}^{\infty} u^2 W^2 d\xi = -\int_{-\infty}^{\infty} [\partial_\xi(uW)]^2 d\xi - \int_{-\infty}^{\infty} (\kappa + 2p_{TW}) u^2 W^2 d\xi \,. \tag{45}$$

Now we multiply this by a positive constant α and add the result to (44):

$$\frac{1}{2}\frac{d}{dt}\int_{-\infty}^{\infty} u^2(1 + \alpha W^2) d\xi \le -\int_{-\infty}^{\infty} u^2(2p_{TW} - a + \alpha\kappa W^2 + 2\alpha p_{TW} W^2) d\xi \,.$$

Now we define ξ_0 by $p_{TW}(\xi_0) = 3a/4$. Then, for $\xi \le \xi_0$, we have

$$2p_{TW} - a + \alpha\kappa W^2 + 2\alpha p_{TW} W^2 \ge \frac{a}{2} + \alpha\kappa W^2 \ge \min\left\{\frac{a}{2}, \kappa\right\}(1 + \alpha W^2) \,,$$

For $\xi \ge \xi_0$, $p_{TW} W^2$ is strictly positive and unbounded as $\xi \to \infty$. Therefore α can be chosen large enough such that

$$2\alpha p_{TW} W^2 \ge \frac{3a}{2} \,.$$

Therefore, for $\xi \ge \xi_0$, again

$$2p_{TW} - a + \alpha\kappa W^2 + 2\alpha p_{TW} W^2 \ge \min\left\{\frac{a}{2}, \kappa\right\}(1 + \alpha W^2) \,,$$

holds. This implies

$$\frac{d}{dt}\int_{-\infty}^{\infty} u^2(1 + \alpha W^2) d\xi \le -\min\{a, 2\kappa\}\int_{-\infty}^{\infty} u^2(1 + \alpha W^2) d\xi \,.$$

By the Gronwall lemma it can be shown that for $u(\xi,0) \in L^2\left((1+W^2)d\xi\right)$, the solution of the linearized equation (43) decays exponentially as $t \to \infty$.

This stability result leaves some questions. What about more general perturbations? In some sense, the slowest solution, i.e. with speed $s = s_0$, is the only stable one. For an initial datum satisfying

$$p(\xi,0) = a \quad \text{for } \xi < \underline{\xi}\,, \qquad p(\xi,0) = 0 \quad \text{for } \xi > \overline{\xi}\,,$$

the solution can be shown to converge to the traveling wave with $s = s_0$ [5].

9 The Turing mechanism

9.1 Destabilization by diffusion

One thing we seem to have learned from the previous section is that diffusion is stabilizing. One of the most important mechanisms for pattern formation, however, uses destabilization by diffusion. It requires a system of at least two coupled reaction-diffusion equations.

We first consider a linear system of two ODEs,

$$\frac{du}{dt} = au + bv\,, \qquad \frac{dv}{dt} = cu + dv\,,$$

with constant coefficients a, b, c, d. The trivial steady state $u = v = 0$ is asymptotically stable, iff both eigenvalues of the coefficient matrix are in the left half plane, which is equivalent to the conditions

$$a + d < 0\,, \qquad ad - bc > 0\,, \tag{46}$$

on the trace and the determinant. Now we add diffusion:

$$\partial_t u = D_u \Delta u + au + bv\,, \qquad \partial v = D_v \Delta v + cu + dv\,,$$

with different diffusivities D_u, D_v (which will be essential). After an appropriate nondimensionalization, this becomes

$$\partial_t u = \Delta u + au + bv\,, \qquad \partial_t v = D\Delta v + cu + dv\,,$$

with $D = D_v/D_u$.

In the spirit of Section 3, we look for solutions of the form

$$u(x,t) = e^{\lambda(k)t + ik\cdot x}\overline{u}\,, \qquad v(x,t) = e^{\lambda(k)t + ik\cdot x}\overline{v}\,,$$

with constants $\overline{u}$ and $\overline{v}$, giving the linear system

$$(\lambda(k) + |k|^2 - a)\overline{u} - b\overline{v} = 0\,, \qquad (\lambda(k) + D|k|^2 - d)\overline{v} - c\overline{u} = 0\,,$$

for $\overline{u}$ and $\overline{v}$, possessing nontrivial solutions, iff

$$\lambda(k)^2 + \lambda(k)(|k|^2(D+1) - a - d) + D|k|^4 - |k|^2(aD+d) + ad - bc = 0\,.$$

This equation determines the dispersion relation. By (46), the coefficients and, thus, the left hand side is strictly positive for $|k| = 0$. The same is true for large values of $|k|$. A positive eigenvalue $\lambda(k)$ only exists, if there are values of k such that

$$D|k|^4 - |k|^2(aD+d) + ad - bc < 0\,,$$

requiring that a and d (and therefore by (46) also b and c) have opposite signs and that the ratio D of the diffusivities is different from 1. W.l.o.g we assume

$$0 < d < -a\,, \quad \text{and } D \text{ small enough such that } aD + d > 2\sqrt{D(ad-bc)}\,.$$

Using D as a bifurcation parameter, the bifurcation point is defined by the equality $aD + d = 2\sqrt{D(ad-bc)}$. The critical wave number k_c (with $\lambda(k_c) = 0$) is then determined by $k_c^2 = (aD+d)/(2D) = \sqrt{(ad-bc)/D}$.

9.2 A predator-prey model

As an example we discuss a two-species population model of predator-prey type. Denoting the prey density by $b(x,t)$ ('Beute') and the predator density by $r(x,t)$, ('Räuber') we consider the reaction-diffusion model

$$\begin{aligned} \partial_t b &= D_b \Delta b + \gamma b - \delta b^2 - \varepsilon r b\,, \\ \partial_t r &= D_r \Delta r + \alpha r^2 b - \beta r\,, \end{aligned}$$

where D_b and D_r are the diffusivities, γ is the growth rate of small prey populations in the absence of predators, γ/δ is a stable equilibrium prey density in the absence of predators, εr is the death rate of prey caused by predators, $\alpha r b$ is the birth rate of predators assuming sexual reproduction and the necessity of favourable conditions caused by the presence of prey, and β is the death rate of predators.

This is only one of many possible predator-prey models chosen such that the Turing mechanism can occur. We start by a nondimensionalisation reducing the number of parameters. Introducing the reference length $\sqrt{D_b/\gamma}$,

the reference time $1/\gamma$, the reference prey density γ/δ, the reference predator density $\beta\delta/(\alpha\gamma)$, and the dimensionless parameters

$$A = \frac{\beta\delta\varepsilon}{\alpha\gamma^2}\,, \quad B = \frac{\beta}{\gamma}\,, \quad D = \frac{D_r}{D_b}\,,$$

the scaled model reads

$$\begin{aligned} \partial_t b &= \Delta b + b - b^2 - Arb\,, \\ \partial_t r &= D\Delta r + B(rb-1)r\,. \end{aligned}$$

We start by analyzing spatially homogeneous solutions, i.e., the corresponding system of ODEs

$$\frac{db}{dt} = b - b^2 - Arb\,, \qquad \frac{dr}{dt} = B(rb-1)r\,.$$

Under the assumption $A < 1/4$ there are 4 steady states in the first quadrant of the (b,r)-plane given by $(0,0)$, $(1,0)$, and $(b_\pm, b_\pm^{-1})$ with $b_\pm = 1/2 \pm \sqrt{1/4 - A}$. By linearization it is easily checked that the origin is a saddle (with the axes as stable and unstable manifolds) and that $(1,0)$ is stable. The point (b_+, b_+^{-1}) is unstable, whereas (b_-, b_-^{-1}) can be made stable by the additional condition $B < b_- = 1/2 - \sqrt{1/4 - A}$ on the parameters, which makes (b_+, b_+^{-1}) a saddle.

Another important question is wether solutions remain bounded. This we shall answer by constructing an invariant region. We start by solving a simpler problem neglecting two of the 'good' terms:

$$\frac{db}{dt} = (1 - Ar)b\,, \qquad \frac{dr}{dt} = Br^2 b\,.$$

Solution trajectories in the (b,r)-phase-plane are given by $b = \bar{b} - 1/(Br) - (A/B)\ln r$ with a constant of integration $\bar{b}$. We shall use these curves for the construction of invariant regions: $(b,r) \in S_M$ iff $b, r \geq 0$ and either $r \leq 1/A$ and $b \leq M$, or $r \geq 1/A$ and

$$b \leq M + \frac{A}{B}\left(1 - \frac{1}{Ar} - \ln(Ar)\right)\,.$$

It is easily seen that for every M, S_M is bounded and that every point in the first quadrant lies in S_M for large enough M. Also $S_{M_1} \subset S_{M_2}$ for $M_1 \leq M_2$. We shall also prove that for $M \geq 1$, S_M is forward invariant, i.e., every trajectory starting in S_M stays there for all positive times. For this pupose

we have to inspect the flow on the boundary. Since the axes are invariant manifolds, we only need to check the boundary parts in the interior of the first quadrant. Obviously, $\frac{db}{dt} = b - b^2 - Arb = (1 - M - Ar)M \le 0$ for $M \ge 1$ and, thus, the direction of the flow is inwards along $\{(M, r) :\ 0 < r < 1/A\}$. We also compute

$$\frac{d}{dt}\left(b + \frac{1}{Br} + \frac{A}{B}\ln r\right) = -b^2 - Br \le 0\,,$$

showing the same for the boundary piece $\{(M + \frac{A}{B}\left(1 - \frac{1}{Ar} - \ln(Ar)\right), r) : r > 1/A\}$.

The dynamics can now be described as follows: The stable manifold of the saddle (b_+, b_+^{-1}) separates the first quadrant into the domains of attraction of the stable steady states $(1, 0)$ and (b_-, b_-^{-1}). In other words, depending on the initial condition, either the predators die out and the prey density converges to 1, or an equilibrium is reached, where predators and prey coexist. This concludes the analysis of spatially homogeneous solutions.

We now concentrate on the steady state (b_-, b_-^{-1}). With the notation of the previous section, linearization gives $a = -b_-$, $b = -Ab_-$, $c = Bb_-^{-2}$, and $d = B$, satisfying the conditions for a Turing instability if the diffusivity of the predators is small enough compared to that of the prey.

Bounded domain, zero flux BC. Determination of the bifurcating state. Geometric examples.

10 Chemotaxis

10.1 A kinetic transport model for *Escheria coli* and its macroscopic limit

$$\varepsilon\partial_t f + \varepsilon v\cdot\nabla_x f = Q(f)\,,$$

with

$$Q(f) = \int_{|v'|=1}[\varphi(\partial_t S + v'\cdot\nabla_x S)f(v') - \varphi(\partial_t S + v\cdot\nabla_x S)f(v)]dv'\,.$$

where φ is positive and strictly decreasing. Assume $\lim_{\varepsilon\to 0} f = f_0$. Then $Q(f_0) = 0$.

$$\int_{|v|=1} Q(f)\varphi f\,dv = \int_{|v|=1}\int_{|v'|=1}(\varphi' f' - \varphi f)\varphi f\,dv'dv$$
$$= \int_{|v|=1}\int_{|v'|=1}(\varphi f - \varphi' f')\varphi' f'\,dv'dv = -\frac{1}{2}\int_{|v|=1}\int_{|v'|=1}(\varphi f - \varphi' f')^2 dv'dv\,.$$

This implies the existence of $h(x,t)$, such that

$$f_0(x,v,t) = \frac{h(x,t)}{\varphi(\partial_t S(x,t) + v \cdot \nabla_x S(x,t))}\,.$$

Mass conservation of the *turning operator* Q, i.e. $\int Q(f)dv = 0$, implies

$$\partial_t \varrho_0 + \nabla_x \cdot \int_{|v|=1} v f_0 \, dv = 0\,,$$

with

$$\varrho_0 = \int_{|v|=1} f_0 \, dv = h \int_{|v|=1} \frac{dv}{\varphi(\partial_t S + v \cdot \nabla_x S)}\,.$$

This gives

$$\partial_t \varrho_0 + \nabla_x \cdot (\varrho_0 \chi(\partial_t S, |\nabla_x S|) \nabla_x S) = 0\,,$$

with $\chi = b/a$, where

$$\int_{|v|=1} \frac{dv}{\varphi(\partial_t S + v \cdot \nabla_x S)} = \int_{|w|=1} \frac{dw}{\varphi(\partial_t S + w_1 |\nabla_x S|)} = a(\partial_t S, |\nabla_x S|)\,.$$

In terms of the v-coordinates, the w_1-direction is $\nabla_x S/|\nabla_x S|$. Similarly,

$$\int_{|v|=1} \frac{v\,dv}{\varphi(\partial_t S + v \cdot \nabla_x S)} = \frac{\nabla_x S}{|\nabla_x S|} \int_{|w|=1} \frac{w_1 dw}{\varphi(\partial_t S + w_1 |\nabla_x S|)} = b(\partial_t S, |\nabla_x S|) \nabla_x S\,.$$

Note that $a, b > 0$ and, thus, $\chi > 0$, by the properties of φ.

10.2 A kinetic transport model for *Dictyostelium discoideum* and its macroscopic limit

$$\varepsilon^2 \partial_t f + \varepsilon v \cdot \nabla_x f = Q(f)\,,$$

with

$$Q(f) = \int_{|v'|=1} [\varphi(S(x+\varepsilon v, t) - S(x,t)) f(v') - \varphi(S(x+\varepsilon v', t) - S(x,t)) f(v)] dv'\,,$$

where φ is positive, strictly increasing, and scaled such that $\varphi(0) = \varphi'(0) = 1$. With the asymptotic expansion $f = f_0 + \varepsilon f_1 + O(\varepsilon^2)$, we obtain

$$Q(f) = Q_0(f_0) + \varepsilon [Q_0(f_1) + \varrho_0 \nabla_x S \cdot v] + O(\varepsilon^2)\,,$$

with $\varrho_0 = \int f_0 dv$ and $Q_0(f) = \int (f' - f) dv'$. Analogously to the previous section, the limiting equation $Q_0(f_0) = 0$ implies

$$f_0(x, v, t) = \frac{\varrho_0(x, t)}{S_d}, \qquad S_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}$$

Comparison of $O(\varepsilon)$-terms gives

$$f_1 = \frac{\varrho_1}{S_d} - \frac{v}{S_d} \cdot \left(\frac{\nabla_x \varrho_0}{S_d} - \varrho_0 \nabla_x S \right).$$

Finally, the $O(\varepsilon^2)$-equation integrated with respect to v leads to the conservation law

$$\partial_t \varrho_0 - \nabla_x \cdot (D \nabla_x \varrho_0 - \chi \varrho_0 \nabla_x S) = 0,$$

with the diffusivity and the chemotactic sensitivity

$$D = \int_{|v|=1} \frac{v_i^2}{S_d^2} dv = \frac{1}{dS_d^2} \int_{|v|=1} |v|^2 dv = \frac{1}{dS_d}, \qquad \chi = DS_d = \frac{1}{d}.$$

10.3 The Keller-Segel model for cell aggregation

Macroscopic model for chemotaxis, where the chemical is produced by the cells:

$$\begin{aligned} &\partial_t \varrho - \nabla_x \cdot (D \nabla_x \varrho - \chi \varrho \nabla_x S) = 0, \\ &\partial_t S - D_S \Delta S = \alpha \varrho - \beta S. \end{aligned}$$

Scaling $x \to l_0 x$, $t \to t_0 t$, $\varrho \to \varrho_0 \varrho$, $S \to S_0 S$ with given ϱ_0 (typical for initial data) and with

$$l_0 = \sqrt{\frac{D_S D}{\alpha \varrho_0 \chi}}, \quad t_0 = \frac{D_S}{\alpha \varrho_0 \chi}, \quad S_0 = \frac{D}{\chi},$$

gives

$$\begin{aligned} &\partial_t \varrho - \nabla_x \cdot (\nabla_x \varrho - \varrho \nabla_x S) = 0, \\ &\tau \partial_t S - \Delta S = \varrho - \delta S, \end{aligned}$$

with the dimensionless parameters

$$\tau = \frac{D}{D_S}, \qquad \delta = \frac{\beta D}{\alpha \varrho_0 \chi}.$$

Stability of homogeneous equilibria – Fourier analysis

Homogeneous equilibria: $S = S_\infty$, $\varrho = \varrho_\infty = \delta S_\infty$. Perturbations: Setting $S - S_\infty = e^{\lambda t + ik\cdot x}\overline{S}$, $\varrho - \varrho_\infty = e^{\lambda t + ik\cdot x}\overline{\varrho}$, and linearization gives

$$A \begin{pmatrix} \overline{\varrho} \\ \overline{S} \end{pmatrix} = \lambda \begin{pmatrix} \overline{\varrho} \\ \overline{S} \end{pmatrix}, \quad \text{with } A = \begin{pmatrix} -|k|^2 & \varrho_\infty |k|^2 \\ 1/\tau & -(|k|^2+\delta)/\tau \end{pmatrix} \tag{47}$$

Since $\mathrm{trace}(A) < 0$, the real parts of the eigenvalues are negative, iff

$$\det(A) = \frac{|k|^2}{\tau}(|k|^2 + \delta - \varrho_\infty) > 0\,.$$

Thus, instability occurs for small wave numbers $|k|$, iff $\varrho_\infty > \delta$.

Inhomogeneous equilibria in 1D bounded domains

For $x \in (0,\pi)$ with no-flux boundary conditions (i.e. $\partial_x \varrho = \partial_x S = 0$ for $x = 0, \pi$), the total number of cells remains constant, and therefore we restrict our attention to solutions satisfying

$$\int_0^\pi \varrho(x,t)dx = M\,,$$

for a fixed given $M > 0$. Then there is a unique homogeneous equilibrium

$$\varrho_\infty = \frac{M}{\pi}\,, \qquad S_\infty = \frac{M}{\delta\pi}\,.$$

The linearized stability analysis leads to the eigenvalue problem

$$\begin{aligned} &\lambda\hat{\varrho} = \hat{\varrho}'' - \varrho_\infty \hat{S}''\,, \qquad \hat{\varrho}'(0) = \hat{\varrho}'(\pi) = 0\,, \qquad \int_0^L \hat{\varrho}\,dx = 0\,, \\ &\lambda\tau\hat{S} = \hat{S}'' + \hat{\varrho} - \delta\hat{S}\,, \qquad \hat{S}'(0) = \hat{S}'(\pi) = 0\,. \end{aligned}$$

The eigenfunctions are given by $\hat{\varrho}_k(x) = \cos(kx)\overline{\varrho}$, $\hat{S}_k(x) = \cos(kx)\overline{S}$, $k = 1, 2, \ldots$ This leads to (47). Using M as bifurcation parameter, the homogeneous equilibrium looses its stability, when M gets larger than

$$M_0 = \pi(1+\delta)\,.$$

At this value of M, a bifurcation occurs. Its character is influenced by the fact that the problem has a flip symmetry. It is invariant under the transformation $x \to -x$. If a symmetry of this kind is present in an ODE $\dot{u} = f(u,r)$ (with parameter r), expressed as invariance under $u \to -u$, this

implies that f is odd as a function of u. In this case, there is always the trivial steady state $u = 0$, and the normal form is given by $f(u, r) = ru \pm u^3$. Considering the *(supercritical)* case

$$\dot{u} = ru - u^3 \,,$$

where solutions remain bounded, the bifurcation can be described as follows: For $r < 0$, the trivial steady state $u = 0$ is the only equilibrium, and it is asymptotically stable. For $r > 0$, there are two more equilibria $u = \pm\sqrt{r}$, which are asymptotically stable, whereas $u = 0$ is unstable. Motivated by the shape of the bifurcation diagram, this is called the *pitchfork bifurcation*.

The bifurcation analysis will be carried out on the stationary problem

$$(\varrho' - \varrho S')' = 0 \,, \quad S'' = \delta S - \varrho \,, \quad \varrho'(0) = \varrho'(\pi) = S'(0) = S'(\pi) = 0 \,,$$

subject to

$$\int_0^\pi \varrho \, dx = M \,.$$

The equation for ϱ can be solved:

$$\varrho(x) = M \frac{e^{S(x)}}{\int_0^\pi e^{S(y)} dy} \,,$$

and the problem is reduced to

$$S'' = \delta S - M \frac{e^S}{\int_0^\pi e^S dy} \,, \quad S'(0) = S'(\pi) = 0 \,.$$

We prescribe a value of M close to the critical value $M_0 = \pi(1+\delta)$, and look for S close to the corresponding homogeneous equilibrium $S_0 = 1 + 1/\delta$:

$$M = M_0 + \varepsilon^2 \,, \qquad S(x) = S_0 + \varepsilon S_1(x) + \varepsilon^2 S_2(x) + \varepsilon^3 S_3(x) + O(\varepsilon^4) \,.$$

The scaling is motivated by the normal form of the pitchfork bifurcation, where the size of the bifurcating solutions is proportional to the square root of the distance of the bifurcation parameter from its critical value.

It is considerable work (but straightforward) to substitute this ansatz and to expand all terms with respect to powers of ε. We therefore skip most of the details. At $O(\varepsilon)$ we obtain

$$S_1'' + S_1 - (1 + \delta)\overline{S_1} = 0 \,, \quad S_1'(0) = S_1'(\pi) = 0 \,,$$

where $\overline{z} = \pi^{-1}\int_0^\pi z(x)dx$, having the solution $S_1(x) = a\cos x$, with an arbitrary constant $a \in \mathbb{R}$. Using this at $O(\varepsilon^2)$, we obtain

$$S_2'' + S_2 - (1+\delta)\overline{S_2} = -\frac{1}{\pi} - a^2\frac{1+\delta}{2}\left(\cos^2 x - \frac{1}{2}\right), \quad S_2'(0) = S_2'(\pi) = 0\,. \tag{48}$$

Before solving this problem, we consider, more generally,

$$u'' + u - (1+\delta)\overline{u} = f\,, \quad u'(0) = u'(\pi) = 0\,,$$

with given right hand side and note, that

$$\int_0^\pi f(x)\cos x\,dx = 0$$

is a necessary and sufficient condition for solvability. It is satisfied by the right hand side in (48) for arbitrary values of a, and the solution is given by

$$S_2(x) = \frac{1}{\delta\pi} - a^2\frac{1+\delta}{6}\left(\cos^2 x - \frac{1}{2}\right) + b\cos x\,,$$

with an arbitrary constant $b \in \mathbb{R}$. Remembering the normal form of the pitchfork bifurcation, it is no surprise that we have to go to $O(\varepsilon^3)$:

$$\begin{aligned} &S_3'' + S_3 - (1+\delta)\overline{S_3} \\ &\quad = -\frac{1}{\pi}S_1 + (1+\delta)\left(\overline{S_1S_2} - S_1S_2 + \frac{1}{\delta\pi}S_1 - \frac{1}{6}S_1^3 + \frac{1}{2}S_1\overline{S_1^2}\right), \\ &S_3'(0) = S_3'(\pi) = 0\,, \end{aligned}$$

The solvability condition is equivalent to the equation

$$a\left(1 - a^2\frac{\pi}{24}(1+\delta)(4+\delta)\right) = 0\,,$$

leading to the bifurcating solutions

$$S(x) = 1 + \frac{1}{\delta} \pm \varepsilon\sqrt{\frac{24}{\pi(1+\delta)(4+\delta)}}\cos x + O(\varepsilon^2)\,.$$

Since the cell density has the same qualitative behaviour as the chemical concentrations, the cells tend to aggregate close to one of the boundary points. Both bifurcating solutions can be expected to be asymptotically stable. It can be shown that stationary solutions with this qualitative behaviour exist for all $M > M_0$. The important ideas and further references can be found in [4].

11 Cell-cell adhesion

Microscopic one-dimensional model for cell-cell adhesion and volume filling [1]:

$$\begin{aligned}\frac{d\varrho_j}{dt} &= T(j+1\to j)\varrho_{j+1} + T(j-1\to j)\varrho_{j-1} \\ &\quad -(T(j\to j+1)+T(j\to j-1))\varrho_j\,,\end{aligned}$$

with $T(j\to j+1) = (1-\varrho_{j+1})(1-\alpha\varrho_{j-1})/h^2$ and $0\le\alpha\le 1$, where the first factor is due to volume filling and the second due to cell-cell adhesion. It is easily shown that $0\le\varrho_j(0)\le 1$ for all $j\in\mathbb{Z}$ implies $0\le\varrho_j(t)\le 1$ for all $j\in\mathbb{Z}$, $t\ge 0$. The equation can also be written as

$$\frac{d\varrho_j}{dt} = \frac{K_{j+1}-2K_j+K_{j-1}}{h^2}\,, \qquad K_j = \varrho_j + \alpha\varrho_j(\varrho_{j-1}\varrho_{j+1}-\varrho_{j-1}-\varrho_{j+1})\,.$$

With $\varrho_j(t)\approx\varrho(jh,t)$, the macroscopic limit $h\to 0$ formally gives

$$\partial_t\varrho = \partial_x^2 K(\varrho)\,, \qquad K(\varrho) = \varrho - 2\alpha\varrho^2 + \alpha\varrho^3\,,$$

which can be written as the nonlinear diffusion equation

$$\partial_t\varrho = \partial_x(D(\varrho)\partial_x\varrho)\,, \qquad D(\varrho) = 1-\frac{4\alpha}{3}+3\alpha\left(\varrho-\frac{2}{3}\right)^2\,. \tag{49}$$

The initial value problem for this equation maybe ill-posed, since for $\alpha > 3/4$, the diffusivity takes negative values in a ϱ-interval around $\varrho = 2/3$. On the other hand, by the boundedness of ϱ_j, a weak limit (as $h\to 0$) $\varrho(x,t)$ of the piecewise constant extension (in space) of $\varrho_j(t)$ exists. In general, it cannot be expected to solve (49) because of the ill-posedness of this equation.

An understanding of the situation for $h\ll 1$ can be achieved by a tool from numerical analysis, called the *modified equation*. When passing from

the microscopic to the macroscopic model, not only the leading order terms are used, but also the first significant corrections. In our case we obtain by Taylor expansion around $x = jh$:

$$K_j = K(\varrho) + \alpha h^2 \varrho \left((\varrho - 1)\partial_x^2 \varrho - (\partial_x \varrho)^2 \right) + O(h^3) \,.$$

The modified equation

$$\partial_t \varrho = \partial_x^2 \left[K(\varrho) + \alpha h^2 \varrho \left((\varrho - 1)\partial_x^2 \varrho - (\partial_x \varrho)^2 \right) \right] ,$$

is of fourth order. Since for $0 \leq \varrho \leq 1$, the leading order coefficient is nonpositive, well posedness can be expected (although it would be difficult to prove). Obviously, the macroscopic limit $h \to 0$ again leads to (49). However, this changes, when the fast variable

$$y = \frac{x}{h\sqrt{\alpha}}$$

is introduced:

$$\alpha h^2 \partial_t \varrho = \partial_y^2 \left[K(\varrho) + \varrho \left((\varrho - 1)\partial_y^2 \varrho - (\partial_y \varrho)^2 \right) \right] ,$$

Now, the limit $h \to 0$ leads to the stationary fourth order equation

$$0 = \partial_y^2 \left[K(\varrho) + \varrho \left((\varrho - 1)\partial_y^2 \varrho - (\partial_y \varrho)^2 \right) \right] , \tag{50}$$

which can be integrated twice. In the first integration we set the constant of integration equal to zero which guarantees a bounded flux in terms of the original variable x. The second integration then leads to

$$c = K(\varrho) + \varrho \left((\varrho - 1)\partial_y^2 \varrho - (\partial_y \varrho)^2 \right) ,$$

with the integration constant c. This equation can be put into Hamiltonian form by the transformation $\varrho = 1 - e^u$:

$$\partial_y^2 u = \frac{c - K(1 - e^u)}{e^{2u}(1 - e^u)} = f(u, c) \,.$$

For $3/4 < \alpha < 1$ (which we assume in the following), there is an interval of c-values such that there are three steady states $u_1(c) < u_3(c) < u_2(c)$ ($f(u_j(c), c) = 0$), where u_1 and u_2 are saddles and u_3 is a center. Generically, there exists a homoclinic orbit encircling u_3, which either connects u_1 or u_2 with itself. For one parameter value $c = c_{crit}$, however, separating the two

generic situations, this degenerates to a heteroclinic cycle consisting of two heteroclinic orbits, connecting u_1 with u_2 and vice versa (see [1] for more details on these statements). For later reference, we introduce

$$\varrho_1 := 1 - e^{u_1(c_{crit})} > \varrho_2 := 1 - e^{u_2(c_{crit})} ,$$

and recall that there exist bounded solutions of the limiting equation (50) for $y \in \mathbb{R}$, connecting ϱ_1 (at $y = -\infty$) to ϱ_2 (at $y = \infty$) and vice versa.

Numerical simulations with the full microscopic model suggest that the periodic solutions of (50) encircling $\varrho_3 = 1 - e^{u_3}$ describe the oscillations observed when parts of the initial data for the density lie in the forbidden interval $(\underline{\varrho}, \overline{\varrho})$, where the diffusivity $D(\varrho)$ is negative. After a while, a coarsening of these oscillations is observed, where the solution shows rapid changes (almost jumps) across the forbidden ϱ-interval. These jumps can be explained analytically by the heteroclinic orbit solutions of (50) connecting ϱ_1 and ϱ_2, which satisfy

$$\varrho_2 < \underline{\varrho} < \overline{\varrho} < \varrho_1 .$$

After this initial coarsening, a purely macroscopic model can be used for the description of the dynamics. In regions, where $\varrho(x,t) < \underline{\varrho}$ or $\varrho(x,t) > \overline{\varrho}$, the limiting diffusion equation (49) can be used. These regions are separated by points $x_0(t)$, where jumps between, e.g., $\varrho(x_0-,t) = \varrho_2$ and $\varrho(x_0+,t) = \varrho_1$ occur. The dynamics of these jump points are a consequence of mass conservation. Integrating (49) with respect to x from a to b with $a < x_0(t) < b$ gives

$$\int_a^b \varrho \, dx + (\varrho_2 - \varrho_1)\dot{x}_0 = (D(\varrho)\partial_x\varrho)(b) - (D(\varrho)\partial_x\varrho)(a) .$$

The limits $a \to x_0-$, $b \to x_0+$ complete the derivation of an ODE for $x_0(t)$:

$$\dot{x}_0 = \frac{(D(\varrho)\partial_x\varrho)(x_0+) - (D(\varrho)\partial_x\varrho)(x_0-)}{\varrho_2 - \varrho_1} .$$

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