Stochastic and spatial structures of dynamical systems

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Stochastic and spatial structures of dynamical systems

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Preface

Recently great progress has been made in the field of dynamical systems. In January 1995, the Royal Netherlands Academy of Arts and Sciences enabled us to organize a meeting aimed at a wide audience consisting of mathematicians, physicists, biologists and economists. This collection of articles comprises the contributions of most of the speakers.

We felt that several new developments in dynamical systems are important or will become so in the near future. We decided to select some areas which are close to applications and related to noise, randomness and spatial structures. Broadly speaking our aim was to centre the meeting around three topics.

- the effect of noise on data generated by dynamical systems and testing whether these dynamical systems adequately model "reality";
- (ii) spatial structures which can be generated by dynamical systems and which act on a network of coupled systems (coupled lattice maps);
- (iii) random differential equations and applications to biology.

Noise and chaotic dynamics

One effect of adding noise to a system with chaotic dynamics is that it can drastically change its attractor. One reason for this is that noise is amplified in a system which is not very hyperbolic: this becomes especially important when some components of the basin of an attractor are extremely small. Of course, one is often interested in the underlying deterministic system of a dynamical system f which has noise. To formalize this, one could define the *deterministic approximation* $x \mapsto f^*(x)$ of a "noisy system" f to be the conditional expected value E(f|x). However, $(f^2)^*$ need not be equal to $(f^*)^2$. As Takens shows in his paper, this implies that it is in some ways meaningless to ask whether a system with noise is really chaotic. (Because $(f^2)^*$ can be chaotic even when f^* is not.)

One approach to systems with noise is estimating correlation integrals. Given some numerical data, one can try to estimate some of these numbers. In Keller and Sporer's article linear regression estimators are discussed for the correlation dimension, entropy and detection of noise. These estimators are applied to data related to the Hénon map.

In the article of Cheng and Tong, delay coordinates from Takens' embedding theorem are discussed in the context of stochastic dynamical systems. More specifically, assume that one has a stochastic dynamical system of the form

$$X_t = F(X_{t-1}, \ldots, X_{t-d_0}) + \epsilon_t$$

where the condition expectation of ϵ_t (given $X_{t-1}, \ldots, X_{t-d_0}$) is zero. Estimates for suitable choices of the lag d_0 and the required sample size are discussed.

Coupled lattice maps

Recently, many numerical studies and some theoretical results have been obtained on *Coupled Lattice Maps* abbreviated frequently as CLM's. These are systems which are meant to model spatial structures where the state of a site is determined dynamically by the previous state at that site and that of its neighbours. Such models have a wide range of applications to physics (crystals), biology (nervous systems, population dynamics), economics (interaction of different markets), reaction-diffusion equations (see Section 2 of the paper of Losson and Mackey) and so on. Numerically, one can observe the formation of waves, patterns, synchronization in which coupling plays an important role. In one class of models the state $x_{n+1}(i)$ at time n + 1 at site i is determined by the states at the neighbouring sites $i - 1, i, i + 1 \in \mathbb{Z}$ at time n. An example of such a one-dimensional nearest site model is

$$x_{n+1}(i) = (1-\epsilon)f(x_n(i)) + \frac{\epsilon}{2}\left[f(x_n(i+1)) + f(x_n(i-1))\right]$$

where $x_n(i)$ is the state of the system at site $i \in \mathbb{Z}$ at time $n \in \mathbb{N}$. If $\epsilon = 0$ then each site *i* has a time dynamics which is completely uncoupled from those at other sites. When $\epsilon \in (0, 1)$ then the dynamics at distinct sites will interact. Of course, the non-linearity of the map *f* also plays an important role. Similar models can also be constructed when $i \in \mathbb{Z}$ is replaced by $(i, j) \in \mathbb{Z} \times \mathbb{Z}$ (the two-dimensional case) in which case the interaction at site (i, j) could be with its nearest neighbours. In many situations one observes random patterns which are "frozen", or "defects" which zigzag in space. Sometimes, also certain regular patterns suddenly break up and one obtains spatiotemporal chaos.

In the paper of Losson and Mackey a survey is given on CLM's. In particular, the effect of adding stochastic perturbations onto a CLM system is discussed. In fact, even without stochastic perturbations a CLM can behave "ergodically". One way of describing these ergodic properties is discussed in Keller's paper: it is shown that if the map f is sufficiently expanding (and itself has a good invariant probability measure) and the coupling is sufficiently small then one has a good invariant probability measure. In his paper, Mackay shows that for a rather general class of CLM's (with coupling parameter ϵ) solutions of the system for $\epsilon = 0$ persist when $\epsilon > 0$. In fact, since the proof of this uses an implicit function theorem, Mackay is able to show that these results even apply for rather large ϵ . This explains why one can have "spatially local" dynamics.

Instead of coupled lattice maps, Mallet-Paret studies coupled lattice differential equations (LDE's). The class of systems Mallet-Paret discusses in his paper, are simplified versions of systems which seem to be able to identify patterns in digitized images (Cellular Neural Networks, studied experimentally by Chua, Hasler and others). Using methods from bifurcation theory, Mallet-Paret shows that - depending on parameters in the model - all kinds of stripe or check pattern solutions exist and discusses the stability of such solutions. In addition, he discusses travelling wave solutions and also defines and describes systems with spatial chaos.

Random differential equations and applications

Many applications are modelled by the telegraph equation

$$u_{tt} + 2\mu u_t = \gamma^2 u_{xx}.$$

This equation is in some senses an interpolation between the wave equation $u_{tt} = \gamma^2 u_{xx}$ (taking $|\mu|$ small) and a diffusion equation $u_t = (\gamma^2/2\mu)$ (taking μ large). Hadeler's article gives an overview of the many applications of the telegraph equation and its connections to random walks. For example, it is shown that the telegraph equation is equivalent to the system

$$u_t^+ + \gamma u_x^+ = \mu(u^- - u^+),$$

$$u_t^- - \gamma u_x^- = \mu(u^+ - u^-)$$

where u_{\pm} are the densities of a particle performing a correlated random walk on the real line with speed $\pm \gamma$ (i.e., $u^{\pm}(t,x) \geq 0$ and $\int_{-\infty}^{\infty} u^{+}(t,x), u^{-}(t,x)) dx = 1$).

Instead of adding noise to a differential equation (as is done in stochastic differential equations), one can also add a term which comes from a chaotic flow. This point of view is considered in Johnson's article. He considers differential equations of the form

$$x' = f(T_t(y), x), \quad y \in Y, x \in \mathbb{R}^n$$

where Y is some topological space with probability measure μ which is ergodic w.r.t. the flow $T_t: Y \to Y$ and $f: Y \times \mathbb{R}^n \to \mathbb{R}^n$ is Lipschitz continuous in the second variable. The notion of exponential dichotomy and its connection with the theorem of Oseledec is discussed. Furthermore, some examples of bifurcations of such systems are considered.

Finally, in an article of Metz e.a. stochastic processes are suggested which model long-term biological evolution.

Clearly, there are many new exciting developments in dynamical systems. Hopefully these proceedings give a good impression of some of these.

Amsterdam, 16 February, 1996,

Sebastian van Strien and Sjoerd Verduyn Lunel

Part I: Statistical and Reconstruction Methods

The effect of small noise on systems with chaotic dynamics

Floris Takens

1 Introduction

In this paper we are concerned with the effect of small noise in dynamical systems, in particular in nonlinear and chaotic dynamical systems — the noise we consider is, what is sometimes called system noise: at each time there is some uncertainty concerning the next state (for simplicity we only consider systems with discrete time). There are several examples which motivate such a study:

Firstly, we may think of (simple) mathematical models, like the Navier-Stokes equation describing the motion of a fluid, but ignoring the effects due to the molecular motion. This molecular motion (and other possible effects which are not taken into account by the Navier-Stokes equations) is then considered as noise. For this type of noise see e.g. [3].

Secondly, twisting the first example, we can consider a numerical scheme, "solving the Navier-Stokes equations", as a deterministic system and the "real solution", or maybe rather the "real fluid motion", as a more or less random perturbation of the numerical solution. These differences between numerical solutions and exact solutions can be made very small in the case of systems with a finite dimensional state space, but for systems described by partial differential equations, this "numerical noise" can be much bigger, since then one *also* has to approximate the infinite dimensional phase space by a finite dimensional one.

Thirdly, one may think of a system, whose laws of motion are unknown to us and for which we derive in a phenomenological way a (simple) deterministic model as a first order approximation (this situation is quite close to the situation considered in the first example, but here the "deterministic approximation" is somewhat arbitrary due to the absence of "laws of nature"). The deviation between model and reality is then considered as noise.

In all these examples there is the important question: how well does the system with noise approximate the system without noise and vice versa. This question has at least two different aspects:

Firstly, how well can the system with noise be used to predict the short term behaviour of the system without noise and vice versa. We talk here only about short term predictions because we know that in the case where the dynamics is chaotic, predictions over long time intervals are impossible, due to the sensitive dependence on initial conditions.

Secondly, how well can the system with noise be used to predict the long term statistical properties of the system without noise and vice versa. For the moment we do not want to give a precise definition of the "long term statistical properties", but in the numerical experiments which we shall discuss, it will be clear what we mean, and in the final section we go into a somewhat more fundamental discussion.

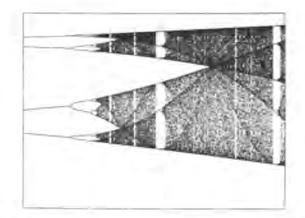


Figure 1: The attractors for the logistic system for μ in [3.5, 3.75].

It is important to keep the difference between these two criteria in mind. This difference is also related with the point that the criteria for a good mathematical model depend on what one wants: there are reasonable models to predict the weather for, say, the next day, but, iterating such a prediction procedure and then averaging over the time to get information about the climate, gives completely non-realistic results [9].

The purpose of this paper is to give a discussion of the above problems. We base this discussion mainly on some numerical experiments with the logistic system. We also provide an example (also related to the logistic system) showing that one cannot make a sharp distinction between systems whose deterministic approximation is chaotic or not. This implies in my opinion that one has to be very careful when assigning numerical invariants, like dimension and entropy, to a system, the dynamics of which is not completely deterministic, via an estimate of an underlying deterministic dynamics.

2 A numerical example

We consider the Logistic system, defined by the map $\varphi_{\mu}(x) = \mu x(1-x)$ for values of μ between 3.5 and 3.75. First we represent the attractors of this system without noise. In figure 1 the horizontal axis is the μ -axis (from 3.5 to 3.75) and the vertical is the x-axis (from 0 to 1). For each of the μ values the following procedure was followed: from a more or less arbitrary initial value of x (here x = .5) we iterate the map φ_{μ} 100 times without plotting anything, then we calculate another 200 iterations for which we plot the corresponding points in the (μ, x) -plane. The idea is that after the first 100 iterations we are on the "attractor" in the sense that the consequences of the particular choice of the initial point are no longer visible. So what is represented graphically are those x-values which continue to occur. This same method of representing graphically

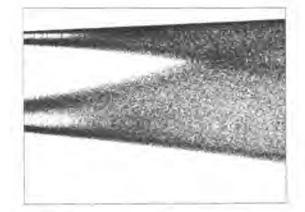


Figure 2: The attractor of the logistic system as in figure 1, but with uniform noise in the interval [-.005, .005].

the dynamics of the logistic system was used e.g. in [1] and by many other authors. In figure 2 we follow the same procedure, only we add, each time we apply the map φ_{μ} , a noise term with average zero and which is uniformly distributed between -.005 and +.005. We see that all fine structure is washed out, even fine structure on a scale much bigger than the amplitude of the noise. So here we have two systems which are very close, in the sense that one can use one to predict what the other will do after one iteration (with an accuracy of .5%), but if we are interested in the question which x-values will continue to occur after many iteration for a given value of μ , then it is very misleading to use one system as a model for the other. Even if we decrease the noise term by a factor 10, see figure 3, there is still fine structure lost on a scale bigger than .5% (the first noise level).

In the next section we want to give an explanation of this dramatic "noise amplification".

Comparing figure 1 with figure 2 we can see that at least in this case it does not make much sense to try to find out whether a "deterministic approximation" of a given system with small noise is chaotic or has a periodic attractor. In a later section we shall substantiate this point with rigorous arguments.

3 Mechanisms of noise amplification

3.1 Linear attractor with noise

We first consider the case of a point attractor of a linear system to which we add noise. This is well known in the theory of linear stochastic systems, e.g. see [7], but we present it here because it explains part of our numerical experiment in the previous section.

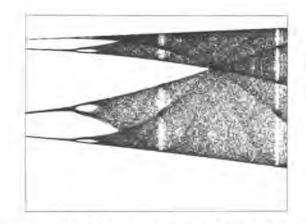


Figure 3: The attractor of the logistic system as in figure 2, but with uniform noise in the interval [-.0005, .0005].

Let $\varphi : \mathbb{R} \to \mathbb{R}$ be a linear contraction by a factor λ , so $\varphi(x) = \lambda x$, with $|\lambda| < 1$. We consider φ as the generator of a dynamical system and we add uncorrelated noise with average zero, standard deviation sd, and maximum absolute value m. For an arbitrary initial point x(0) we then get an evolution of the form $x(n) = \varphi(x(n-1)) + \varepsilon(n)$, where $\varepsilon(n)$ is the contribution of the noise at time n. For large values of n, x(n) will have average zero, standard deviation $sd/\sqrt{|1-\lambda^2|}$, and absolute value at most $m/(1-|\lambda|)$.

This follows from the fact that

$$\begin{aligned} x(n) &= \lambda x(n-1) + \varepsilon(n) \\ &= \lambda^2 x(n-2) + \lambda \varepsilon(n-1) + \varepsilon(n) \\ &= \lambda^3 x(n-3) + \lambda^2 \varepsilon(n-2) + \lambda \varepsilon(n-1) + \varepsilon(n) \text{ etc.}. \end{aligned}$$

So for large n and x(0) fixed, we have the following approximation:

$$x(n) \sim \sum_{i\geq 0} \lambda^i \varepsilon(n-i).$$

Due to the fact that $|\lambda| < 1$, the error in this approximation goes to zero as n goes to ∞ .

This simple calculation shows that a weak contraction $(|\lambda||$ close to one) leads to a strong noise amplification. We have calculated the effect on both standard deviation and maximum absolute value: from the statistical point of view the standard deviation may be more relevant but for the graphical representations we gave, the maximum absolute value could be more important (at least if we take very many iterates).

The above calculation applies to our numerical experiment in the following way. For many values of the parameter μ there are periodic attractors with contracting factor (as such one can define the derivative of φ_{μ}^{n} at a point of a periodic attractor with period n) going to 1 in absolute value. Near these parameter values one expects, on the basis of linear approximations, a strong noise approximation. These parameter values at which the contracting factor in absolute value reaches 1 occur in the following places: at the values of period doubling (e.g. see the left hand side of figure 1 where we see successive doublings from period four to eight, then to sixteen, etc.) and in general at the endpoints of the intervals in the μ -axis for which φ_{μ} has a hyperbolic periodic attractor (also in the right half of figure 1). Where the absolute value of the contracting factor actually reaches 1, our calculation, based on a linear system, is clearly no longer valid. Below, we discuss, and illustrate with numerical experiments, the situation at the so-called Feigenbaum value (this is the μ -value which is the limit of the μ -values for which the successive period doublings, refered to above, occur) for this value of μ , the logistic map has an attractor on which the logarithm of the absolute value of the first derivative is in average equal to zero. In agreement with the above arguments we see in a numerical experiment a very strong noise amplification.

3.2 Small domains of attraction

By the above arguments we have explained *part* of the noise amplification but not all: apart from parameter values at which the contracting factor is arbitrarily close to one in absolute value, there are also parameter values at which the contracting factor is even zero. Here our argument, based on linear approximation, gives no noise amplification. It turns out however that, due to *nonlinearities*, the connected components of the domains of attraction of periodic orbits, the period of which is not too low, can become extremely small, so that even small noise is capable to drive a point out of the domain of attraction of the periodic attractor. Below we shall illustrate this effect by a a numerical experiment.

4 Noise amplification illustrated by numerical experiments

4.1 Noise amplification for μ at the Feigenbaum value

As we have mentioned before, the Feigenbaum value F is the limiting value to which the μ -values converge for which we have transitions from periodic attractors of period 2^n to period 2^{n+1} . In the numerical experiments we use for F the value 3.5699457, based on [1]. The map φ_F has a scaling property. To formulate this scaling property we define the renormalization transformation \mathcal{T} for a mapping φ of the real line to itself as: first replace φ by φ^2 and then apply a conjugacy, magnifying the "state space" \mathbb{R} by a factor λ^{-1} with center in .5, where $\lambda = -.3995\cdots$ is one of the Feigenbaum constants. So

$$(\mathcal{T}\varphi)(x) = \lambda^{-1}((\varphi^2((x-.5)\lambda+.5)) - .5) + .5.$$

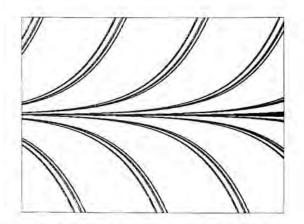


Figure 4: The attractor of the logistic system at the Feigenbaum value. A magnification has been applied by a factor which depends exponentially on the horizontal coordinate.

According to the scaling property, the result of repeated application of the period doubling operator to φ_F gives attractors which converge (and even converge very quickly). Assuming that the convergence is immediate, this means that if we magnify the "attractor" of φ_F by a factor λ^{-1} from the centre x = .5, and restricting to the interval [0,1] we get the same picture. We first illustrate this scaling with a numerical experiment, which we repeat later with noise added in a next experiment. The result of the first experiment is given in figure 4 which was obtained in the following way. In each vertical line we plot the attractor of φ_F in the same way as we plotted attractors in figure 1. The value of μ is now fixed (at F); on the horizontal axis we have the magnifying factor: if we count the pixels on the horizontal axis from 0 to 639, then for the 0^{th} pixel we have x ranging from 0 to 1; this range decreases in an exponential way: for each 100 pixels it decreases by a factor $|\lambda|$. So we expect to see a periodicity in the sense that shifting 100 pixels to the right and turning the picture up side down should give the same picture again (in the "limit"). This periodicity is indeed clearly visible. (In order to compensate for the fact that when making the x-range small most points will fall outside the picture, we also increased the number of iterations exponentially when moving to the right on the horizontal axis: a factor 2 for each 100 pixels.)

Now we repeat the same experiment but with noise added. One may ask how to decrease the maximal amplitude of the noise (which we always take to have average zero and uniform distribution between \pm its maximum amplitude) as a function of the magnifying factor so that the visible effect remains the same. According to the computations in [2], one has to reduce the maximum amplitude by a factor .151 for each period corresponding to the renormalization (so in our case a factor .151 for each 100 pixels on the horizontal axis). The result is given as figure 5.

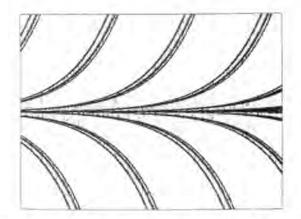


Figure 5: The attractor of the logistic system at the Feigenbaum value as in figure 4, but with noise added.

We see that the relative effects of the noise remains the same (as far as one can conclude from the figure). Since the calculations in the above paper are based on the standard deviation, and not on the maximal absolute value of the effect of the noise, this indicates that it is the standard deviation which is important for this graphical representation.

The factor .151 implies that the ratio between the variance of the effect and the variance of the noise goes to infinity for small noise: each reduction of the length scale with .3995, the absolute value of the scaling constant λ , corresponds to a reduction of the standard deviation of the noise by a factor .151. So for μ at the Feigenbaum value we have a very strong noise amplification, at least for small noise.

4.2 Small basins of (strict) attraction of the superstable period 5 orbit

Here we show with a numerical experiment how the effect of "small basins of attraction" works. We investigate this for the value of μ for which there is a periodic attractor with period 5 and contraction factor 0. This value is obtained by solving the equation $\varphi_{\mu}^{5}(.5) = .5$ — the periodic attractor of period 5 can be seen in figure 1, see also figure 2 and 3, near the right border. We call this μ value S (periodic points with contraction factor 0 are often called Super stable); we use the numerical approximation S = 3.73891. It is known that for almost any initial point $x \in [0, 1]$, in the sense of Lebesgue, the corresponding evolution $\varphi_{S}^{n}(x)$ converges to the periodic attractor of period 5. This convergence can however go in 5 different ways depending on the value of *i* (modulo 5) for which $\lim_{n\to\infty} \varphi^{5n+i}$ is equal to .5; we say that there are 5 different phases in which one can convergence to the period 5 attractor. The regions for which the different possibilities occur are strongly interwoven so that if

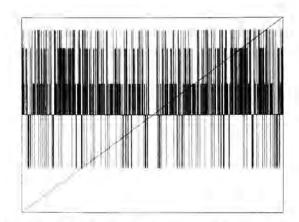


Figure 6: The regions in [0, 1] of initial points with different phase of convergence to the super stable attractor of period 5.

one takes an initial point with not to great accuracy, it is unpredictable which of the five cases will occur (like in the case one throws a dice where also the outcome is unpredictable or at least hard to predict). These different regions are separated by a set which has Lebesgue measure zero, but still is uncountable and forms a Cantor set. These types of situations were studied by Grebogy et al. [5] as fractal basin boundaries.

In order to visualize this aspect we show in figure 6 the map which assigns to each point $x \in [0,1]$ the phase in which it converges to the periodic attractor in the following way. The horizontal axis represents the points of the unit interval [0, 1] for each of these points we calculated 2000 iterates of the map φ_S to arrive (practically) at one of the five points of the attractor (which of the five determines in which phase we approach the attractor). In order to get a clearer visual representation we represent the result by a vertical line, above the x-value in question on the horizontal axis, connecting the point of the attractor with the point with height .5 (the vertical axes, like the horizontal axis, represents the interval [0, 1]). To this we add the diagonal so that we can find the *domains of strict attraction*: with this we mean the connected intervals around each of the 5 points of the periodic attractor, consisting of the points which remain forever (under iteration of φ_S) in phase with the corresponding point of the periodic orbit. These domains of strict attraction can be seen in figure 6 as the plateaus intersecting the diagonal (because the number of iterations (2000) is a multiple of the period (5)). We see that this domain around .5 is rather big, but the others, especially for the highest and lowest value of x, are very small. This means that in these domains a small amount of noise can "break" the periodicity. So here we have a form of noise amplification which is due to nonlinearity.

5 Ambiguity of the dynamical class of a deterministic approximation

In this section we point out the difficulty *in principle* to decide the question whether a system (with only small) noise has an "underlying deterministic dynamics" which is chaotic or not. We shall discuss this in a context as simple as possible, but the implications also hold for more general systems.

We consider dynamical systems with state space \mathbb{R} or a closed interval in \mathbb{R} and with discrete time (like in the case of the logistic system). We suppose that the dynamics of the system is given in terms of a probability measure on the state space (defined by the density of the points of a typical evolution of the system) and a probability measure on the Cartesian product of the state space with itself (defined by the density of the pairs (x(n), x(n+1)) of successive states for a typical evolution of the system). These measures, which are defined and discussed in more detail in the next section, are denoted by M_1 and M_2 respectively. From the measure M_2 one can obtain the conditional probability measures M_x , for x in the support of M_1 : M_x describes the probability distribution for x(n+1), given that x(n) = x.

Giving a deterministic approximation of such a stochastic system means to replace (or to approximate) the conditional probability distributions M_x each by a single value $\varphi(x)$ which is the image of x under the function defining the deterministic approximation. There are various ways of approximating a probability distribution on \mathbb{R} by a single number: one can take the average (or expectation value) or one can take the median (the value such that the probability of being smaller than this value is .5). In the present context, where we are thinking in terms of nonlinear systems, and where one usually considers systems equivalent if they can be transformed into one another by a nonlinear change of coordinates (or conjugacy), the only good choice seems to be to use the medium value since that is independent of the linear structure in \mathbb{R} and only depends on the order structure. This choice of the medium value to construct a deterministic approximation is not very essential however: also if one uses expectation values the construction below remains valid (but the arguments need slight modifications).

For the formulation of our result we need one more definition. If we have a system with noise in the above sense, i.e. with a one dimensional state space and described in terms of the probability measures M_1 and M_2 , we define the square of the system as the system with the same state space, the same measure M_1 , but the measure M_2 replaced by the measure M_2^* defined by the density of the pairs (x(n), x(n+2)) for a typical time series of the original system. If the original system were deterministic and defined by the map φ , then the squared system would also be deterministic and would be defined by the map φ^2 — this is why we call this construction "squaring the system". In other words, squaring a system means that we consider two time steps of the old system as one time step of the new system.

Example There is a deterministic system such that, with arbitrarily small perturbations one obtains systems (with arbitrarily small noise) such that the deterministic approximation is not chaotic while the deterministic approximation of the square is chaotic. This deterministic system is defined by a map which has a saddle node whose (locally) unstable set returns, under iterated plication of the map, back to the (local) domain of attraction of the saddle node (with criticality in the sense of [6], see below).

This is the sense in which the question whether a system with small noise is chaotic or not is meaningless (at least in some cases): the answer should not change when squaring the system.

Remark: Before starting the actual construction, we observe that for hyperbolic systems, e.g. see [4], one does not expect such examples. This is due to the fact that such systems are structurally stable, though structural stability only holds for C^1 -small perturbations while we may have here even C^0 -small perturbations.

Construction For the construction of this example we need a one parameter family ψ_{ν} of maps of the interval such that for $\nu < 0$ almost all points of the interval are attracted, when iterating ψ_{ν} , to an attracting orbit of period k, while for $\nu > 0$ there is no orbit of period k; moreover we assume that for $\nu = 0$ the period k orbit undergoes a saddle node bifurcation and that the (locally) unstable set of the saddle node orbit returns, under repeated iteration of ψ_{ν} to the local basin of attraction of the saddle node with *criticality* (with this we mean that the iterate of ψ_{ν} which maps the local unstable set of the saddle node back to its local domain of attraction has critical points which we assume to be non-degenerate). Due to this last property, ψ_{ν} has chaotic dynamics for arbitrarily small positive values of ν , e.g. see [6] for the saddle node cycle with criticality.

Examples of such one parameter families can be obtained from the Logistic family in the form $\psi_{\nu} = \varphi_{\mu(\nu)}$ for some reparameterization $\mu(\nu)$: if we consider e.g. the μ -interval on which φ_{μ} has a periodic attractor with period 5, then, when μ moves out of the interval to the left (i.e. towards lower values) then the period 5 orbits disappear through a saddle node bifurcation, which has all the required properties.

From this one-parameter family of mappings we obtain a two-parameter family of systems with noise: for an evolution of such a perturbed system, denoted by $\Psi_{\varepsilon,\nu}$, given x(n), the corresponding probability distribution for x(n+1) is a uniform distribution on the interval with endpoints $\psi_{\nu}(x(n)) \pm \varepsilon$ (in fact the construction is slightly more complicated: the distribution is uniform on such an interval, but with respect to a new coordinate which is adapted to the saddle node bifurcation in a way which we describe below). All these systems can be obtained from ψ_0 by small perturbations (if ε and ν are close to 0). It is clear that the deterministic approximation, as discussed above, of the system $\Psi_{\varepsilon,\nu}$ is again given by the map ψ_{ν} (note that the notion of deterministic approximation is invariant under changes of coordinates). Next we square the system $\Psi_{\varepsilon,\nu}$ and denote the map, defining its deterministic approximation, by $\psi_{\varepsilon,\nu}^{\star}$. It is not hard to see that, for $\varepsilon \to 0$, $\psi_{\varepsilon,\nu}^{\star}$ converges (with derivatives) to ψ_{ν}^{2} . This implies that, for ε sufficiently small, also $\psi_{\varepsilon,\nu}^{\star}$ has a generically unfolding saddle node bifurcation, and has, for ν -values arbitrarily close to the value for which there is a saddle node bifurcation, chaotic dynamics. The important point, which we shall prove below, is that for positive ε , the map $\psi_{\varepsilon,0}^{\star}$ has no orbit of period k, in other words, the saddle node bifurcation occurs for negative ν -values. This implies that there are arbitrarily close to zero values $\varepsilon > 0$ and $\nu < 0$ such that the dynamics of $\psi_{\varepsilon,\nu}^{\star}$ is chaotic. This means that for these values we obtain the announced systems with non-chaotic deterministic approximation while the square has a deterministic approximation with chaotic dynamics. This is because the mean of the second iterate of a stochastic system need not be the same as the second iterate of the mean of the same stochastic system.

So the only thing left is the proof that $\psi_{\varepsilon,0}^*$ has no periodic point of period k near the period k periodic saddle node of Ψ_0 . We first consider the case that k = 1, where the saddle node bifurcation occurs at a fixed point, say at \bar{x} . Then, for ν near zero and x near \bar{x} we have $\psi_{\nu}(x) = x + a(x - \bar{x})^2 + b\nu$ plus terms of higher order, where a and b are non-zero and have the same sign. This means that for $\nu = 0$, all points near \bar{x} , except \bar{x} itself, move in the same direction. This implies that for $\psi_{\varepsilon,0}^*$ all points near \bar{x} , including \bar{x} itself, move in the same direction implying that we are already beyond the saddle node.

In the case k > 1 we denote the points of the bifurcating periodic orbit by $\{p_1, \dots, p_k\}$ so that $\psi_0(p_i) = p_{i+1}$, where the indices are taken modulo k. Then, near each of the points of the periodic orbit, we define the "positive direction" to be the direction in which the points move under ψ_{ν}^{k} for small $\nu > 0$. Then we construct smooth maps A_i from neighbourhoods of p_i to neighbourhoods of p_{i+1} in such a way that $A_i(p_i) = p_{i+1}$, such that in p_i the derivative of ψ_0 is equal to the derivative of A_i (note that this implies that A_i maps positive directions to positive directions), such that $A_k \circ A_{k-1} \circ \cdots \circ A_1$ is the identity on a neighbourhood of p_1 , and such that for all points x near p_i , but different from p_i , $\psi_0(x)$ can be obtained from $A_i(x)$ by shifting it in the positive direction (for this last requirement it is enough to adjust the second order derivatives of the maps A_i in the points p_i). Once we have these maps A_i we choose a new coordinate such that, with respect to this new coordinate, the maps A_i are, on small neighbourhoods of p_i , affine (this can be done by taking a C^1 small perturbation of the standard coordinate on \mathbb{R}). If we use this new coordinate to define the systems with noise, then the arguments, used above for the case k = 1remain valid.

6 General formulation for higher dimensional systems

In this section we discuss how to formalize the different concepts which came up in connection with the numerical experiments discussed before. We want these considerations also to be applicable to systems of dimension bigger than one. Even for higher dimensional systems, the dynamic behaviour can often be described in terms of time series $\{x(n)\}_{n\in\mathbb{N}}$ with x(n) in \mathbb{R} . One can think of a deterministic system defined by a rule

$$x(n) = f(x(n-1), \cdots, f(n-k)),$$

or one may think of a dynamical system with state space P, evolution map $\varphi: P \to P$ (i.e. if the state at time n is $p \in P$, then the state at time n + 1 is $\varphi(p)$) and read out function Y (i.e. if the state at time n is p, then the corresponding value of the time series is x(n) = Y(p)). By the reconstruction theorem, see [10] and [8], both these interpretations of time series from deterministic dynamical systems are essentially the same. We disregard here the possibility that different initial states (in the above interpretations the first k values of the time series, respectively, the first value $p \in P$ of the evolution in P) can lead to completely different time series due to the fact that they are in the domains of attraction of different attractors.

7 Reconstruction measures and predictability

The following considerations concerning time series are independent of the question whether they are generated by deterministic or stochastic dynamical systems. Our main concern is to give a correct description of the two aspects of mathematical models as mentioned in the introduction. They were good for either predicting one time step ahead, or good for predicting the long term statistical behaviour. For similar considerations see [11].

First we define the notion of *stationarity*. We call a time series stationary if for each continuous function $g: \mathbb{R}^k \to \mathbb{R}$ the average

$$\mathcal{E}(g) = \lim_{N \to \infty} N^{-1} \sum_{i=1}^{N} g(x(i), \cdots, x(n+k))$$

is well defined and finite (for all k). We note that this definition is somewhat different from the usual definition in the theory of stochastic processes. The present definition has the advantage that it can be applied to one single time series instead of an "ensemble". What follows below, however, also makes sense with the usual definitions.

The above averages define a Borel probability measure μ_k on \mathbb{R}^k , for each k, such that for each g as above, $\mathcal{E}(g) = \int g d\mu_k$ — these measures have bounded support. The existence of these measures follows from the theorem of Riesz. The heuristic meaning of these measures is the following: if a region in \mathbb{R}^k has a heigh density for the measure μ_k then it often happens that one meets in the time series a segment of k successive values which define a vector which belonging to that region. So the measures μ_k describe the asymptotic properties of the time series in the sense that they describe the statistics of the occurrence of finite segments. Since vectors, having as components k successive values of a time series, are called k-dimensional reconstruction vectors, we call μ_k the k-dimensional reconstruction measure.

From the k+1-dimensional reconstruction measure, one obtains the order k prediction measures P_{x_1,\dots,x_k} for (x_1,\dots,x_k) in the support of μ_k : P_{x_1,\dots,x_k} is the probability distribution, according to μ_{k+1} , of the last component of the vector $x(n-k),\dots,x(n)$, given that the first k components are $x(n-k) = x_1,\dots,x(n-1) = x_k$. So the order k prediction measures describe the optimal predictions based on the previous k elements in the time series.

So the two aspects discussed in this paper: prediction of the next state and the asymptotic statistical properties correspond to the prediction measures respectively the reconstruction measures. As we have seen, the order k-prediction measures can be obtained from the k + 1-dimensional reconstruction measures. Also the k + 1-dimensional reconstruction measure can be obtained from the order k prediction measures: one just constructs a time series $\{y(n)\}$ such that $y(1), \dots, y(k)$ are in the support of μ_k and then one continues with values y(k + 1), y(k + 2) etc. which are obtain as random choices of the relevant prediction measures. Then, with probability 1, one obtains a time series having the same reconstruction measures of dimension up to dimension k + 1.

The findings in this paper indicate that the reconstruction measures may depend sensitively on the corresponding prediction measures.

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Remarks on the linear regression approach to dimension estimation

Gerhard Keller and Ralph Sporer

Abstract

We discuss some statistical theory of the simultaneous estimation of correlation integrals from dynamical data with varying radii and embedding dimensions. Thereby we focus on the estimation of the covariance matrix of these estimators taking into account the finite sample size and the correlation time effects observed by Theiler [23]. As applications we discuss linear model statistics like linear regression estimates of correlation dimension and entropy and the detection of noise.

1 Introduction

Let X_1, X_2, X_3, \ldots be a real-valued stationary time series that is mixing in a sense to be made precise later. Typical examples would be a) independent identically distributed (i.i.d.) random observations, b) observation on a "chaotic" dynamical system, c) observations on a noisy system. In particular there may be some interesting dependence between consecutive observations that can be studied by looking at the distribution μ_{ℓ} of blocks

$$Y_i^{\ell} := (X_i, \ldots, X_{i+\ell-1}) \in \mathbb{R}^{\ell} .$$

The length ℓ of the blocks is called the *embedding dimension*, and for fixed ℓ the sequence $Y_1^{\ell}, Y_2^{\ell}, Y_3^{\ell}, \ldots$ is again stationary and mixing.

Some aspects of the geometry of the distribution μ_l can be described by means of the correlation integrals

$$C(r, \ell) := \int \int \mathbb{1}_{\{ \|y-y'\| < r\}} d\mu_\ell(y) \, d\mu_\ell(y')$$

where ||y - y'|| denotes the euclidean (or any other suitable) distance of y and y'. Grassberger and Procaccia [14] used the functional dependence of $\log C(r, \ell)$ on r and ℓ to describe quantitative features of *deterministic* chaotic systems. They observed that in many cases there are real numbers $\nu > 0$ and h > 0 such that

$$\log C(r,\ell) = \begin{cases} \nu \cdot \log r + o(\log r) & \text{as } r \to 0 \text{ when } \ell \text{ is large,} \\ -\ell \cdot h + o(\ell) & \text{as } \ell \to \infty \text{ when } r \text{ is small.} \end{cases}$$
(1)

 ν is called the *correlation dimension* and h is an entropy like quantity. Cutler [10] gives a rather comprehensive review of much of the underlying theory.

If, on the other hand, the X_i are i.i.d. observations and if ||y - y'|| denotes the maximum norm of y - y', then $C(r, \ell) = (C(r, 1))^{\ell}$ such that the following model assumption makes sense

$$\log C(r,\ell) = \ell \cdot \nu_1 \cdot (\log r + o(\log r)) \quad \text{as } r \to 0, \tag{2}$$

where ν_1 denotes the correlation dimension of the distribution μ_1 of the X_i , see [6]. The two model assumptions (1) and (2) differ drastically in the sense that (1) describes a finite entropy situation whereas (2) reflects the in general infinite entropy of true random observations.

The above considerations motivate the following decomposition of $\log C(r, \ell)$ into a linear part with constant term and a (hopefully small) nonlinear remainder $\delta(r, \ell)$:

$$\log C(r,\ell) = \nu \cdot \log r - h \cdot \ell + \nu_1 \cdot \ell \cdot \log r + C + \delta(r,\ell) .$$
(3)

This model, although appropriate if ||y - y'|| denotes the maximum norm, can be improved if the euclidean distance is used by replacing $\log r$ with $\log \frac{r}{\sqrt{t}}$, *i.e* by using dimension scaled distances, see [13].

In practice the unknown coefficients ν, h, ν_1, C must be estimated from a finite number of observations X_1, \ldots, X_N . Therefore (3) (or any other linear or nonlinear model describing $\log C(r, \ell)$) can be fitted only on finitely many parameter pairs $(r_1, \ell_1), \ldots, (r_p, \ell_p)$ the appropriate choice of which depends on the sample size and the nature of the observed data. In particular we make no attempt to calculate limits as $r \to 0$ or $\ell \to \infty$. Using the notation

$$(\underline{r},\underline{\ell}) = \begin{pmatrix} r_1 & \ell_1 \\ \vdots & \vdots \\ r_p & \ell_p \end{pmatrix}, \quad Z(\underline{r},\underline{\ell}) = \begin{pmatrix} \log C(r_1,\ell_1) \\ \vdots \\ \log C(r_p,\ell_p) \end{pmatrix}, \quad \delta = \begin{pmatrix} \delta(r_1,\ell_1) \\ \vdots \\ \delta(r_p,\ell_p) \end{pmatrix}$$

we write our model (3) as

$$Z(\underline{r},\underline{\ell}) = M\beta + \delta \tag{4}$$

where M is a matrix involving only the controlled parameters $\log \underline{r}$ and $\underline{\ell}$ and where $\beta = (\nu, h, \nu_1, C)^t$ is that coefficient vector that yields the best fit in (4) in the least squares sense, i.e.

$$\beta = B \cdot Z(\underline{r}, \underline{\ell})$$
 where $B = (MM^t)^{-1}M^t$

Our aim is to estimate this coefficient vector β from observed data.

Suppose now that $\hat{Z} = \hat{Z}(X_1, \ldots, X_N) \in \mathbb{R}^p$ is a "suitable" estimator for the *p*-vector $Z(\underline{r}, \underline{\ell})$ of logarithms of correlation integrals, suitable in the following sense:

$$Z = Z(\underline{r}, \underline{\ell}) + \epsilon = M\beta + \delta + \epsilon$$

where ϵ is approximately $\mathcal{N}(\underline{0}, V)$ -distributed (approximately in the sense of a central limit theorem), and there is a reliable (*i.e.* "consistent" in statistical terms) estimate $\hat{V} = \hat{V}(X_1, \ldots, X_N)$ of V. Then $\hat{\beta} = B\hat{Z}$ is the least squares estimator for β and $\hat{\epsilon} = \hat{Z} - M\hat{\beta} = (1 - MB)\hat{Z}$ are the corresponding residues. The distributions of $\hat{\beta}$ and $\hat{\epsilon}$ are known, namely $\hat{\beta} \sim \mathcal{N}(\beta, BVB^t)$ and $\hat{\epsilon} \sim \mathcal{N}(\delta, SVS^t)$ where S = 1 - MB. All this is well known, see *e.g.* [24]. Replacing V by the consistent estimate \hat{V} we can *e.g.* calculate confidence bounds for β , test the hypothesis " $\nu_1 = 0$ ", *i.e.* the absence of true randomness on the scale of radii r_1, \ldots, r_p , or discriminate between the systematic error δ of our linear model (3) and the statistical error ϵ . In section 3 we illustrate this by the results of some numerical simulations. Beforehand we turn to the problem of how to obtain good estimates \hat{Z} of $Z(\underline{r}, \underline{\ell})$ and \hat{V} of V. Remarks on the linear regression approach to dimension estimation

2 Covariance estimates

2.1 The covariance matrix of the correlation integrals

Recall that $C(r, l) = \int \int h(y, y') d\mu_l(y) d\mu_l(y')$ where $h(y, y') = \mathbb{1}_{\{||y-y'|| < r\}}$. Quantities represented by integrals in this way are usually estimated by a so called U-statistic

$$\frac{1}{N(N-1)} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} h(Y_i, Y_j) \; .$$

In the case of i.i.d. observations Y_i the U-statistic is an asymptotically normal unbiased minimal variance estimator of C(r, l), see [15]. These properties essentially persist if the observations are mixing with exponentially decaying correlations. The concept of mixing which is most useful in this context is that of *absolute regularity*, see [25] for a purely probabilistic treatment and [12] for its applicability to chaotic dynamical systems. Although strong mixing properties like this one are difficult to verify on a theoretically level in the case of non-uniformly hyperbolic systems, one can expect that many chaotic systems show the same central limit behaviour. In the last section of this note we discuss this aspect in some more detail.

For computational purposes we assume that the observations Y_i^{ℓ} are *t*-dependent, *i.e.* Y_i^{ℓ} and Y_j^{ℓ} are independent, if |i-j| > t. For a given data set *t* should be carefully chosen. In our Hénon example in the next section t = 10 seems to be a good choice. We modify the U-statistic estimator of C(r, l) accordingly:

$$U_N(r,l) = \frac{1}{\pi(N,t)} \sum_{i=1}^{N} \sum_{\substack{j=1\\|j-i|>2t}}^{N} h(Y_i^{\ell}, Y_j^{\ell}) .$$
(5)

Here $\pi(N,t) = (N-2t)(N-2t-1)$ is the number of pairs in the sum. The minimal index distance 2t (instead of t) will help to avoid some dependencies when we calculate the variance of $U_N(r,l)$. As we are going to estimate $C(r_1,\ell_1),\ldots,C(r_p,\ell_p)$ simultaneously, we have indeed to calculate the covariance matrix of the \mathbb{R}^p -valued estimator

$$U_N(\underline{r},\underline{\ell}) = \begin{pmatrix} U_N(r_1,\ell_1) \\ \vdots \\ U_N(r_p,\ell_p) \end{pmatrix} .$$

A tedious, though elementary calculation yields the following expression for the covariance matrix K of $U_N(\underline{r}, \underline{\ell})$:

$$K = 4 \cdot \left(N^{-1}P + N^{-2} \left(\frac{1}{2}Q - R - (1+2t)P \right) + O(N^{-3}) \right)$$
(6)

where P, Q and R are $p \times p$ -matrices, that can be described as follows: For u = 1, ..., p let

$$h^{(u)}(y,y') = 1_{\{\|y-y'\| < r_u\}}$$

$$h_0^{(u)} = \int \int h^{(u)}(y, y') d\mu_{\ell_u}(y) d\mu_{\ell_u}(y') \ (= C(r_u, \ell_u))$$

$$h_1^{(u)}(y) = \int h^{(u)}(y, y') d\mu_{\ell_u}(y')$$

$$h_2^{(u)}(y, y') = h^{(u)}(y, y') - h_1^{(u)}(y) - h_1^{(u)}(y') + h_0^{(u)}.$$

Then for $u, v = 1, \ldots, p$

Remarks:

- (i) In the case of a single radius and embedding dimension the formula for K reduces to that of Theiler [23] if t = 0, *i.e.* if the Y_i are independent, namely K = 4(N⁻¹P + N⁻²(¹/₂Q P)).¹
- (ii) As we assume Y_i and Y_{i+k} to be independent for |k| > t, we have the following relation between $P_{u,u}$ and Theiler's correlation time τ : $P_{u,u} = \tau \cdot E\left[(h_1^{(u)}(Y_i^{\ell_u}))^2\right]$
- (iii) Asymptotically (as $N \to \infty$) the N^{-1} -term in the decomposition of K dominates. However, for small radii r_u , $P_{u,u}$ tends to be much smaller than $Q_{u,u}$ such that the N^{-2} -term may be comparable in size to the N^{-1} -term even for N = 10000. In the case of independent observations the statistic $U_N(r_u, \ell_u) h_0^{(u)}$ can be decomposed into a sum of two random variables in analogy to the decomposition of its variance into an N^{-1} and N^{-2} -term. The first part is asymptotically normal, the second one is a weighted sum of squares of normal random variables, see [11, Example 2.2.7]. Therefore, if the N^{-2} -term is not neglectable, $U_N(r_u, \ell_u) h_0^{(u)}$ is not close to an exact normal but to a slightly skewed normal distribution. It seems impossible, however, to estimate the size of this effect from the data.

As $U_N(\underline{r},\underline{\ell}) - C(\underline{r},\underline{\ell})$ is approximately $\mathcal{N}(0,K)$ -distributed, standard results from probability theory guarantee that $\log U_N(\underline{r},\underline{\ell}) - \log C(\underline{r},\underline{\ell})$ is approximately $\mathcal{N}(0,V)$ distributed where $V_{u,v} = K_{u,v}/(C(r_u,\ell_u)C(r_v,\ell_v))$, $u,v = 1,\ldots,p$. Higher order correction terms which occur also in this approximation are small compared to the leading term and can be neglected.

¹Theiler gives $(\frac{1}{2}Q + \frac{1}{2}P)$ instead of $(\frac{1}{2}Q - P)$, but as P occurs also at the order of N^{-1} , this is practically meaningless.

Remarks on the linear regression approach to dimension estimation

2.2 An estimator for the covariance matrix

An unbiased and consistent estimator for $P_{u,v}$ is

$$\sum_{k=-t}^{t} \frac{1}{N-k} \sum_{i=1}^{N-k} \left(h_1^{(u)}(Y_i^{\ell_u}) \cdot h_1^{(v)}(Y_{i+k}^{\ell_v}) - h_0^{(u)} \cdot h_0^{(v)} \right) \ .$$

As the $h_0^{(u)}$ and $h_1^{(u)}(Y_i^{\ell_u}) = \int h^{(u)}(Y_i^{\ell_u}, y') d\mu_{\ell_u}(y')$ are not explicitly known (they are defined in terms of the unknown distribution μ_{ℓ_u}), we replace them through estimators

$$H_0^{(u)} := U_N(r_u, \ell_u) \quad \text{and} \quad H_{1,i}^{(u)} := \frac{1}{N - 2t - 1} \sum_{\substack{j=1\\|j-i| > t}}^N h^{(u)}(Y_i^{\ell_u}, Y_j^{\ell_u}) \tag{7}$$

and denote

$$\hat{P}_{u,v} := \sum_{k=-t}^{t} \frac{1}{N-k} \sum_{i=\max\{1,1-k\}}^{\min\{N,N-k\}} \left(H_{1,i}^{(u)} \cdot H_{1,i+k}^{(v)} - H_{0}^{(u)} \cdot H_{0}^{(v)} \right) .$$
(8)

Another tedious but elementary calculation shows that

$$E[4N^{-1}\hat{P}] = 4 \cdot \left(N^{-1}P + N^{-2}(Q - R - 5(1 + 2t)P) + O(N^{-3})\right)$$

= $K + 2N^{-2}Q - 16(1 + 2t)N^{-2}P + O(N^{-3})$,

i.e. $4N^{-1}\hat{P}$ is not an unbiased estimator for P. As a matter of fact, the correction term can be both, negative or positive, depending on the particular situation. An unbiased estimator for Q is easily found:

$$\hat{Q}_{u,v} := \frac{1}{\bar{\pi}(N,t)} \sum_{\substack{i,j=1\\|j-i|>3t}}^{N} \sum_{p,q=-t}^{t} \left(h^{(u)}(Y_i^{\ell_u}, Y_j^{\ell_u}) \cdot h^{(v)}(Y_{i+p}^{\ell_v}, Y_{j+q}^{\ell_v}) - H_0^{(u)} \cdot H_0^{(v)} \right)$$
(9)

where $\tilde{\pi}(N,t) = (N-3t)(N-3t-1)$. The importance of the "p = q"-terms in $\hat{Q}_{u,v}$ for deterministic data is obvious: If $Y_j^{\ell_u}$ is close to $Y_i^{\ell_u}$ (because the system returned close to a previously attained state), also $Y_{j+p}^{\ell_v}$ and $Y_{i+p}^{\ell_v}$ are likely to be close to each other for small p. The " $p \neq q$ "-terms contribute to $\hat{Q}_{u,v}$ if the system spends some time near a fix point or a periodic orbit of small period.

To summarize: $\hat{K} := 4N^{-1}(1 + 4(1 + 2t)N^{-1})\hat{P} - 2N^{-2}\hat{Q}$ is an estimator for the covariance matrix K of $U_N(\underline{r}, \underline{\ell})$ which is unbiased up to terms of order $O(N^{-3})$. It is defined by (8) and (9).

As the computation of \hat{Q} involves about $p^2(2t+1)^2N^2$ terms, we determine only the diagonal terms $\hat{Q}_{u,u}$ and use the following modified estimator \hat{K}' for K: Decompose $4N^{-1}\hat{P} = D^{1/2}CD^{1/2}$ where D is the diagonal matrix made up from the diagonal

elements of $4N^{-1}\hat{P}$. Thus *C* is the correlation matrix corresponding to $4N^{-1}\hat{P}$. We modify *D* by subtracting the diagonal elements of $2N^{-2}\hat{Q}$: $D'_{u,u} := D_{u,u} - 2N^{-2}\hat{Q}_{u,u}$, and obtain the estimator $\hat{K}' := D'^{1/2}CD'^{1/2}$ for *K*. The diagonal of \hat{K}' coincides with that of \hat{K} whereas its correlation structure is that of the leading term $4N^{-1}\hat{P}$ of \hat{K} . This leads us finally to the following estimator \hat{V} for the covariance matrix of $\log C(\underline{r}, \underline{\ell})$:

$$\hat{V}_{u,v} := \frac{\hat{K}'_{u,v}}{U_N(r_u,\ell_u) U_N(r_v,\ell_v)}$$

3 Simulations

We tested the reliability of the statistical procedures described in the previous sections on Hénon time series. More exactly: X_1, \ldots, X_N are the *x*-coordinates of N consecutive iterates of a Hénon system with parameters a = 1.4 and b = 0.3. (In some cases noise was added, see below.) We always used a set of radii r_0, \ldots, r_{20} ranging from $r_0 = 0.01$ to $r_{20} = 0.41$. Instead of working with the maximum-norm distance we used dimension scaled euclidean distances, see [13]. Based on the observed decay of correlations for the random variables $H_{1,i}^{(u)}$ from (7) we assumed that X_i and X_j are independent if |i - j| > t = 10.

(i) Fixed embedding dimension $\ell = 4$; no noise; N = 1000 and N = 10000:

We performed 100 independent runs recording for the *j*-th run the estimated logarithms of the correlation integrals $Z_j(r_i) = \log C_j(r_i)$ and their estimated standard deviations $\sigma_j(r_i)$. The averages of these quantities over all runs are denoted $\overline{Z}(r_i)$ and $\overline{\sigma}(r_i)$, respectively. The sample standard deviation of the $Z_j(r_i)$ is denoted by S_i . The comparison of $\overline{\sigma}(r_i)$ and S_i in Figure 1, where we give both, the values of $\overline{\sigma}_i$ we obtained using the uncorrected variance estimator $\hat{P}_{u,u}$ and those using the corrected estimator $\hat{Q}_{u,u}$, shows that, at least for small radii the corrected estimates for the standard deviation are on the average closer to the sample standard deviation than the uncorrected values. As to be expected, this effect is much stronger for N = 1000 than for N = 10000. We remark that for N = 1000 there were 4 runs where the corrected estimator for $\sigma_j^2(r_i)$ took negative values for some radii. As this estimator is the difference of two values, it is not surprising that this happened a few times. For our further calculations we set these values to 0.

From the same data we calculated 100 estimates ν_j for the correlation dimension and their estimated standard deviations σ_j and denoted their 95%-confidence intervals by $J_j = [\nu_j - 1.96 \sigma_j, \nu_j + 1.96 \sigma_j]$. As the true value of ν is not known we could not simply count the number of runs where the true value is inside the confidence interval. Instead we counted the number of runs where $\bar{\nu} = \frac{1}{100} \sum_{j=1}^{100} \nu_j$ is in this interval². As long as the distribution of the σ_j^2 is close

²The average correlation dimension was $\bar{\nu} = 1.19330 \pm 0.00111$ for $r_0 - r_{10}$ and $\bar{\nu} = 1.20881 \pm 0.00078$ for $r_{10} - r_{20}$

to normal one can approximately calculate the expected number of successes. The observed success probabilities with the expected ones in brackets are:

	N = 1000		N = 10000	
	$r_0 - r_{10}$	r10-r20	$r_0 - r_{10}$	r10-r20
uncorrected	0.99 (0.934)	0.95 (0.930)	0.98 (0.945)	0.98 (0.945)
corrected	0.93		0.96 (0.941)	0.96 (0.945)

(The corrected σ_j^2 for N = 1000 were so non-normal that no useful expected value of the success probabilities could be calculated.) So, except for large radii and small numbers of observations, the uncorrected values seem to give too pessimistic confidence intervals whereas the corrected ones work very well for N = 10000 but tend to give slightly too small confidence intervals for N = 1000. Compared to other approaches that provide confidence intervals for correlation integrals or the correlation dimension (e.g. [21, 17]) we neither need parametric assumptions on the dynamical system producing the data nor very large sample sizes in order to produce reasonable estimates.

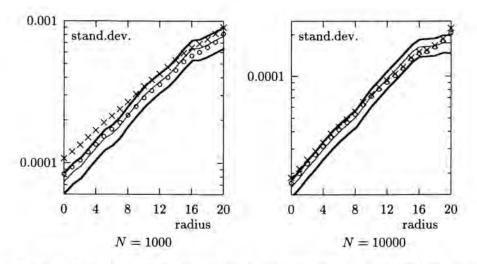


Figure 1: Comparison of the average estimated standard deviation $\bar{\sigma}(r_i)$ to the sample standard deviation S_i for time series of length 1000 and 10000. Logarithmic plot. Lines: S_i with 95%-confidence intervals. Crosses: uncorrected variance estimator. Circles: corrected variance estimator.

(ii) Simultaneous estimation of ν, h, and ν₁; l = 4,...,7; N = 10000: We performed single runs on estimating ν, h, and ν₁ from the linear model
(3) using the radii r₀ = 0.01,...,r₁₀ = 0.064. In all cases we calculated 95%-confidence intervals: (a) No noise: As ν₁ was not significantly different from 0 (interpretation: no noise!) we excluded the variable ν₁ from the model and estimated ν and h again:

	ν	h	ν_1
			[-0.013, 0.025]
ν_1 excluded	[1.077, 1.188]	[0.277, 0.313]	

(b) 1% noise in the system: As ν was not significantly different from 0 we excluded the variable ν from the model and estimated h and ν_1 again:

	ν	h	ν_1
ν included	[-0.050, 0.441]	[2.471, 2.992]	[0.445, 0.560]
ν excluded	-	[2.789, 2.963]	[0.520, 0.553]

(c) 1% measurement noise: As ν was not significantly different from 0 we excluded the variable ν from the model and estimated h and ν_1 again:

	ν	h	ν_1
ν included	[-0.216, 0.224]	[2.717, 3.167]	[0.531, 0.631]
ν excluded	-	[2.868, 3.022]	[0.567, 0.596]

 (iii) Discrimination between systematic and statistical errors; fixed embedding dimension ℓ = 4; r₀,...,r₁₀; N = 10000;

Recall from the introduction that the residues $\hat{\epsilon} = \hat{Z} - M\hat{\beta}$ are normally distributed with mean δ (= the systematic error) and a degenerate covariance matrix SVS^t (representing the statistical error) that can be estimated from the data. In particular, the euclidean length of the difference vector $\hat{\epsilon} - \delta$ has a distribution that can approximately be determined by simulations with normal random numbers. This distribution can be compared to the actually observed length $|\hat{\epsilon}|$ of $\hat{\epsilon}$. In our numerical example we found $|\hat{\epsilon}| = 0.0533$. At the same time a 95%-confidence interval for $|\hat{\epsilon} - \delta|$ was [0, 0.0129]. Indeed, the largest among 500 simulated values of $|\hat{\epsilon} - \delta|$ was 0.0210. So more than 2/3 of the length of the observed residue vector is due to the nonlinearity of the function $\log r \mapsto \log C(r)$ and only a smaller part of it can be explained by statistical fluctuations.

4 Remarks on mixing in chaotic systems

In [12, 9, 22] the following framework for statistics on data from dynamical system was considered: Let $T: M \to M$ describe a time-discrete, deterministic dynamical system on a metric space (M, d). Suppose there is an ergodic, *T*-invariant Borel probability measure *P* on *M*, and fix a finite partition $\mathcal{Z} = (Z_1, \ldots, Z_\ell)$ of *M*. Then

$$\begin{array}{lll} X_n(\omega) &:= & T^n(\omega) & \text{and} \\ \xi_n(\omega) &:= & j & \text{if} & X_n(\omega) \in Z_j & (\omega \in M) \end{array}$$

define ergodic stationary processes on the probability space (M, P). Here the index n ranges over $I = \mathbb{Z}$ if T is invertible and over $I = \mathbb{N}$ otherwise.

Sometimes it is possible to recover the process $(X_n)_{n \in I}$ from the label process $(\xi_n)_{n \in I}$ via a functional $\Phi : \{1, \ldots, \ell\}^I \to M$ for which there are real constants C > 0 and $\alpha \in (0, 1)$ such that for *P*-a.e. ω

$$d\left(\Phi((k_i)_{i\in I}) - X_n(\omega)\right) \le C \cdot \alpha^m,\tag{10}$$

whenever $k_i = \xi_{n+i}(\omega)$ for all $i \in I$ with $|i| \leq m$. In particular, $\Phi((\xi_{n+i}(\omega))_{i \in I}) = X_n(\omega)$.

In such a situation good mixing properties of the process $(\xi_n)_{n \in I}$ guarantee the asymptotic normality of $U_N(\underline{r}, \underline{\ell})$. In particular it suffices that the process $(\xi_n)_{n \in I}$ is absolutely regular with mixing coefficients β_n decreasing at a rate of $n^{-(2+\delta)}$ or faster. In the language of ergodic theory this means that \mathcal{Z} is a weak Bernoulli partition for (T, P) with mixing rate β_n .

The asymptotic normality of the \mathbb{R}^p -valued process $U_N(\underline{r}, \underline{\ell})$ and the structure and estimability of its limiting covariance matrix are discussed in [12, 9]. Indeed, besides the absolute regularity and property (10) a mild regularity assumption on the measure P is needed, see [12, Theorem 1]. For our particular U-statistic $U_N(\underline{r}, \underline{\ell})$ it is not hard to show that condition (3.6) of [12] is satisfied if the functions $r \mapsto C(r, \ell)$ are Hölder continuous, a very reasonable assumption in the context of dimension estimation.

Absolute regularity (with even exponentially decreasing β_n) and property (10) are known since long for many uniformly hyperbolic or uniformly expanding systems such as mixing torus automorphisms, Axiom-A-diffeomorphisms [5], piecewise expanding interval maps [16] and others. For non-uniformly hyperbolic dynamical systems the situation is much more complicated, but results for two prototype systems indicate that also for such systems the statistical approach to dimension estimation via Ustatistics is justified: For Collet-Eckmann maps (i.e. quadratic interval maps where the critical point has a positive Lyapunov exponent) it was essentially proved in [8] that there exists an absolutely continuous f-invariant probability measure μ on [0, 1]. Without essential loss of generality one may assume that (f, μ) is mixing, cf. [4]. The exponential weak Bernoulli property of the partition $([0, \frac{1}{2}], (\frac{1}{2}, 1])$ for the system (f, μ) is proved in [9] (building on results from [19]), and the approximation property (10) is an immediate consequence of [20]. In view of the work of Benedicks and Carleson [1] one might hope that the Collet-Eckmann property is in a sense typical for unimodal maps which have no stable attractor. In the case of the Hénon family there is not yet a complete theoretical justification for the statistical approach, but the relevant results obtained during the last years are nevertheless impressive: For a set of parameters of positive Lebesgue measure in the Hénon family Benedicks and Young [3] proved (building on results from [2]) the existence of a SBR-measure (that is a physically observable invariant measure), and more recently they proved exponential decay of correlations and a Central Limit Theorem for Hölder continuous observables of these systems ³. Finally we mention the work of Chernov [7] who offers a kind of tool-box to investigate mixing properties of a broad class of dynamical systems.

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On delay co-ordinates in stochastic dynamical systems

Bing Cheng and Howell Tong

Abstract

We study the asymptotic distribution of the cross-validatory estimate of the delay co-ordinates in a stochastic dynamical system. By studying the tail probabilities of under-fitting and over-fitting, we obtain an estimate of the sample size requirement under realistic conditions.

1 Introduction

For the analysis of deterministic dynamical systems, the delay co-ordinates approach due to Takens (1981) is now firmly established and is one of the most frequently employed techniques in the dynamical systems literature. Although the actual mechanics of delay co-ordinates construction was pre-dated by the statistical literature (notably Yule, 1927), it is only through the celebrated embedding theorem of Takens that we understand the full impact of such a construction.

Nowadays, delay co-ordinates are so widely used in the dynamical systems literature that they are often applied even when the system noise (also called the intrinsic noise or the dynamic noise) is present. Strictly speaking, this situation is beyond the scope of Takens' theorem. The primary motivation of Takens' delay co-ordinates construction is the recruitment of a finite and minimally sufficient set of past observations with which we analyse the dynamical system (e.g. the attractors) and Takens' embedding theorem assures us of the existence of such sets which preserve all the essential features of the deterministic dynamical system under generic conditions. The recruitment process can also be likened to an information condensation process: the recruitment of redundant past observations provides no additional information. It is pertinent to discuss the purpose and the methodology of a similar delay co-ordinates construction within the wider context of stochastic dynamical systems, in which system noise (or noise for short) is present.

2 Delay Co-ordinates

Let $\{X_t\}$ be a discrete-time stationary time series with $EX_t^2 < \infty$. The conditional expectation of X_t given $(X_{t-1}, ..., X_{t-d})$ will be denoted by $E[X_t|X_{t-1}, ..., X_{t-d}]$. Define the prediction error variance by

$$\sigma^2(d) = E[X_t - E[X_t | X_{t-1}, ..., X_{t-d}]]^2, \quad d \ge 1.$$
(1)

Define the generalized partial autocorrelation function (PACF) by

$$\phi(d) = \{1 - \sigma^2 (d+1) / \sigma^2 (d)\}^{1/2}.$$
(2)

Definition 2.1 $\{X_t\}$ is said to be generated by a stochastic dynamical system with d_0 delay co-ordinates, in short $SDS(d_0)$, if \exists a non-negative integer $d_0 < \infty$ such that $\phi(d_0 - 1) \neq 0$ and $\phi(d) = 0$ for all $d \geq d_0$. If no such finite d_0 exists, then $\{X_t\}$ is said to be generated by a stochastic dynamical system with infinite number of delay co-ordinates, or $SDS(\infty)$.

The underlying idea is the recruitment of past observations for the purpose of one-step-ahead prediction by the least-square method. The function $\phi^2(d)$ measures the percentage reduction in the prediction error variance in adding X_{t-d-1} to the recruitment set consisting of $X_{t-1}, ..., X_{t-d}$. Clearly, an $SDS(d_0)$ may be modelled as

$$X_t = F_{d_0}(X_{t-1}, ..., X_{t-d_0}) + \epsilon_t,$$
(3)

where

$$E[\epsilon_t | X_{t-1}, ..., X_{t-d_0}] = 0.$$
(4)

A more general idea is to identify d_0 as the minimum integer such that the vector time series $\{X_t^{(d_0)}\}$ is a Markov chain on \mathbb{R}^{d_0} . Here, $X_t^{(d_0)} = (X_{t-1}, ..., X_{t-d_0})^T$. We shall pursue this more general idea elsewhere.

Example 2.1 Consider the stochastic logistic map

$$X_t = A_t X_{t-1} (1 - X_{t-1}) + \eta_t g(X_{t-1}), \ X_0 \in (0, 1),$$

where $\{\eta_t\}$ is a sequence of independent and identically distributed random variables, each with zero mean, finite variance and finite support, g(.) is any suitable function which ensures that $X_t \in (0, 1), \forall t \ge 1$, and η_t is independent of $X_s, s < t$. Moreover, A_t is a random variable with mean $\alpha, (0 \le \alpha \le 4)$, finite variance and compact support and is independent of $X_s, s < t$. Clearly,

$$\phi(d) = 0, \quad (d \ge 1). \tag{5}$$

Therefore, we have an SDS(1). Note that we have incorporated a non-additive system noise process as well as parameter uncertainty in the above map. Further, we note that $(F_1(x_1), x_1)^T$ traces a parabola in \mathbb{R}^2 , whilst $(F_d(x_d, ..., x_1), x_d, ..., x_1)^T$ traces a parabolic cylinder in \mathbb{R}^{d+1} for each $d \geq 2$. It is clear that the cylindrical structure will prevail even if we consider general maps (of possibly higher dimensions and with more exotic "shape".) \Box

The fact that redundancy is characterized by a cylindrical structure suggests that cylinder hunters will reap great rewards in the face of noisy data.

3 Distance Function

Recall that $X_t^{(d)} = (X_{t-1}, ..., X_{t-d})$ and that $E[X_t|X_t^{(d)}]$ is denoted by $F_d(X_t^{(d)})$. Let $\mathcal{L}_2(\mathbb{R}^d)$ denote the set of all square-integrable measurable functions on \mathbb{R}^d . Obviously, $\mathcal{L}_2(\mathbb{R}^1) \subset \mathcal{L}_2(\mathbb{R}^2) \subset ... \subset \mathcal{L}_2(\mathbb{R}^d) \subset ...$

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Denote

$$\mathcal{L}_{2}(X_{t}^{(d)}) = \{F(X_{t}^{(d)}) | F \in \mathcal{L}_{2}(\mathbb{R}^{d})\}.$$
(6)

Then

$$\mathcal{L}_2(X_t^{(1)}) \subset \mathcal{L}_2(X_t^{(2)}) \subset \dots \subset \mathcal{L}_2(X_t^{(d)}) \subset \dots$$

$$\tag{7}$$

and $F_d(X_t^{(d)})$ is the orthogonal projection of X_t in $\mathcal{L}_2(X_t^{(d)})$. For integers $0 < d_1 \leq d_2$, we have

$$F_{d_1}(X_t^{(d_1)}) \in \mathcal{L}_2(X_t^{(d)}) \subset \mathcal{L}_2(X_t^{(d_2)})$$

and

$$F_{d_2}(X_t^{(d_2)}) \in \mathcal{L}_2(X_t^{(d_2)}).$$

Our objective is to define a suitable distance function on $N \times N$ which enables us to determine d_0 . Clearly, the Euclidean distance is not appropriate for many "discrete" problems such as ours. For example, Akaike (1974) has used instead the Kullback-Leibler information to construct a suitable distance function for linear autoregressive order determination. For our purpose, it turns out that a feasible non-Euclidean distance emerges if we consider the Euclidean distance between two cylinder sets of dimensions say d_1 and d_2 ($d_1 \leq d_2$) in the space of square-integrable functions on \mathbb{R}^{d_2} . This motivates the following definition of the function $\Delta(.,.)$ on $N \times N$, which will serve as our choice of a non-Euclidean (squared) distance on $N \times N$.

$$\Delta(d_1, d_2) = E[F_{d_1}(X_t^{(d_1)}) - F_{d_2}(X_t^{(d_2)})]^2, \tag{8}$$

where the expectation is taken with respect to the distribution of $X_t^{(d_2)}$. Note that F_d is uniquely determined once d is defined. Thus, $\Delta(.,.)$ is well defined.

Definition 3.1 The time series $\{X_t\}$ is an $SDS(d_0)$, $(d_0 \ge 1)$, if and only if

- (i) $\Delta(d, d_0) \neq 0$ for all $d < d_0$, and
- (ii) $\Delta(d, d_0) = 0$ for all $d \ge d_0$.

Proposition 3.1

- (i) $\Delta^{1/2}$ is a properly defined distance function on $\mathbb{N} \times \mathbb{N}$, i.e. $\Delta^{1/2}(d_1, d_2) = \Delta^{1/2}(d_2, d_1), \ \Delta^{1/2}(d, d) = 0, \ \Delta^{1/2}(d_1, d_3) \leq \Delta^{1/2}(d_1, d_2) + \Delta^{1/2}(d_2, d_3).$
- (ii) If for each $d \ge 1$, F_d has bounded first partial derivatives on \mathbb{R}^d , then $\Delta(d_2, d_1) \le c|d_2 d_1|$, where c is a constant.
- (iii) For $d_1 \leq d_2 \leq d_3$, $\Delta(d_2, d_3) \leq \Delta(d_1, d_3)$. That is for fixed d_3 , $\Delta(d, d_3)$ is a decreasing function in d.

- (iv) For any $d_1 \leq d_2$, we have $\Delta(d_1, d_2) = \sigma^2(d_1) \sigma^2(d_2)$.
- (v) $\sum_{d=1}^{\infty} \Delta(d, d+1) < \infty$.
- (vi) There are infinitely many d for which $\Delta(d, d+1) \leq \kappa/d$, where κ is a constant.
- (vii) $\forall d \leq D < \infty, \exists \kappa_D, 0 < \kappa_D < \infty$, such that $\Delta(d, d+1) \leq \kappa_D/d$.

The proofs are given in Cheng and Tong (1994).

Note that the bound in (vi) is almost sharp because, for example,

$$\sum_{d=2}^{\infty} d^{-1} (\ln d)^{-2} < \infty \ \text{ and } \ \sum_{d=1}^{\infty} d^{\epsilon-1} = \infty,$$

where $\epsilon > 0$.

Note also that for continuous parameters such as the bandwidth parameters in kernel smoothing, we may use the Euclidean distance as an appropriate distance function for parameter (e.g. bandwidth) choice. However, as mentioned earlier, for many discrete cases, the Euclidean distance is found to be inappropriate. For our case, we have obtained an appropriate non-Euclidean distance function, namely $\Delta^{1/2}(.,.)$ on N × N, based on the projection of the skeleton from a low dimensional space to a high dimensional space as described earlier. Proposition 3.1 (ii) reveals the relation between $\Delta(.,.)$ and the Euclidean distance.

4 Estimation

Henceforth we suppose that $\{X_t\}$ is a bounded time series (Cf. Chan and Tong, 1994). Let $\mathbb{B}_s^t(X)$ denote the sigma algebra generated by $(X_s, ..., X_t)$ and suppose that the following conditions are satisfied:

- (a) $E[\epsilon_t | \mathbb{B}^{t-1}_{-\infty}(X)] = 0$, almost surely.
- (b) $E[\epsilon_t^2 | \mathbb{B}_{-\infty}^{t-1}(X)] = \sigma^2$, a strictly positive constant, almost surely.
- (c) For each d, $E[X_t|X_{t-1}, ..., X_{t-d}]$ is Hölder continuous.
- (d) Let the probability density function of (X_t,..., X_{t-d}) be strictly positive and Lipschitz continuous on a compact set in R^d.
- (e) Let k denote a probability density function with compact support on \mathbb{R}^1 , and $\forall x, y \in \mathbb{R}^1, |k(x) k(y)| \leq c_3 |x y|.$
- (f) For every $t, s, \tau, t', s', \tau' \in \mathbb{N}$, the joint probability density function of $(X_t, X_s, X_{\tau}, X_{t'}, X_{s'}, X_{\tau'})$ is bounded.
- (g) Let 1/p + 1/q = 1. For some p > 2 and $\delta > 0$ such that $\delta < 2/q 1$, $E|\epsilon_s|^{2p(1+\delta)} < \infty$ and $E|F(X_1)|^{2p(1+\delta)} < \infty$.
- (h) For each d, F_d has bounded first partial derivative.

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(i)

$$\sup_{i\in\mathbb{N}} \left(E[\sup_{A\in\mathbb{B}^{\infty}_{i+j}(X)} \{ |P(A|\mathbb{B}^{i}_{1}(X)) - P(A)| \}] \right) = \bigcirc (\beta^{j}), 0 < \beta < 1.$$

Without loss of generality, let $d_2 \ge d_1$. Let M be a pre-specified maximum lag in the delay co-ordinate construction. Equation (9) suggests that a natural estimate of $\Delta(d_1, d_2)$ is

$$\hat{\Delta}(d_1, d_2) = RSS(d_1) - RSS(d_2), \tag{9}$$

where

$$RSS(d) = (N - M + 1)^{-1} \sum_{t=M}^{N} \{X_t - \hat{F}_{d,N}(X_t^{(d)})\}^2,$$
(10)

with $\hat{F}_{d,N}$ being the Nadaraya-Watson kernel estimate of F_d based on the observations $X_1, ..., X_N$, namely

$$\hat{F}_{d,N}(x_1,...,x_d) = \frac{\sum_{t=M}^{N-1} X_{t+1} k(\frac{x_1-X_t}{h}) k(\frac{x_2-X_{t-1}}{h}) \dots k(\frac{x_d-X_{t-d+1}}{h})}{\sum_{t=M}^{N-1} k(\frac{x_1-X_t}{h}) k(\frac{x_2-X_{t-1}}{h}) \dots k(\frac{x_d-X_{t-d+1}}{h})}.$$

Here, $h \equiv h_{d,N} \in [aN^{-(1/(2d+1))-\xi}, bN^{-(1/(2d+1))+\xi}]$, with a and b being arbitrary real positive constants and ξ any real positive constant strictly less than $\binom{2(d+1)(2d+1)}{2}$. Chang and Tang (1002) have proved the following theorem.

 $\{2(d+1)(2d+1)\}^{-1}$. Cheng and Tong (1992) have proved the following theorem.

Theorem 4.1 Under the above conditions,

$$RSS(d) = \sigma_N^2(d) \{ 1 - (2\alpha - \beta)/(Nh^d) + o_p(1/(Nh^d)) \},\$$

where

$$\sigma_N^2(d) = (N - M + 1)^{-1} \sum_{t=M}^N \{X_t - F_d(X_t^{(d)})\}^2,$$
(11)

$$\alpha(d) = \{k(0)\}^d \text{ and } \beta(d) = \{\int k^2(u) du\}^d.$$

Now, using this theorem, we may easily deduce that for each $d \ge d_0$ and $h_{d,N} = N^{-1/(2d+1)}$

$$\hat{\Delta}(d, d+1) = RSS(d) - RSS(d+1)$$
(12)

$$= \sigma_N^2(d_0) \{ 2\alpha(d+1) - \beta(d+1) \} N^{-(d+2)/(2d+3)}$$
(13)

$$+o_p(N^{-(d+2)/(2d+3)}).$$
 (14)

This analysis shows that if we use $\hat{\Delta}(d, d+1)$ to obtain an estimate of d_0 , we have to decide where the former cuts off. Recall that $\Delta(d, d+1) = 0$ for $d \ge d_0$. (Cf. equation

(9).) Thus, we are facing a statistical problem of the same type as described in Akaike (1974). A conventional statistical approach prior to Akaike's innovation would be along the line of testing a class of null hypotheses: $\Delta(d, d+1) = 0, d \in \{1, 2, ..., M\}$. In the present setting of a nonparametric autoregression, Robinson (1989) has adopted the conventional approach by considering the problem of testing the null hypothesis that d takes a specified value say \tilde{d} versus the alternatives $d > \tilde{d}$. Presumably, one would then have to "scan" \tilde{d} over the set say $\{1, 2, ..., M\}$ in a suitable manner, which has to be specified. Recently, Cheng and Tong (1992, 1994) have adopted an approach in the spirit of Akaike (1974). Specifically, they have proposed a cross-validatory method: replace $\hat{F}_{d,N}(X_t^{(d)})$ in equation (11) by an estimate which is obtained from the observed sample but with X_t deleted. Let $\hat{F}_{d,N,\backslash t}(X_t^{(d)})$ denote this delete-one estimate and

$$CV(d) = (N - M + 1)^{-1} \sum_{t=M}^{N} \{X_t - \hat{F}_{d,N,\backslash t}(X_t^{(d)})\}^2.$$
(15)

Effectively the "delete-one" device penalizes model complexity and Cheng and Tong (1992) have shown that $argmin_{1 \leq d \leq M} CV(d)$, or \hat{d}_{CV} for short, yields a consistent estimate of d_0 provided $d_0 \leq M$, i.e. $Pr\{\hat{d}_{CV} = d_0\} \rightarrow 1$ as $N \rightarrow \infty$. Briefly, from Cheng and Tong (op. cit.) we can easily deduce that for bounded time series, (i.e. X_t is bounded.)

$$CV(d) - CV(d_0) = \sigma_N^2(d) - \sigma_N^2(d_0) + \sigma_N^2(d^*)\beta(d^*)N^{-(d^*+1)/(2d^*+1)}$$
(16)

$$+o_n(N^{-(d^*+1)/(2d^*+1)}),$$
 (17)

where $d^* = \max\{d, d_0\}$. Note that $\sigma_N^2(d) = \sigma_N^2(d_0)$ for $d \ge d_0$ and that for $1 \le d \le M$, $\sigma_N^2(d) \to \sigma^2(d)$ almost surely as $N \to \infty$. Consistency then follows.

5 Tail Probabilities

It would be pertinent to investigate the limiting distribution of d_{CV} further. First we notice that

$$\begin{aligned} P(\{\hat{d}_{CV} = d_0\}) &= P(\{CV(d_0) \le CV(d), 1 \le d \le M\}) \\ &= P(\{CV(d_0) \le CV(d), 1 \le d < d_0\}) + P(\{CV(d_0) \le CV(d), d_0 \le d \le M\}) \\ &- P(\{CV(d_0) \le CV(d), 1 \le d < d_0\} \bigcap \{CV(d_0) \le CV(d), d_0 \le d \le M\}). \end{aligned}$$

Now, let $\theta(d) = (2d+1)/(d+1)$.

Case 1: $(d < d_0)$ We have

$$CV(d) - CV(d_0) = \hat{\Delta}(d, d_0) - RSS(d_0) \times 2\alpha N^{-\theta^{-1}(d_0)} + o_p(N^{-\theta^{-1}(d_0)})$$

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$$= \Delta(d, d_0) - \Delta(d, d_0) + \Delta(d, d_0) - RSS(d_0) \times 2\alpha N^{-\theta^{-1}(d_0)} + o_p(N^{-\theta^{-1}(d_0)}).$$

Since

$$\theta^{-1}(d_0) = \frac{d_0+1}{2d_0+1} = \frac{1}{2-1/(d_0+1)} > \frac{1}{2}$$

the above is equal to

 $\Delta(d, \ d_0) \ + \ o_p(N^{-\frac{1}{2}}).$

This implies that

$$\sqrt{N(CV(d) - CV(d_0))} \sim_{asym} \mathcal{N}(\sqrt{N\Delta(d, d_0)}, \Sigma).$$

So, for $1 \leq d < d_0$,

$$P(\{CV(d_0) \le CV(d)\}) = P(\{\sqrt{N}(CV(d_0) - CV(d)) \le 0\}) \\ =_{asym} P(\xi_d \le 0),$$

where $\xi_d \sim_{asym} \mathcal{N}(-\sqrt{N}\Delta(d, d_0), \Sigma)$. Hence, we have the formula $P(\xi_d \leq 0) = 1 - t_u$ for $d < d_0$, where t_u is the tail probability of underfitting.

Case 2: $(d > d_0)$ We have $\epsilon_t^{(d)} = \epsilon_t^{(d)}$, a.s., Using formula (16), we have for $d > d_0$

$$CV(d) - CV(d_0) = \sigma_N^2(d_0)\beta N^{-\theta^{-1}(d)} + o_p(N^{-\theta^{-1}(d)}),$$

where $\sigma_N^2(d_0) = \frac{1}{N} \sum_{i=1}^{N} [\epsilon_t^{(d)}]^2$.

By the standard Central Limit Theorem, we have

$$\sqrt{N(\sigma_N^2(d_0) - \sigma^2(d_0))} \sim \mathcal{N}(0, \Sigma)$$

and by a high-order expansion, we may obtain

$$\sqrt{N}N^{\theta^{-1}(d)}(CV(d) - CV(d_0)) = \sqrt{N}\sigma_N^2(d_0)\beta + \nabla + o_p(1),$$

where ∇ is a constant. Therefore,

$$P(\{CV(d_0) \le CV(d)\}) = P(\{\sqrt{N}N^{\theta^{-1}(d)}(CV(d_0) - CV(d)) \le 0\}) \sim_{aymp} P(\eta_d \le 0),$$

where $\eta_d \sim_{asym} \mathcal{N}(-\sqrt{N}\sigma^2(d)\beta + \nabla, \ \overline{\Sigma}).$

Putting the two results together, we have that

$$\begin{split} P(\hat{d}_{CV} = d_0) &\leq \max\{(1 - \text{tail prob of underfitting}), \\ &(1 - \text{tail prob of overfitting})\} \\ &= \max\{1 - t_u, 1 - t_o\}, \end{split}$$

where $t_u = P(\xi_d \ge 0)$ and $t_o = P(\eta_d \ge 0)$. Now, we show that by using the above tail probabilities, we obtain a similar formula for the sample requirement as that reported in Cheng and Tong (1994). First, we need a simple lemma.

Lemma Let Z be a normal random variable with mean -M (M > 0) and variance σ^2 . Then

$$P(Z \ge 0) = \int_{M}^{+\infty} e^{-\frac{x^2}{2\sigma^2}} dx = O(Me^{-\frac{1}{2}M^2}).$$

Now, for the tail probability of underfitting, t_u , $M = \sqrt{N}\Delta(d, d_0)$ and for the tail probability of overfitting, t_o , $M = \sqrt{N}\beta\gamma\sigma^2(d_0)$. To control the tail probabilities at level $\epsilon > 0$, we need to have

$$Me^{-\frac{1}{2}M^2} \leq \epsilon$$
 asymptotically.

Since $\beta = \beta(d_0)$ has a complicated form, the tail probability of overfitting is not so helpful. However, for the tail probability of underfitting, since $M = \sqrt{N}\Delta(d, d_0)$, it is easy to see that

$$N \geq \Delta^{-2}(d, d_0) \log(\frac{1}{\epsilon}).$$

In particular, choosing $d = d_0 - 1$, we readily have $\Delta(d_0 - 1, d_0) = O(\sigma^2(d_0)/d_0)$ as in Cheng and Tong (1994). Therefore, we obtain

$$N = N(d_0) \geq \frac{d_0^2 log(1/\epsilon)}{\sigma^4(d_0)}.$$

6 Conclusion

Using an argument based on controlling the tail probabilities, we have arrived at the same sample size requirement under realistic conditions as that obtained in Cheng and Tong (1994) for the construction of delay co-ordinates in a stochastic dynamical system.

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Part II: Coupled Map Lattices

Thermodynamic properties of coupled map lattices

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Abstract

This chapter presents an overview of the literature which deals with applications of models framed as coupled map lattices (CML's), and some recent results on the spectral properties of the transfer operators induced by various deterministic and stochastic CML's. These operators (one of which is the wellknown Perron-Frobenius operator) govern the temporal evolution of ensemble statistics. As such, they lie at the heart of any thermodynamic description of CML's, and they provide some interesting insight into the origins of nontrivial collective behavior in these models.

1 Introduction

This chapter describes the statistical properties of networks of chaotic, interacting elements, whose evolution in time is discrete. Such systems can be profitably modeled by networks of coupled iterative maps, usually referred to as coupled map lattices (CML's for short). The description of CML's has been the subject of intense scrutiny in the past decade, and most (though by no means all) investigations have been primarily numerical rather than analytical. Investigators have often been concerned with the statistical properties of CML's, because a deterministic description of the motion of all the individual elements of the lattice is either out of reach or uninteresting, unless the behavior can somehow be described with a few degrees of freedom. However there is still no consistent framework, analogous to equilibrium statistical mechanics, within which one can describe the probabilistic properties of CML's possessing a large but finite number of elements. The results presented in this chapter illustrate some recent attempts to partially fill this theoretical void.

1.1 Coupled map lattices: Initial presentation

Models framed as coupled discrete time maps are not a novelty. Caianiello [10] proposed his "neuronic equations", which are coupled iterative maps, as generalizations of the McCulloch and Pitts neural networks more than three decades ago. Similarly, the work of Denman [22], trying to characterize the dynamics of interacting pressure and electromagnetic waves in plasmas, made use of coupled discrete maps, and related models were used in the early theory of transmission lines [82]. However, the modern body of work dealing with coupled map lattices can be traced back to the beginning of the eighties (*cf.* work by Kaneko [39], Waller and Kapral [98, 99] and Deissler [20]) as phenomenological models to study the behavior of large collections of coupled chaotic elements (we will return to more precise descriptions of these and more recent investigations of CML dynamics).

1.1.1 Deterministic CML's

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In their most general form, deterministic coupled map lattices are mappings Φ : $\mathbb{R}^N \mapsto \mathbb{R}^N$ governing the evolution of a state vector $\mathbf{x}_t = (x_t^1, \cdots, x_t^N)$,

$$\mathbf{x}_{t+1} = \Phi(\mathbf{x}_t) \quad t = 0, 1, \cdots.$$
 (1)

More specifically, the evolution of a component $x_t^{(i)}$ of the state vector \mathbf{x}_t is governed by the difference equation

$$x_{t+1}^{(i)} = \Phi_{ ext{local}}^{(i)}(x_t^{(i)}) + \Phi_{ ext{neighbours}}^{(i)}(\cdots, x_t^{i-1}, x_t^{i+1}, \cdots)$$

where $\Phi_{\text{local}}^{(i)}$ models the local dynamics at site *i*, and $\Phi_{\text{neighbours}}^{(i)}$ denotes the mechanisms acting on *i* from a specified neighbourhood. If those mechanisms are the same for all sites on the lattice, and if they are locally modeled by the map $S : \mathbb{R} \mapsto \mathbb{R}$, and in the neighbourhood by the map $T : \mathbb{R} \mapsto \mathbb{R}$ one can write

$$x_{t+1}^{(i)} = S(x_t^{(i)}) + \sum_{\substack{\text{some} \\ \text{neighbourhood}}} T(x_t^j).$$

In many situations of interest, it is possible to further simplify the formulation of the models by letting $T \equiv S$, and using a linear coupling scheme between the elements¹. In these circumstances, we have

$$x_{t+1}^{(i)} = (1-\varepsilon)S(x_t^{(i)}) + \frac{\varepsilon}{p} \sum_{\substack{p \\ n \in ghbours}} S(x_t^j)$$
(2)

where $\epsilon \in [0, 1]$ is the coupling term. Again, *i* denotes a discrete spatial index (of arbitrary finite dimension), and *t* denotes discrete time.

In our description of CML's, we view the sites of the lattice as being located on the nodes of a regular body centered cubic lattice, and in this chapter periodic boundary conditions are always enforced. There are investigations of coupled map lattices in which the underlying lattice is not as simple as the body-centered-cubic example chosen here, and possesses intrinsically "complex" (sometimes called hierarchical) structure. In these cases, it was demonstrated [18, 19] that the bifurcation structure of the CML can depend on the topology of the lattice, but we will not dwell on this point, since most of the analytical tools discussed in this chapter do not depend on the properties of the underlying lattice topology.

We consider cases where the phase space X of Φ is a restriction of \mathbb{R}^N to the *N*-dimensional hypercube: $\mathbb{X} = [0,1] \times \cdots \times [0,1]$. In two spatial dimensions, the evolution of each site of a deterministic coupled map lattice with linear interelement coupling is given by

$$x_{t+1}^{(kl)} = \Phi^{(kl)}(\mathbf{x}_t) = (1-\varepsilon)S(x_t^{(kl)}) + \frac{\varepsilon}{p} \sum_{\substack{p \text{ nearest}\\ neighbours}} S(x_t^{(ij)}), \quad \varepsilon \in (0,1),$$
(3)

¹The coupling scheme of equation (2) is called *linear* because $x_{t+1}^{(i)}$ is linearly proportional to $S(x_t^{(i)})$. Some authors [46] would call such architectures nonlinear but we will adhere to this convention.

where $S : [0,1] \mapsto [0,1]$ describes the local dynamics. When p = 4, the coupling in (3) mimics a discrete version of the diffusion operator, and when the *p*-neighbourhood encompasses the entire lattice, the coupling is known as mean-field.

To allow for the possibility that stochastic perturbations influence the evolution of the CML, we now introduce a class of stochastic CML's which will be investigated numerically and analytically in Section 5.

1.1.2 Stochastic CML's

It is of interest to understand and clarify the influence of noisy perturbations on the evolution of these CML's. The perturbations considered here are random vectors of N numbers (for an N element CML), whose components are independent of one another, each being distributed according to a one dimensional probability density g. The density g of the vector random variable $\boldsymbol{\xi} = (\xi^{(1)}, \dots, \xi^{(N)})$ will therefore be constructed as the product of independent (identical) components:

$$\mathbf{g}(\boldsymbol{\xi}) = \prod_{i=1}^{N} g^{(i)}(\boldsymbol{\xi}^{(i)}) = \prod_{i=1}^{N} g(\boldsymbol{\xi}^{(i)}).$$
(4)

There are various ways in which a stochastic perturbation can influence the evolution of a coupled map lattice: the perturbation can be additive or multiplicative, and it can be applied constantly or randomly. The influence of the noise on the dynamics depends on which of these is considered.

When the stochastic perturbations are applied at each iteration step, they can be either added to, or multiply, the original transformation Φ . In the former case, the evolution of a lattice site is given by a relation of the form

$$x_{t+1}^{(kl)} = \Phi^{(kl)}(\mathbf{x}_t) + \xi_t^{(kl)} \equiv \Phi^{(kl)}_{add}(\mathbf{x}_t)$$
(5)

and $\boldsymbol{\xi}$ is then referred to as *additive* noise. In the latter, we have

$$x_{t+1}^{(kl)} = \Phi^{(kl)}(\mathbf{x}_t) \times \xi_t^{(kl)} \equiv \Phi^{(kl)}_{mul}(\mathbf{x}_t)$$
(6)

and $\boldsymbol{\xi}$ is then referred to as *multiplicative* or *parametric noise*. In general, the effects of additive and multiplicative noise on CML's can be different, since they model different perturbing mechanisms. The density (4) of the perturbations present in (5) and (6) is always defined so that the phase space of the perturbed transformations remains the N dimensional hypercube X defined above. In other words, $\Phi_{add} : X \mapsto X$ and $\Phi_{mul} : X \mapsto X$.

The developments which followed the introduction of CML's have established the usefulness of these models to investigate the dynamics of a wide variety of systems in various areas of research ranging from population dynamics to solid state physics. Our own research was motivated in part by this activity, and we therefore give a fairly extensive though by no means exhaustive review of the literature before proceeding to a description of CML thermodynamics.

2 Overview of models framed as CML's

Two collections of papers on the subject, both edited by K. Kaneko [38, 24] are available, so the present section focuses primarily on some of the more recent published works on CML dynamics.

2.1 Biological applications

There are many biological systems which can be thought of as collections of interacting elements with intrinsic nontrivial dynamics. When this is case, and if the local dynamics can reasonably be modeled by discrete time maps, it is feasible to introduce models framed as CML's.

This approach has been fruitful in population dynamics, in which the discrete time occurs naturally if generations do not overlap (insect populations constitute one possible example). The investigations of Solé et al. [87, 88] have led these authors to conclude that CML's provided the simplest models for discrete ecological models. Franke and Yakubu [26] have recently proposed a CML to investigate the inter-species competition of large bird populations. These CML's are crude models for the evolution of species competing for shared resources, which are obtained by straightforward (albeit not very realistic) multidimensional generalizations of proposed one-dimensional maps [70, 96]. They open the way for more realistic population competition models which could be framed as CML's in which the underlying lattice is not regular, perhaps taking into account some of the spatial features observed in the field. Ikegami and Kaneko [45] have also proposed a model for host-parasitoid networks, and their study of the corresponding CML have led them to introduce a generalization of the idea of homeostasis. The proposed alternative, "homeochaos", describes an asymptotic state reached by networks of evolving and mutating host-parasite populations in which chaotic fluctuations in the numbers of hosts and parasites are observed at equilibrium.

Beyond population dynamics, the mathematical description of neural behavior has also benefited from discrete time, discrete space models. The foundations of the modeling of cortical function were laid in two seminal papers by Wilson and Cowan [102, 103]. However, the original models presented by these authors are computationally costly, and are not easily amenable to analytic investigations. As a result, there have been attempts to reduce the original networks of integro-differential equations to simpler spatially extended models. Reduction to CML's are presently being considered by some of the same authors [68]. In its methodology, this work [*ibid*] is typical of investigations in which the CML is proposed as a discrete-time version of previously considered continuous-time systems. For example, Molgedey *et al.* [71] made use of coupled map lattices to examine the effects of noise on spatiotemporal chaotic behavior in a neural network which was originally proposed (in its continuoustime version) by Sompolinsky *et al.* [89]. Following a similar path, Nozawa [73] has presented a CML model, obtained by using the Euler approximation to the original Hopfield equations.

One of the outstanding problems motivating this neural oriented research is the

identification of organizing principles to explain the synchronization of large populations of neurons possessing individually complex dynamics. Such synchronizations are thought to take place in pathological situations (e.g. epileptic seizures) as well as in the normal brain. For example, Andersen and Andersson [1], and later Steriade and Deschenes [90] have hypothesized that such a synchronized activity of the reticular thalamic nucleus (RTN) acted as a pacemaker for the so-called "spindle oscillations" observed during various sleep stages. Models of the RTN framed as networks of coupled differential delay equations have been proposed by Destexhe [23], and these can be reduced, by a straightforward singular perturbation procedure [34], to CML's. Models of the RTN framed as coupled ODE's have also been considered recently, and provide a motivation for the theoretical description of globally coupled arrays of oscillators [27]. An interesting review of the mathematical description of cortical behavior in terms of coupled nonlinear units is given in [104]. A less recent, but somewhat broader view of the contemporary efforts to mathematically describe the behavior of neural networks using the conceptual tools of nonlinear dynamics is presented in [84]. For the sake of completeness, we also refer the reader to the review by Herz [30], which describes some of the earlier neural modeling attempts which made use of CML's, as well as some of the models based on delay differential equations.

At the molecular level, Cocho et al. [15] proposed a CML model to describe the evolution of genetic sequences. A comprehensive account of the development of this idea can be found in [16]. In this simplified formalism, each genetic sequence is made up of m nucleotides, which come in four flavors. The latter is determined by which of four possible bases (guanine, cytosine, adenine, thymine) complements the phosphate and deoxyribose groups which make-up the nucleotide. The building block of a genetic sequence is then a triplet of nucleotides, called a codon (which codes for an amino acid). Cocho et al. established that for certain viruses, it is relevant to restrict attention to sequences containing only two types of codons, denoted type I and II. Hence a sequence of length L = m/3 codons is uniquely characterized by the number i_I of type I codons it possesses. i_I can also be thought of as a position index in a configuration space, and in this case two sequences are "close" if they differ by a small number of codons. Under specified fitness constraints (whose meaningful definition imposes the most important limits on this approach), sequences can mutate: a type I codon becomes type II, or vice-versa. The CML model for genetic sequence evolution describes the evolution of the number of sequences at location i_I in the configuration space, and therefore, local interactions are due to mutations, whereas ecological constraints (i.e. coming from limited food supplies) generate long range coupling. Recently [17], the same authors have extended this approach to study the mutations of the HIV1 virus, and their predictions concerning the regularity of the chemical compositions of this virus' RNA sequences agree with statistical analyses of gene data.

The use of CML's, though interesting from the mathematical biologist's point of view, is not restricted to biological models. Contemporary developments in the theory of image processing have led to the introduction of various algorithms which are in fact coupled map lattices.

2.2 Image processing applications

One of the basic challenges in image processing is the so-called "shape from shading" problem [8], which surfaces both in computer graphics, where shading is used to enhance realism, and computer vision, where the study of shading is crucial for the proper interpretation of a pattern's two dimensional projection (its picture). In computer vision, a typical task is the classification of patterns into classes (*e.g.* faces *vs.* landscapes), where the input patterns possess underlying "shapes" describing their essential features (nose, eyes, *vs.* trees or clouds) which are immersed in secondary information due to the shading of the image.

Several approaches to this problem [8, 92, 97] make use of algorithms which are coupled map lattices, although there appears to be no explicit awareness in this literature of the link between the structure of the algorithms and their formulation as CML's. We illustrate this link with a frequently encountered model used to approach shape from shading, which was introduced by Brooks and Horn and is known as the B-H algorithm [7]. To derive the model, the shape of an object is thought of as a function which minimizes a given functional. After minimization of the proper errors [97], the B-H algorithm is written

$$x_{t+1}^{(ij)} = \bar{x}_t^{(ij)} + \frac{\varepsilon^2}{4\lambda} \left(E^{(ij)} - x_t^{(ij)} \cdot \mathbf{S} \right) \mathbf{S}$$
(7)

where $E^{(ij)}$ is the shading, $x_t^{(ij)}$ is the surface normal at site (i, j) of the image, λ and ε describe the role of a smoothness constraint, and **S** is the light source vector (the light source being responsible for the presence of shade), and $\bar{x}_t^{(ij)}$ is the average of the normals in a neighbourhood of site (i, j). The local coupling comes from this latter term, and as a result, the evolution of the initial image under the action of the B-H shade from shading algorithm is akin to the evolution of an initial vector under the action of a CML. There are more recent descriptions of this problem which do not make use of the variational techniques used to derive (7), and which lead to different CML's (one example is given in [97]).

The treatment of fuzzy images is not limited to the shape from shading problem. In fact, prior to this analysis, "dirty" images, possibly obtained with remote sensing equipment must be "cleaned". This procedure, known as the segmentation of an image, is an attempt to highlight edges while smoothing the noise in regions devoid of edges. A "physicist-friendly" presentation of the segmentation problem is given by Price *et al.* [78]. They introduce a coupled map lattice designed as an alternative to the costlier and more unstable segmentation algorithms obtained by the minimization of a cost function. Their work is an additional illustration of the potential benefits to the image-processing community which could follow from an increased awareness of the wealth of dynamics displayed by high-dimensional nonlinear discrete time maps: the stability properties of the algorithms, and their possible pathological treatments of real images can sometimes be determined beforehand by an in-depth investigation of the corresponding CML.

2.3 Phenomenological models

In spite of the obvious interest generated by CML's for their many potential applications, the main motivation for their investigation from a physicist's point of view undoubtedly lies in their use as phenomenological models for the study of more general spatially extended systems

2.3.1 Spatiotemporal intermittency and weak turbulence

An example of the fruitful application of CML's to study fluid dynamics is given by the work of Chaté and Manneville, concerning the transition to turbulence via spatiotemporal intermittency [11, 12]. In this work, the CML's are constructed to reflect what are thought to be the essential features of a fluid undergoing the transition from laminar flow to turbulent flow via the so-called intermittency scenario, according to which a laminar flow gradually becomes turbulent by the growth of regions in the laminar regime in which the flow is turbulent. Hence, the essential features of the Chaté-Manneville models are the partition of the local phase space into two regimes: one laminar, and the other turbulent. Their analysis of the corresponding CML's lead to the identification of universality classes describing the "contamination process" of the laminar flows by turbulent "islands" [11, 13, 12]. The usefulness of the CML approach is that these models capture much of the phenomenology while remaining amenable to extensive numerical simulations.

The destabilization of laminar flows does not always occur via spatiotemporal intermittency. Various convective instabilities can result in alternate destabilizing mechanisms, and some of the recent work on CML's focuses on the dynamics of these instabilities in so-called "open flow" models [21]. Convective instabilities grow as they are transported downstream, and they are localized in the sense that a laboratory observer sees them pass by from upstream to downstream as localized defects [66]. Such situations are encountered, for example, in the modeling of shear flows and boundary layers, and they provide situations in which spatial order can be coexistent with temporal chaos. Given the complexity of the full equations of motion, it has been helpful to consider reduced models framed as CML's. In [4], Biferale et al. describe the convective instabilities of a unidirectionally coupled CML by focusing on the tangent vector associated with a trajectory of the CML. This analysis resulted in a relatively simple description of the localization of temporal chaos around the defects of the lattice. Other descriptions of asymmetrically coupled CML's include the works of Jensen [37, 36], Aranson et al. [2], and Willeboordse [101]. In all these, the coupling between the elements of the CML is not isotropic, and there is a preferred spatial direction in the lattice along which information is more easily transmitted. More recently, we have used CML's with unidirectional coupling to investigate the statistical properties of some differential delay equations [61].

2.3.2 Reaction diffusion models

Reaction-diffusion models play an important role in the description of real spatially extended systems because the competition between these two general mechanisms is ubiquitous in nature. In one dimension, they are modeled by the generic PDE

$$\frac{du(x,t)}{dt} = D\nabla^2 u(x,t) + F(u(x,t)), \tag{8}$$

where F is the reaction term. In a seminal work, Turing [95] established that this competition was at the origin of many pattern-forming instabilities. Reaction diffusion systems have been the subject of many descriptions in terms of CML's because diffusion is approximated by a nearest neighbour coupling in CML's of the form (2) (examples of this reduction are given by Puri et al. [81] for the one dimensional Cahn-Hilliard equation, and by some of the same authors for the Fischer equation [75]). We note that the reduction of models framed as PDE's to their CML counterparts is usually not a rigorous procedure, although there are special circumstances (for some externally forced models) in which the CML provides a close approximation to the PDE [48]. As mentioned in [58], the benefits of using CML's in the majority of investigations stem from the fact that they reproduce most of the interesting phenomenology, without requiring the prohibitively large computing resources associated with PDE simulations. In addition, it is likely that as those resources increase with technological breakthroughs, so will the complexity of the problems considered by the modeling community, so that there is some intrinsic virtue in trying to understand reduced systems, such as CML's, to help in the study of more complicated ones.

Because of their computational efficiency, CML's are well-suited for the introduction of new quantifiers of spatiotemporal dynamics, or for the multidimensional generalizations of one-dimensional concepts [93] (this was an important motivation for the early discussions [20, 98, 99]). In this spirit, Kaneko has introduced such concepts as the "comoving mutual information flow" [40], and various "pattern entropies" and "pattern distribution functions" [41], to mention a few of the frequently encountered statistical descriptors of the motion. Reaction diffusion CML's are then usually of the form (2) with p = 2 in one spatial dimension, or p = 4 in two dimensions, and used to explore in great detail the behavior of the quantifiers of spatio-temporal motion more efficiently than if PDE's were considered.

Similar lattices have been used to simulate interfacial phenomena in reaction diffusion systems [58]. In these investigations, the CML's usually arise from the phenomenological simplification of PDE's of the form (8), and they provide the simplest models which retain the disparate length and time scales necessary for the appearance of rich interfacial dynamics. Other typical examples of this approach are given for crystal growth by Oono and Puri [74] and for chemical waves by Barkley [3]. A phenomenological description of interfacial phenomena was recently given by Kapral *et al.* [47], using a piecewise linear CML (with a branch with slope zero in the local map) which displays some of the interfacial structures associated with continuous time, continuous space models. In a similar spirit, the behavior of liquids at the boiling transition was studied by Yanagita [105] with another reaction-diffusion CML. To conclude, we refer the interested reader to the comprehensive review of the applications of CML's to capture the essential features of pattern formation in chemically reacting systems given by Kapral in [46]

2.3.3 Arrays of globally coupled oscillators

The introduction of all-to-all (or mean-field, or global) coupling in theoretical physics to investigate the dynamics of spatially extended systems is not novel; it has always been one of the standard techniques used to describe the magnetic properties of spin systems. As experimentalists probe ever deeper into the behavior of systems with a large number of degrees of freedom, new models of globally coupled oscillator arrays are introduced, in which the individual oscillators are either continuous or discrete in time. Some of the experimental situations in which global coupling arises naturally are related to nonlinear optics, with examples ranging from solid-state laser arrays [107], to multimode lasers [35]. In electronics, a number of experiments on Josephson junction arrays coupled in series or in parallel have indicated the presence of very rich dynamics, often related to the multiplicity of attractors, or the linear stability properties of fully synchronized states (cf. [72] and references therein). The majority of models proposed to describe these dynamics are framed as globally coupled sets of ordinary differential equations [29, 85, 91]. The ODE's are usually not rigorously reduced to CML's, and the introduction of the discrete-time map lattices is often motivated by the desire to improve the phenomenological insight into the evolution of the continuous-time oscillators. For example, Wiesenfeld and Hadley [100] found that CML's provided useful reduced systems to investigate the effects of low levels of noise on large globally coupled arrays which possess an even larger number of attractors. More recently, discrete maps were used to describe the dynamical properties of periodic attractors in arrays of p - n diode junctions [25], and the stability regions of various solution types for the CML's agreed qualitatively with the experimental data obtained from two coupled diode junctions. We close this admittedly incomplete presentation of some contemporary discussions of global coupling in the physical sciences, by mentioning that CML's have recently been used to study theoretically the remarkable phenomenon of mutually destructive fluctuations in which the activity of the mean field is observed to have a much smaller variance than the individual trajectories [72]. This phenomenon is extremely interesting for researchers trying to understand the role of noise in the transmission of information in spatially extended processing systems. For example, it is well known that the behavior of individual neurons can sometimes be more erratic than that of the average behavior of a population of neurons [69].

We now turn to the presentation of some of the conceptual tools which will be used throughout the remainder of this chapter to discuss the statistical properties of models framed as CML's.

3 CML's and probability densities

Suppose that the dynamics of a physical system are modeled by a (deterministic or stochastic) dynamical system denoted by $\mathcal{T} : \mathbb{X} \to \mathbb{X}$ (many examples of such situations are described in Sections 2 and 2.3). Suppose further that some observable $\mathcal{O}(\mathbf{x}_n)$, which depends on the state \mathbf{x}_n of \mathcal{T} , is being measured at time n (The observable \mathcal{O} is arbitrary, though it must be a bounded measurable function). The

expectation value of this observable, denoted by $E(\mathcal{O}_n)$, is the mean value of $\mathcal{O}(\mathbf{x}_n)$ when the measurement is repeated a large (ideally infinite) number of times. Mathematically it is given by

$$E(\mathcal{O}_n) = \int_{\mathbf{X}} \mathbf{f}_n(\mathbf{y}) \mathcal{O}(\mathbf{y}) \, d\mathbf{y},\tag{9}$$

where $f_n(\mathbf{x})$ is the density of the variable \mathbf{x}_n , *i.e.* the probability $p(\mathbf{x}'_n)$ of finding \mathbf{x}_n between \mathbf{x}'_n and $\mathbf{x}'_n + \delta \mathbf{x}'_n$, is

$$p(\mathbf{x}'_n) = \int_{\mathbf{x}'_n}^{\mathbf{x}'_n + \delta \mathbf{x}'_n} \mathbf{f}_n(\mathbf{y}) \, d\mathbf{y}.$$

All extrinsic functions which characterize the thermodynamic properties of a system are observables whose expectation values are defined by (9) since \mathcal{O} was arbitrary. Therefore, the thermodynamic state of the CML \mathcal{T} at time *n* is completely characterized by the density function \mathbf{f}_n . Hence a complete description of the thermodynamics of \mathcal{T} must focus on the behavior and properties of \mathbf{f}_n . To this end, we introduce the transfer operator associated with \mathcal{T} , denoted by $\mathcal{P}_{\mathcal{T}}$, which governs the time evolution of \mathbf{f}_n

$$\mathbf{f}_{n+1}(\mathbf{x}) = \mathcal{P}_{\mathcal{T}} \mathbf{f}_n(\mathbf{x}), \quad n = 0, 1, \cdots.$$
(10)

To draw an analogy with more familiar physical systems, the transfer operators discussed here describe the arbitrary dynamical system \mathcal{T} much as the Liouville equation describes the ensemble dynamics of ODE's, the Fokker Planck equation those of the Langevin equation (which is a stochastic ODE), or the Perron-Frobenius operator (defined in Section 3.1) those of deterministic maps (cf. Table 1.1).

Description of the model	Description of ensemble dynamics
Deterministic maps	The Perron-Frobenius operator
Stochastic maps	The transfer (Markov) operator
Deterministic ODE's	The generalized Liouville equation
Stochastic ODE's (white noise)	The Fokker Planck equation
Stochastic ODE's (non-white noise)	The Kramers- Moyal equation
Differential delay equations	The Hopf equation for the characteristic functional

TABLE 1.1:

Brief summary of the probabilistic descriptions associated with various types of discrete and continuous-time models.

3.1 The Perron-Frobenius operator \mathcal{P}_{Φ}

A discrete-time nonsingular transformation $\Phi : \mathbb{X} \longrightarrow \mathbb{X} (\mathbb{X} \subset \mathbb{R}^N)$ induces an operator denoted \mathcal{P}_{Φ} which acts on probability densities, and which is defined implicitly by the relation

$$\int_{\mathbf{A}} \mathcal{P}_{\Phi} \mathbf{f}(\mathbf{x}) \, d\mathbf{x} = \int_{\Phi^{-1}(\mathbf{A})} \mathbf{f}(\mathbf{x}) \, d\mathbf{x}, \quad \text{for all } \mathbf{A} \subset \mathbb{X}, \tag{11}$$

Thermodynamic properties of coupled map lattices

and all probability densities \mathbf{f} . \mathcal{P}_{Φ} is called the Perron-Frobenius operator induced by Φ , and a study of its properties will be the cornerstone of our probabilistic description of deterministic CML's. If the transformation Φ is piecewise diffeomorphic, it is possible to give a more explicit definition of \mathcal{P}_{Φ} by performing a change of variable in the above definition.

Define Π to be a partition of the phase space X which contains $s(\Pi)$ elements denoted $\pi_1, \pi_2, \dots, \pi_{s(\Pi)}$. Let $\Phi_{|i}$ be the monotone restriction of Φ to the set $\pi_i \subset$ X, $i = 1, \dots, s(\Pi)$ (with $\bigcup_{i=1}^{s(\Pi)} \pi_i = X$). Let $\tilde{\pi}_i$ denote the image of the set π_i : $\tilde{\pi}_i \equiv \Phi_{|i}(\pi_i)$. The Perron-Frobenius operator induced by Φ can be written

$$\mathbf{f}_{n+1}(\mathbf{x}) \equiv \mathcal{P}_{\Phi} \mathbf{f}_n(\mathbf{x}) = \sum_{i=1}^{s(\Pi)} \frac{\mathbf{f}_n(\Phi_{|i}^{-1}(\mathbf{x}))}{\mathcal{J}_{\Phi_{|i}}(\Phi_{|i}^{-1}(\mathbf{x}))} \chi_{\bar{\pi}_i}(\mathbf{x}), \tag{12}$$

where $\chi_{\tilde{\pi}_i}(\mathbf{x}) \equiv 1$ iff $\mathbf{x} \in \tilde{\pi}_i$, and 0 otherwise, and $\mathcal{J}_{\tau}(Z)$ is the absolute value of the Jacobian of transformation τ , evaluated at Z. It should be clear from our presentation that the asymptotic properties of the sequence $\{\mathbf{f}_n\}$ of the iterates of an initial density \mathbf{f}_0 under the action of \mathcal{P}_{Φ} determine the thermodynamic behavior of the dynamical system Φ . These asymptotic properties of $\{\mathbf{f}_n\}$ are themselves dependent on the spectral characteristics of the operator \mathcal{P}_{Φ} , and our investigations of CML thermodynamics will in fact focus on the spectral properties of \mathcal{P}_{Φ} .

There have been several attempts to use the Perron-Frobenius operator to describe the dynamics of CML's [32, 33, 42, 77], but these have all concentrated on the properties of an operator acting on one-dimensional densities. The "proper", or complete description is given instead by the N-dimensional operator, and it will be the object of our attention.

Remark 1 The invariant density f_* is implicitly defined by the relation

$$\mathbf{f}_{*} = \mathcal{P}_{\Phi} \mathbf{f}_{*},$$

and it plays a special role in the thermodynamic description of any dynamical system, since it describes the state(s) of thermodynamic equilibrium(ia). Uniqueness of the invariant density implies uniqueness of the state of thermodynamic equilibrium for the system, and the approach of the sequence $\{f_n\}$ to f_* describes the non-equilibrium behavior of the dynamical system.

3.2 The transfer operators $\mathcal{P}_{\Phi_{\text{add}}}$ and $\mathcal{P}_{\Phi_{\text{mul}}}$

When considering stochastic CML's like the ones introduced in Section 1.1.2, an operator governing the evolution of ensemble densities can be defined in analogy with the definition of the Perron-Frobenius operator of the previous section. The main difference in the derivation of this operator is that (11) does not hold since the system is no longer deterministic. This equality must be replaced by one which equates the expectation to be in a given preimage at a time t, with the expectation to be in the image at time t + 1. More precisely, we introduce an arbitrary bounded measurable

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function $h: \mathbb{X} \longrightarrow \mathbb{R}$ which can be written

$$h(\mathbf{x}) = \prod_{i=1}^{N} h^{(i)}(x^{(i)}).$$

The expectation value of $h(\mathbf{x}_{t+1})$ is given by

$$E(\boldsymbol{h}(\mathbf{x}_{t+1})) = \int_{\mathbf{X}} \boldsymbol{h}(\mathbf{x}) \mathbf{f}_{t+1}(\mathbf{x}) \, d\mathbf{x}.$$
 (13)

In the additive noise case, we also have

$$E(h(\mathbf{x}_{t+1})) = E(h(\Phi_{\text{add}}(\mathbf{x}_{t})))$$

= $\int_{\mathbf{X}} \int_{\mathbf{X}} \mathbf{f}_{t}(\mathbf{y}) \prod_{i=1}^{N} h^{(i)}(\Phi^{(i)}(\mathbf{y}) + z^{(i)}) g(z^{(i)}) d\mathbf{z} d\mathbf{y},$ (14)

while in the multiplicative case,

$$E(h(\mathbf{x}_{t+1})) = E(h(\Phi_{mul}(\mathbf{x}_t)))$$

=
$$\int_{\mathbf{X}} \int_{\mathbf{X}} \mathbf{f}_t(\mathbf{y}) \prod_{i=1}^N h^{(i)}(z^{(i)} \Phi^{(i)}(\mathbf{y})) g(z^{(i)}) \, d\mathbf{z} d\mathbf{y}.$$
 (15)

Using (14) and (15) in conjunction with the right hand side of (13), one can obtain the explicit expression for the transfer operators governing the evolution of ensemble densities in CML's perturbed by additive or multiplicative noise. For CML's perturbed as in (5), the expression is [55]:

$$\mathcal{P}_{\Phi_{\mathbf{s}dd}}\mathbf{f}_t(\mathbf{x}) \equiv \mathbf{f}_{t+1}(\mathbf{x}) = \int_{\mathbf{X}} \mathbf{f}_t(\mathbf{y}) \mathbf{g}(\mathbf{x} - \Phi(\mathbf{y})) \, d\mathbf{y}, \quad n = 0, 1, \cdots.$$
(16)

For CML's perturbed as in (6), we have [62]

$$\mathcal{P}_{\Phi_{mul}}\mathbf{f}_t(\mathbf{x}) \equiv \mathbf{f}_{t+1}(\mathbf{x})$$

$$= \int_{\mathbf{x}^{(N)}}^1 \cdots \int_{\mathbf{x}^{(1)}}^1 \mathbf{f}_t(\mathbf{y}) \prod_{i=1}^N \left[g\left(\frac{\mathbf{x}^{(i)}}{\Phi^{(i)}(\mathbf{y})}\right) \frac{1}{\Phi^{(i)}(\mathbf{y})} \right] d\mathbf{y} \qquad (17)$$

It is not difficult to show (cf. [55, 62]) that the operators defined in (16) and (17) are Markov, and defined implicitly by stochastic kernels. [recall that \mathcal{P} is a Markov operator if it is linear, and if for all probability densities f it satisfies (1) $\mathcal{P}f \ge 0$ for $f \ge 0$, (2) $\|\mathcal{P}f\|_{L^1} = \|f\|_{L^1}$].

In Section 5.2, these observations are used to gain insight into the thermodynamic properties of the corresponding CML's. It is useful at this point to recall some basic notions which will be needed as we proceed.

3.3 Ergodicity, mixing and asymptotic periodicity

Here we discuss the behavior of the sequence of densities $\{\mathbf{f}_n\}$ which is intimately linked to the equilibrium and nonequilibrium statistical properties of the CML. For example, \mathcal{T} is ergodic if and only if the sequence is *weak Cesàro convergent* to the invariant density $\mathbf{f}_*(\mathbf{x})$,

$$\lim_{n\to\infty}\frac{1}{n}\sum_{k=0}^{n-1}\int_{\mathbf{X}}\mathbf{f}_k(\mathbf{x})\mathbf{q}(\mathbf{x})\ d\mathbf{x}=\int_{\mathbf{X}}\mathbf{f}_*(\mathbf{x})\mathbf{q}(\mathbf{x})\ d\mathbf{x},\ \text{ for all }\mathbf{q}\in L^\infty(\mathbb{X}),$$

and all initial probability densities $f_0(x)$. A stronger (and more familiar) property, mixing, is equivalent to the *weak convergence* of the sequence to f_* :

$$\lim_{n\to\infty}\int_{\mathbf{X}}\mathbf{f}_n(\mathbf{x})\mathbf{q}(\mathbf{x})\ d\mathbf{x} = \int_{\mathbf{X}}\mathbf{f}_\star(\mathbf{x})\mathbf{q}(\mathbf{x})\ d\mathbf{x}, \ \text{ for all } \mathbf{q}\in L^\infty(\mathbb{X})$$

and all initial probability densities $f_0(\mathbf{x})$. An even stronger type of chaotic behavior, known as *exactness* (or asymptotic stability) is reflected by the *strong convergence* of the sequence $\{\mathbf{f}_n\}$ to the invariant density \mathbf{f}_* :

$$\lim_{n\to\infty} \left\| \mathcal{P}_{\mathcal{T}} \mathbf{f}_n - \mathbf{f}_{\star} \right\|_{L^1} = 0$$

for all initial probability densities $\mathbf{f}_0(\mathbf{x})$. Exactness implies mixing and is interesting from a physical point of view because it is the only one of the properties discussed so far which guarantees the evolution of the thermodynamic entropy of \mathcal{T} to a global maximum, irrespective of the initial condition \mathbf{f}_0 [65].

The hierarchy of chaotic behaviors

$$Exactness \implies Mixing \implies Ergodicity$$

is discussed here because it is shown in Sections 4 and 5.2 that some deterministic and many stochastic CML's are either exact, or possess a another dynamical property, known as *asymptotic periodicity*, of which exactness is a special case.

Asymptotic periodicity is a property of certain Markov operators which ensures that the density sequence $\{f_n\}$ converges strongly to a periodic cycle.

Definition 1 (Asymptotic Periodicity) A Markov operator \mathcal{P} is asymptotically periodic if there exist finitely many distinct probability density functions v_1, \dots, v_r with disjoint supports, a unique permutation γ of the set $\{1, \dots, r\}$ and positive linear continuous functionals $\Gamma_1, \dots, \Gamma_r$, on $L_1(\mathbb{X})$ such that, for almost all initial densities \mathbf{f}_0 ,

$$\lim_{n \to \infty} \left\| \mathcal{P}^n \left(\mathbf{f}_0 - \sum_{i=1}^r \Gamma_i[\mathbf{f}_0] v_i \right) \right\|_{L^1} = 0$$
(18)

$$\mathcal{P}v_i = v_{\gamma(i)}, \quad i = 1, \cdots, r.$$

Clearly, if \mathcal{P} satisfies these conditions with r = 1, it is exact (or asymptotically stable). If r > 1 and the permutation γ is cyclical, asymptotic periodicity also implies

ergodicity [65]. The early papers discussing asymptotically periodic Markov operators are [52, 51, 56, 57, 53]. A somewhat more intuitive presentation is given in [54]. Ξ

Remark 2 The phase space density \mathbf{f}_n of an AP system at any (large) time n is a linear combination of "basis states" (denoted v_i above) with disjoint supports, and at every time step the coefficients (Γ_i) of this linear combination are permuted by γ . Therefore, the density evolution in such systems is periodic, with a period bounded above by r!, but with the exact cycle depending on the initial preparation since the Γ_i 's are functionals of the initial density (*cf.* (18)). A direct consequence of asymptotic periodicity is that the thermodynamic equilibrium of the system consists in a sequence of metastable states which are visited periodically. It was shown in [54] that AP systems are ergodic if and only if the permutation γ is cyclical.

4 Deterministic CML's

As mentioned in Section 2, there are numerous motivations for investigating the dynamics of coupled map lattices. When these dynamics are temporally and/or spatially chaotic, it is natural to turn to a probabilistic description in terms of the Perron-Frobenius operator. For example, there is now ample evidence [67, 60] that CML's can possess different phases which correspond to qualitatively different behavior of statistical averages, and it is legitimate to try and understand the connection between the presence of these different phases and the properties of the Perron-Frobenius operator. Before proceeding with the analysis, it is instructive to numerically illustrate this multi-phase phenomenology in a relatively simple toy model.

Consider a lattice of the form (2) with $S : [0:1] \mapsto [0:1]$ given by the tent map $S(z) = \min(az, a(1-z))$, and with p = 4 (to mimick diffusive coupling in two spatial dimensions). As the slope of the local transformation is varied in the interval (1,2], for fixed $\varepsilon \in [0,1]$, one observes a sequence of "bifurcations": on both sides of the bifurcation point, the lattice evolves chaotically in time, but the number of "bands", or simply connected subsets of [0,1] on which the activity of a site is supported, changes abruptly. This behavior is observed in the single tent map, where it can be shown to reflect a change in the degeneracy of the Perron-Frobenius operator's eigenvalues of unit modulus (*i.e.* a change in r in (18); for a detailed discussion see [79, 106]). The extension of these results for one-dimensional maps to lattices with arbitrarily large numbers of elements has proven to be a major theoretical challenge, which has only been met in rather small regions of parameter space.

4.1 Phenomenology of the tent CML

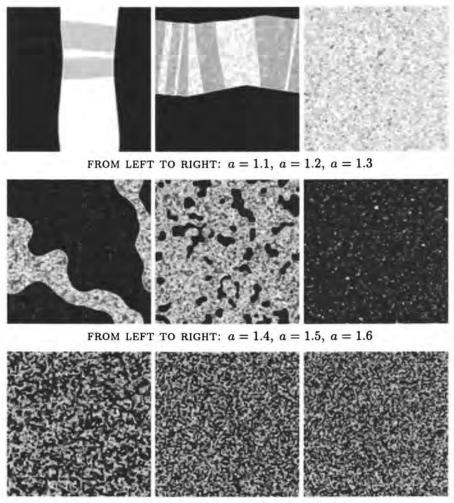
Here we focus on the model (2) with local map defined by either the tent map, defined in the previous paragraph. For the tent map lattice two qualitatively different types of statistical behavior are evidenced in Figure 2. The first is characterized by the evolution of large scale patterns from the random initial conditions; this is the clustered, or ordered state $a = 1.1, \dots, 1.5$. The panel a = 1.3 presents an interesting

limiting case for which the "cluster" covers the entire area of the lattice; different initial conditions for such parameter values evolve to the more usual large scale patterns. Note that the lattices are not at equilibrium in the panels displayed in this figure. It is not possible to observe the true equilibrium because of the astronomically large transients typical of a lattice of 40000 elements. The point of our investigation is not to describe explicitly the presence, stability and asymptotic behavior of the patterns presented here, but to understand how the thermodynamics of these lattices should be investigated. Although the problem of pattern formation in CML's is fascinating, it is not the focus of our investigation, and we will therefore not spend more time discussing the pattern dynamics *per se*. The interesting observation from our point of view is that the pattern-forming behavior associated with small values of *a* is also accompanied by statistical cycling in the lattice. This is illustrated by the behavior of various statistical quantifiers of the motion discussed below, rather than by the snapshots of Figure 2.

The second phase is described statistically by a unique invariant measure generated by almost all initial conditions. This corresponds to the spatiotemporally chaotic state described rigorously by Bunimovich and Sinai [9] in infinite lattices.

Before proceeding, we should note that this oscillatory behavior of macroscopic observable has also been observed in lattices of logistic maps, as well as in more complex, biologically motivated models [63]. In fact, in the recent literature [76, 14], this behavior has been referred to as *periodic collective behavior*, and understanding its origin in various spatially extended models is an on-going endeavour.

We propose as a possible mechanism that the Perron-Frobenius operator induced by lattices such as the tent CML in the statistically periodic regime are in fact asymptotically periodic and possess the cyclical spectral decomposition (18). At present, proving this statement is only possible in very limited cases, namely, in lattices perturbed by noise (as in Section 5), and in lattices of piecewise linear, expanding maps (see the contribution of Keller in this issue for more on this topic). Nevertheless, this working hypothesis is interesting because it provides some insight into the dynamics underlying periodic collective behavior (cf the last paragraph of the next section).



FROM LEFT TO RIGHT: a = 1.7, a = 1.8, a = 1.9

FIGURE 2:

Snapshots of the activity at the surface of a 200×200 lattice of diffusively coupled tent maps when the coupling is constant ($\varepsilon = 0.45$) but the local slope is increased from a = 1.1 to a = 1.9. For all panels, the transient discarded is of length 10^5 . The 256 grey scales range from black when $x^{i,j} = x_{min}$ to white when $x^{i,j} = x_{max}$ where x_{min} and x_{max} are the lower and upper bounds of the attracting subinterval of [0, 1] respectively. The initial values on the lattice were in all cases given by a random number generator yielding uniform distributions on the unit interval. The transition from statistical cycling to statistical equilibrium occurs between a = 1.5 and a = 1.6for this value of the coupling. This observation is not made from Figure 2 but with the help of other the statistical quantifiers (cf. Figure 3 for example).

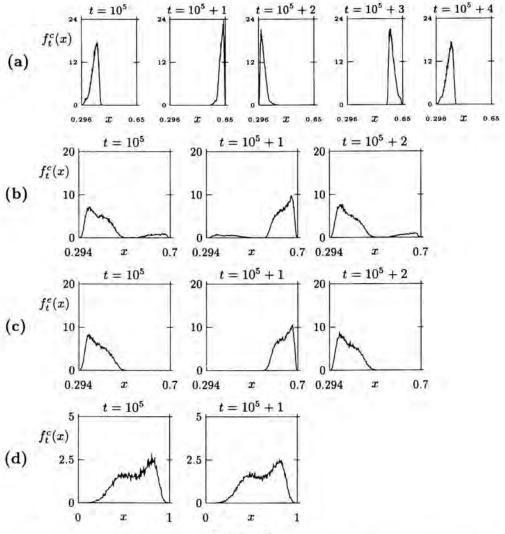


FIGURE 3:

The collapsed density f_t^c for a 200 × 200 lattice of diffusively coupled tent maps with $\varepsilon = 0.45$. The first 10^5 iterations were discarded as transients. In a) the cycle is of period 4, and a = 1.3. The initial density was uniformly distributed on [0.3:0.4]. In b) the cycle is of period 2, a = 1.4 and the initial density was uniformly distributed on [0:1]. In c), the parameters are as in b) but the initial density was supported on [0.39:0.43]. This illustrates the dependence of the density cycle on the initial density. d) the slope of the map is a = 1.99 and the initial density is uniform on [0:1]. This density is numerically reached for all densities.

4.2 Discussion

Until now, most attempts at constructing the statistical mechanics of high dimensional chaotic dynamical systems have followed two broad and intersecting paths. One is the extension of the so-called thermodynamic formalism of Ruelle [83], Bowen [5] and Sinai [86] to high dimensional hyperbolic dynamical systems, which has led to various proofs of existence of Gibbs measures describing spatio-temporal chaos in such models [9]. The other is an operator-theoretic approach which focuses on the Perron-Frobenius operator (11) as an operator acting on some suitably defined function space [6, 50]. The kinds of results that are sought are again the existence and uniqueness of invariant measures which are associated with fixed points of the Perron-Frobenius equation, and the properties of the system's relaxation to equilibrium when it is started out of equilibrium. Given that the Perron-Frobenius operator is a Markov operator, this information is given by its spectral properties. Obviously, these depend on the function space on which \mathcal{P}_{Φ} operates. We always consider here \mathcal{P}_{Φ} acting either on $L^1(\mathbb{X})$ ($\mathbb{X} \subset \mathbb{R}^n$), or on a subspace of $L^1(\mathbb{X})$. So far most investigations have actually focused on Banach spaces "properly" embedded in $L^1(\mathbb{X})$, where "properly" means here that one can then apply a now-famous theorem of Ionescu-Tulcea and Marinescu [94] to study the spectral properties of \mathcal{P}_{Φ} acting on the embedded space. Examples of such spaces are BV(X), the space of functions of bounded variation (discussed in some detail in Chapter 5 of [16]), and the related $GH(\mathbb{X})$, the space of Generalized Hölder continuous functions (described in [64]).

If this second approach is followed, the objective is to place conditions on the parameters of the CML such that the conditions of the Ionescu-Tulcea and Marinescu theorem are satisfied. If one considers $\mathcal{P}_{\Phi} : BV(\mathbb{X}) \longmapsto BV(\mathbb{X})$, then it is possible to obtain conditions on the parameters of an expanding Φ such that \mathcal{P}_{Φ} satisfies (18) (see for example [28, 50, 61]). The weakness of this approach is that the conditions are usually extremely complicated, and they require very detailed geometrical knowledge of the transformation Φ (for example one needs to know a lot about the geometry of sets on which Φ is strictly monotone).

For a description of the operator-theoretic approach, and a discussion of its applications and limitations, the interested reader is referred to the contribution of Keller (this issue). One important step in this theoretical analysis is that the CML's which can be studied effectively with this operator-theoretic approach are product dynamical systems, which are close, in some clearly defined sense, to a direct product of independent low dimensional dynamical subsystems. This indicates that CML's which display periodic collective behavior, far from "synchronizing" in some loosely defined, and poorly understood manner, in fact *desynchronize* into a collection of statistically independent "clusters", each containing a few degrees of freedom. If this hypothesis holds, the statistical properties of a single CML's trajectory then approximate the ensemble properties of those low dimensional clusters. This in turn motivates the analysis of the cluster's Perron-Frobenius operator. The programme outlined in this paragraph, which is a direct consequence of the "cluster working hypothesis" is the subject of ongoing research [59].

We now turn our attention to the probabilistic description of CML's whose evo-

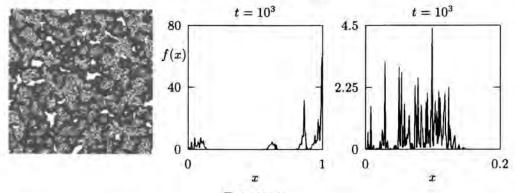
lution is stochastically perturbed.

5 The statistics of stochastic CML's

The transfer operators for the stochastic CML's (5) and (6) were introduced in Section 3.2. The study of these operators is greatly simplified by the observation that they are Markov operators defined by stochastic kernels [54]. Before proceeding to their analysis, we will briefly describe some of the observed phenomenology in models like (5) and (6), since these are less frequently described than their deterministic counterparts in the literature.

5.1 Some numerical observations

Here we focus on the effects of additive noise on a piecewise linear toy model originally introduced by Keener [49]. The purpose is not to give an overview of the effects of stochastic perturbations on the dynamics of CML's, but to illustrate with a simple example that sometimes the presence of a little noise can have dramatic consequences which can, at first glance, seem rather counterintuitive.





Left: Grey scale representation of the state of a 200×200 lattice of diffusively coupled Keener maps without noise, at time $t = 10^3$ with a = 0.5, b = 0.571 and $\varepsilon = 0.45$. The 256-level grey scale is such that if $x_{10^3}^{(kl)} = 0$, it is represented by a black pixel, while if $x_{10^3}^{(kl)} = 1$ it is represented by a white pixel. Center panel: 200-bin histogram of the state of the lattice displayed on the left panel. The fractal nature of the support of this distribution is suggested by the right panel, which was obtained from a larger lattice (10^6 sites) and a larger number of bins on [0, 1] (10^3).

The example considered here is a perturbation of a two-dimensional lattice of diffusively coupled "Keener maps"

$$\begin{aligned} x_{t+1}^{(i,j)} &= (1-\varepsilon)S(x_t^{(i,j)}) + \frac{\varepsilon}{4} \left[S(x_t^{(i+1,j)}) + S(x_t^{(i-1,j)}) + S(x_t^{(i,j+1)}) + S(x_t^{(i,j-1)}) \right], \end{aligned}$$
(19)

where the local map (a slight generalization of the r-adic map) was considered by Keener [49]

$$S(z) = (az + b) \mod 1, \quad a, b \in (0, 1), \quad x \in [0, 1].$$
(20)

Before considering the dynamics of the lattice, it is useful to recall some basic properties of the single map. There exists a range of values for the parameters a and b such that the trajectories are chaotic in the sense that they attracted to a subset of [0, 1]of zero measure (a Cantor set) [49]. Numerically, this is reflected by the fact that if the histogram along a trajectory is constructed, the number of histogram peaks will increase as the bin size decreases. In this case, the Perron Frobenius operator does not possess a fixed point in the space of probability densities. In fact, it asymptotically transforms almost all initial probability densities into generalized functions. A rigorous treatment of such operators is possible, and studying the nonequilibrium statistical properties of the corresponding CML's involves the reformulation of the problem in terms of the evolution of measures. Figure 4 shows that the fractal nature of the attractor of the single map survives diffusive coupling.

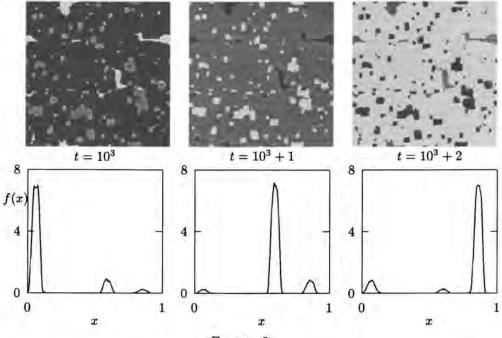


FIGURE 5:

Noise induced statistical cycling in a lattice of 200×200 noisy "Keener maps" (21), with a = 0.5, b = 0.571, $\varepsilon = 0.1$ and ξ uniformly supported on [0, 0.05]. The top panels display three successive iterations, and the bottom panels display the corresponding histograms (produced with 200 bins). The grey scale for the top row is the same as in Figure 4.

This picture is greatly simplified when the local transformation is replaced by

$$S_{\xi}(z) = (az + b + \xi) \mod 1 , \quad a, b \in (0, 1), \quad x \in [0, 1]$$
(21)

where ξ is a random variable distributed with density g. Figure 5 displays the remarkable behavior of the lattice (19) when the map S is replaced by S_{ξ} . Note that the noise present in (21) is multiplicative. The activity of the lattice no longer seems to be supported on a set of measure zero, and furthermore, it appears that the evolution of the histogram of activity on the lattice is periodic with period 3. To understand the origin of this simplification of the dynamics as a result of stochastic perturbations, one must focus on the properties of the transfer operators defined in Section 3.2.

5.2 Analytic results

In this section it is shown that under rather general circumstances, the transfer operators induced by stochastic coupled map lattices are asymptotically periodic.

5.2.1 Additive noise

Consider the CML (5), for which the density of the noisy perturbation satisfies

$$\mathbf{g}(\boldsymbol{\xi}) = \prod_{i=1}^{N} \chi_{[b,c]}(\boldsymbol{\xi}^{(i)}), \quad 0 \le b < c \le 1,$$
(22)

where the indicator function χ is defined by $\chi_{[b,c]}(x) = (c-b)^{-1}$ if $x \in [b,c]$ and $\chi_{[b,c]}(x) = 0$ otherwise. This form for g is chosen here to simplify the statement of the proof of Theorem 1 below, but more general forms can be treated in exactly the same way.

Theorem 1 If the CML Φ_{add} is written in the form (5), where the density of the perturbation $\boldsymbol{\xi}$ is given by (22), and the local map S of (3) is bounded and nonsingular then $\mathcal{P}_{\Phi_{add}}$ defined by (16) is asymptotically periodic.

The proof consists in showing that $\mathcal{P}_{\Phi_{add}}$ is a Markov operator defined by a stochastic Kernel which satisfies the conditions of theorem 5.7.2 of [55]. It is discussed in [62]. This is a general result. The two main assumptions which are necessary for its derivation are that S be nonsingular and bounded. This generic nature of the result explains the ubiquitous presence of statistical cycling which has been reported in stochastic CML's elsewhere [62].

5.2.2 Multiplicative noise

Here the transformation Φ_{mul} is given by (6). In this section it is proved that multiplicative noise induces the spectral decomposition (18) in a large class of CML's. Our presentation is inspired by the treatment of one-dimensional maps perturbed by parametric noise given by Horbacz [31].

Theorem 2 Let $\mathbf{K} : \mathbb{X} \times \mathbb{X} \longrightarrow \mathbb{R}$ be a stochastic kernel and \mathcal{P} be the Markov operator defined by

$$\mathcal{P}\mathbf{f}(\mathbf{x}) = \int_{\mathbf{x}^{(N)}}^{1} \cdots \int_{\mathbf{x}^{(1)}}^{1} \mathbf{K}(\mathbf{x}, \mathbf{y}) \mathbf{f}(\mathbf{y}) \, d\mathbf{y}.$$
 (23)

Assume that there is a nonnegative $\lambda < 1$ such that for every bounded $\mathbb{B} \subset \mathbb{X}$ there is a $\delta = \delta(\mathbb{B}) > 0$ for which

$$\int_{\mathbf{A}} \mathbf{K}(\mathbf{x}, \mathbf{y}) \, d\mathbf{x} \leq \lambda \quad \text{for } \mu(\mathbb{A}) < \delta, \quad y \in \mathbb{B}, \quad \mathbb{A} \subset \mathbb{B}.$$
(24)

Assume further there exists a Lyapunov function $V: \mathbb{X} \longmapsto \mathbb{R}$ such that

$$\int_{\mathbf{X}} V(\mathbf{x}) \mathcal{P} \mathbf{f}(\mathbf{x}) \, d\mathbf{x} \le \alpha \int_{\mathbf{X}} V(\mathbf{x}) \mathbf{f}(\mathbf{x}) \, d\mathbf{x} + \beta, \ \alpha \in [0, 1), \ \beta > 0$$
(25)

for every density **f**. Then \mathcal{P} is asymptotically periodic, and therefore admits the representation (18). [Recall that a nonnegative function $V : \mathbb{X} \mapsto \mathbb{R}$ is known as a Lyapunov function if it satisfies $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$.]

The proof of the theorem is based on demonstrating that the operator defined by (23) is *contractive*. This property, in turn, was shown by Komorník [51] to imply asymptotic periodicity. The complete proof is given in [62].

The connection with stochastic CML's of the form (6) should now be clear: the operator $\mathcal{P}_{\Phi_{\text{mul}}}$ can easily be shown to satisfy the conditions of Theorem 2 under rather general circumstances. More precisely, we have the following corollary:

Corollary 1 A CML of the form (6), perturbed by the noise term $\boldsymbol{\xi}_t$ distributed with density (4) will induce a transfer operator $\mathcal{P}_{\Phi_{mul}}$ defined by (17). If the deterministic part of the transformation (denoted Φ) is bounded and nonsingular, then $\mathcal{P}_{\Phi_{mul}}$ is asymptotically periodic.

In light of this result, we can interpret the statistical cycling displayed in Figure 5 as an illustration of the cyclical spectral decomposition (18) of the transfer operator $\mathcal{P}_{\Phi_{mul}}$. In addition, the presence of asymptotic periodicity in this model, and in the large class of models which satisfy the conditions of Theorem 1 or Corollary 1, has some interesting applications for the construction of statistical mechanics for these models. Before exploring these, we briefly note that the results presented in this section do not allow us to predict the periodicity observed numerically in the evolution of histograms of activity (cf. Figure 5). The periodicity of these density cycles stems from stable period 3 orbits of the isolated Keener maps for certain values of the parameters (cf [80] for details).

6 Conclusion

This chapter has described the statistical dynamics of CML's by focusing on the properties of the transfer operators induced by these models. For deterministic CML's, the spectral characteristics of the Perron-Frobenius operator are investigated using some well-known bounded-variation techniques. When the CML's are perturbed by noise, the transfer operators are Markov and defined by stochastic kernels. This allows us to treat them using some basic results of the theory of Markov operators, and we show that in many cases of interest they are asymptotically periodic.

Thermodynamic properties of coupled map lattices

Asymptotic periodicity is an intriguing dynamical property which has several important implications for the construction of statistical mechanics for these high dimensional dynamical systems. The first one is that when the period of the density cycle in (18) is greater than one, the asymptotic ensemble statistics of the CML depend on the initial ensemble. This is due to the dependence of the functionals Γ_i on f_0 in (18), and it generalizes the usual dependence of trajectory dynamics on the initial conditions, to the evolution of ensemble probability densities. Another consequence of the presence of AP is the possible presence of phase transitions in the system: If the period of a density cycle changes as a control parameter is tuned, then the model undergoes a qualitative change in the behavior of its statistical quantifiers.

More importantly, some of the usual misconceptions concerning the true meaning of ergodicity are exacerbated when supposed consequences of ergodicity are violated by systems which turn out to be asymptotically periodic. Observations of the coherent behavior of globally coupled and some locally coupled CML's reported by Kaneko [43, 44] and Perez et al. [76] have led to a controversy in the recent literature concerning an apparent violation of the law of large numbers in these models. In fact, since the law of large numbers is a theorem, it cannot be violated, but its verification for CML's must performed with care. As explained by Pikovsky and Kurths [77], it is important when considering this law for ergodic systems which are non mixing, to compute the relevant averages with respect to ensemble densities, and not with respect to densities constructed from trajectories. Even if a system is ergodic, the two constructions will not in general be equivalent when it comes to verifying the law of large numbers. This is because the type of convergence to equilibrium guaranteed by ergodicity (cf. Section 3.3) is not strong enough to imply the equality of the two types of averages (trajectory vs. ensemble) when the system is started out of equilibrium. In most circumstances this would seem like a technical mathematical objection, not of great relevance to the practicing physicist, because one would nevertheless expect the system to relax to a state described by the invariant density. But if it is asymptotically periodic, a system will almost surely not converge to equilibrium, and in that case, the verification of the law of large numbers must necessarily be performed with ensemble densities.

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Coupled map lattices via transfer operators on functions of bounded variation

Gerhard Keller

Abstract

We describe the transfer operator approach to coupled map lattices (CML) in cases where the local map is expanding but has no Markov partition (e.g. a general tent map). The coupling is allowed to be non-local, but the total influence of all sites $j \neq i$ on site *i* must be small. The main technical tool are lattice-size independent estimates of Lasota-Yorke type which show that the transfer (Perron-Frobenius) operator of the coupled system is quasicompact as an operator on the space of functions of bounded variation.

1 Introduction

The purpose of this note is to summarize results from [11] and from the unpublished thesis [12]. Let L be a finite or countable index set, e.g. $L = \mathbb{Z}$ or $L = \mathbb{Z} \setminus d\mathbb{Z}$. We investigate time-discrete dynamics on the state space $X = [0,1]^L$ that are composed of independent chaotic actions on each component [0,1] of X followed by some weak interaction that does not destroy the chaotic character of the whole system. More specifically, let $\tau : [0,1] \to [0,1]$ be monotone and C^2 on each component of $[0,1] \setminus$ $\{\zeta_0 = 0, \zeta_1, \ldots, \zeta_{N-1}, \zeta_N = 1\}$. We assume that $\tau''/(\tau')^2$ is bounded and that τ satisfies the following combined expansion and regularity assumption:

There are $M \in \mathbb{N}$ and $\kappa_M > 2$ such that $|(\tau^M)'| \ge \kappa_M$ and such that

$$\tau^{m}(0), \tau^{m}(\zeta_{1}\pm), \dots, \tau^{m}(\zeta_{N-1}\pm), \tau^{m}(1) \notin \{\zeta_{1}, \dots, \zeta_{N-1}\}$$
(1)

for m = 0, ..., M - 1.

Now a map $S_0: X \to X$ describing the uncoupled dynamics is defined by $(S_0x)_i = \tau(x_i)$ $(i \in L)$ and coupled maps $S_{\epsilon} := \Phi_{\epsilon} \circ S_0$ are introduced using appropriate continuous couplings $\Phi_{\epsilon}: X \to X$ close to the identity on X. The regularity assumption in (1) is unavoidable if a weakly coupled system S_{ϵ} is to behave like a small perturbation of S_0 , because weak couplings affect each individual map τ like a small perturbation, and it is known that in the absence of the above assumption arbitrarily small perturbations can change the dynamics of τ completely, see the examples in [9] and [1].

In the sequel we consider C^2 -couplings $\Phi_{\epsilon}(x) = x + A_{\epsilon}(x)$, and we call Φ_{ϵ} an (a_1, a_2) -coupling, if a_1, a_2 are positive constants such that

$$|A_{\epsilon}|_{\infty} \leq \epsilon, \quad \|DA_{\epsilon}\|_{\infty} \leq a_{1}\epsilon, \quad \|D_{i}DA_{\epsilon}\|_{\infty} \leq a_{2}\epsilon.$$

$$(2)$$

Here D denotes the total derivative, D_i the partial derivative with respect to x_i , $| \cdot |_{\infty}$ the maximum-norm for vectors, and $|| \cdot ||_{\infty}$ the corresponding operator norm for matrices (maximal row sum). The main result is:

Theorem 1 [11, 12] Given a local map τ satisfying (1) and $a_1, a_2 > 0$ there exists $\epsilon_{\max} > 0$ such that for each $\epsilon \in [0, \epsilon_{\max}]$ the following holds:

- If L is finite and if Φ_{ϵ} is an (a_1, a_2) -coupling, then the coupled system S_{ϵ} has an invariant probability density h_{ϵ} .
- If $L = \mathbb{Z}^r$ and if Φ_{ϵ} is a shift-invariant (a_1, a_2) -coupling, then the coupled system S_{ϵ} has an invariant probability measure whose finite-dimensional marginals are absolutely continuous with respect to Lebesgue measure.

Remarks: a) The proof of this theorem relies on a spectral analysis of the transfer operator associated with S_{ϵ} . Details are provided in the next sections.

b) Φ_{ϵ} is called shift-invariant if $\Phi_{\epsilon} \circ \sigma = \sigma \circ \Phi_{\epsilon}$ for each shift σ on $X = [0, 1]^{\mathbb{Z}^{r}}$.

c) For the tent map $\tau(\xi) = a \cdot (1 - |2\xi - 1|)$ with constant couplings $\Phi_{\epsilon}(x) = x + \epsilon B x$ where B is a $L \times L$ -matrix with $||B||_{\infty} = 2$ and $\sum_{j \in L} b_{ij} = 0$ for each row i, Künzle [12] estimates ϵ_{\max} as follows:

If a = 0.9, then M = 2, $\kappa_M = 3.24$ and $\epsilon_{\max} \ge 0.035$.

If a = 0.7, then M = 3, $\kappa_M = 2.744$ and $\epsilon_{\max} \ge 0.0029$.

d) In [11] two additional assumptions were made: The most important one was $|\tau'| > 2$ (*i.e.* M = 1 in assumption (1)), which excludes *e.g.* tent maps. The other one concerned only infinite lattices $L = \mathbb{Z}^r$: It was required that the couplings have finite range, *i.e.* that there is a constant w > 0 such that $(DA_{\epsilon})_{ij} = 0$ if |i-j| > w. Both restrictions are removed in [12].

2 Functions of bounded variation

2.1 Finite lattices

The variation of a C^1 -function $f:[0,1] \to \mathbb{R}$ can be defined as

$$ext{var}\,(f) = \int_0^1 |f'(\xi)|\,d\xi\,\,.$$

Approximating this integral by Riemann sums yields the more common expression var $(f) = \sup\{\sum_{i=1}^{r} |f(\xi_i) - f(\xi_{i-1})|\}$ where the supremum extends over all finite partitions $\xi_0 < \xi_1 < \ldots < \xi_r$ of [0, 1]. More important for our purposes is a third characterization which is a consequence of the integration by parts formula: Let $\mathcal{T} := \{\varphi \in C^1([0, 1]) : \varphi(0) = \varphi(1) = 0, |\varphi| \leq 1\}$ be the set of C^1 -test functions bounded by 1. Then

$$\mathrm{var}\left(f
ight) = \sup_{arphi \in \mathcal{T}} \int_{0}^{1} f'(\xi) arphi(\xi) \, d\xi = \sup_{arphi \in \mathcal{T}} \int_{0}^{1} f(\xi) arphi'(\xi) \, d\xi \, \, .$$

Just as the previous one this characterization can be used for defining the variation of any measurable function (and not merely that of C^1 -functions). Besides that it has

an immediate extension to functions of several variables: For $U \subseteq \mathbb{R}^d$ open and $f \in C^1(U; \mathbb{R})$ define

$$\operatorname{var}_{U}(f) := \frac{1}{d} \int_{U} |Df(x)|_{1} \, dx = \frac{1}{d} \sum_{j=1}^{d} \int_{U} |D_{j}f(x)| \, dx \, . \tag{3}$$

 $(| . |_1 \text{ denotes the sum-norm of the row vector } Df.)$ Let

$$\mathcal{T} := \{ \varphi \in C^1(U; \mathbb{R}) : \varphi_{|\partial U} = 0, |\varphi| \le 1 \} .$$

As in the 1-dimensional case $\operatorname{var}_U(f)$ can be equivalently characterized as

$$\operatorname{var}_{U}(f) = \frac{1}{d} \sup \left\{ \int_{U} f(x) \operatorname{div}\varphi(x) \, dx : \varphi = (\varphi_{1}, \dots, \varphi_{d})^{t}, \varphi_{j} \in \mathcal{T} \right\}$$
(4)
$$= \frac{1}{d} \sum_{j=1}^{d} \sup_{\varphi \in \mathcal{T}} \int_{U} f(x) D_{j}\varphi(x) \, dx ,$$

and again this yields a definition of variation applicable to each measurable $f: U \to \mathbb{R}$.

An immediate consequence of (4) is that $\operatorname{var}_U(f) = \operatorname{var}_U(g)$ if f = g Lebesgue a.e. Therefore (4) can be used as a definition of variation for equivalence classes of measurable functions, and we can define the space of functions of bounded variation on U

$$BV(U) := \{f \in L^1(U) : \operatorname{var}_U(f) < \infty\}.$$

Let $||f||_{BV} := \operatorname{var}_U(f) + ||f||_{L^1}$. Then

 $(BV(U), \| . \|_{BV})$ is a Banach space, and if U is bounded with "piecewise smooth" boundary, then the unit ball of $(BV(U), \| . \|_{BV})$ is a compact subset (5) of $(L^1(U), \| . \|_{L^1})$. (This is true in particular for open rectangles in \mathbb{R}^d .)

This and further properties of functions of bounded variation can be found in [7] and [16].

Remarks: a) Our notion of variation is not invariant under isometries Ψ of \mathbb{R}^d , i.e. $\operatorname{var}_U(f \circ \Psi)$ and $\operatorname{var}_{\Psi U}(f)$ do not necessarily coincide. This invariance can be achieved by using the euclidean 2-norm of the gradient instead of the 1-norm in (3). Later we refer to this as "euclidean variation". Indeed, several basic results in [11] are derived for general *p*-norm variations. Of course, BV-norms based on different *p*-norms are equivalent, but constants appearing in various estimates are different, and they are crucial for the application we envisage.

b) Usually the variation is not normalized by $\frac{1}{d}$. This is unessential for fixed d but rather convenient for the asymptotics $d \to \infty$ we have in mind.

If, in the context of coupled map lattices, $X = [0,1]^L$ with some finite index set L, we write $\operatorname{var}^L(f)$ instead of $\operatorname{var}_{(0,1)^L}(f)$. The importance of $\operatorname{BV}(X)$ is that it contains the invariant probability densities h_{ϵ} from Theorem 1.

2.2 Infinite lattices

If the index set L is countable, it is not so obvious how to generalize the idea that an invariant probability measure for S_{ϵ} should have a "density" f of bounded variation. Indeed, each generalization that requires f to be a function in the strict sense is useless for our purposes: Suppose that $L = \mathbb{Z}$ and that τ has a unique absolutely continuous invariant probability measure ν that is mixing (this is the case e.g. for the tent map with $a > \frac{1}{\sqrt{2}}$). If μ is an invariant probability measure for the uncoupled system S_0 and if μ has absolutely continuous finite-dimensional marginals, then μ is necessarily the infinite product measure ν^L . Hence μ is absolutely continuous with respect to the infinite product Lebesgue measure λ^L on X if and only if $\mu = \lambda^L$, *i.e.* if ν itself is Lebesgue measure on [0, 1]. More generally, as λ^L is ergodic under the shift transformation, there is no other shift-invariant probability measure absolutely continuous with respect to λ^L on X. But for a shift-invariant coupling Φ_{ϵ} this is just the class of measures in which we hope to find S_{ϵ} -invariant ones.

Therefore we look at those (signed) measures μ on X whose finite-dimensional marginals μ_J are absolutely continuous with a density f_J of bounded variation. (Here $J \subset L$ is finite and μ_J is the projection of μ to a measure on $[0, 1]^J$.) Denote by $|\mu|(X)$ the total variation of μ , i.e. the sum of the masses of the positive and the negative part of μ .¹ It is proved in [11, Lemma 2.4] that

$$\int |f_J(x)| \, dx \nearrow |\mu|(X) \quad \text{for } J \nearrow X \; . \tag{6}$$

So it makes sense to think about a signed measure μ on X with absolutely continuous marginals as a projective family $f = (f_J)_{J \in \mathcal{F}(L)}$ of marginal densities where $\mathcal{F}(L)$ is the collection of all finite subsets of L. We denote the space of these families f by $L^1(X)$ and remark that $L^1(X)$ is a closed linear subspace of the space of all signed Borel measures on X equipped with the total variation norm. The variation of $f \in L^1(X)$ is now defined naturally as

$$\operatorname{var}(f) := \sup \{ \operatorname{var}^J(f_J) : J \in \mathcal{F}(L) \} .$$

Remark: If $L = \mathbb{Z}^r$, if μ is a shift-invariant measure on X and if $J_1 \subset J_2 \subset \ldots \subset L$ is an increasing sequence of cubes centered at 0, then $\operatorname{var}^{J_1}(f_{J_1}) \leq \operatorname{var}^{J_2}(f_{J_2}) \leq \ldots$, see [12, Lemma 3.6].

Let $BV(X) := \{f \in L^1(X) : var(f) < \infty\}$ and define $||f||_{BV} := var(f) + ||f||_{L^1}$ for $f \in BV(X)$, where $||f||_{L^1} := \sup_{J \in \mathcal{F}(L)} ||f_J||_{L^1}$ is just the total variation of the measure represented by f, see (6). It is not hard to prove that $(BV(X), || \cdot ||_{BV})$ is a Banach space, but in contrast to the finite-dimensional situation (5) the unit ball of $(BV(X), || \cdot ||_{BV})$ is not a compact subset of $(L^1(X), || \cdot ||_{L^1})$. Therefore the spectral arguments developed in the next section for finite lattices do not carry over to infinite lattices. There is however a weaker type of compactness which still allows to find invariant measures in BV(X): Define a family of seminorms on L^1 by

¹I apologize for the two distinct meanings of the word "variation" which just reflect common usage.

Coupled map lattices via transfer operators on functions of bounded

 $||f||_J := ||f_J||_{L^1}$ $(J \in \mathcal{F}(L))$. These seminorms define a locally convex topology on $L^1(X)$, and using (5) one proves [11, Theorem 2.5]:

The unit ball of $(BV(X), \| \cdot \|_{BV})$ is compact in $(L^1(X), \{\| \cdot \|_J\}_{J \in \mathcal{F}(L)})$. (7)

3 Transfer operators

3.1 Finite lattices

The map $S_{\epsilon}: X \to X$ induces a transformation S_{ϵ}^{*} on the set of all signed measures ν on X by $S_{\epsilon}^{*}\nu = \nu \circ S_{\epsilon}^{-1}$. If L is finite, S_{ϵ}^{*} transforms absolutely continuous measures into absolutely continuous ones as long as $\epsilon < a_{1}^{-1}$ because S_{ϵ} is nonsingular, see (2). Therefore we may interpret S_{ϵ}^{*} as an operator on $L^{1}(X)$ transforming densities to densities. This is just the well known transfer operator, defined explicitly by

$$S_{\epsilon}^{*}f = \sum_{Z \in \mathbb{Z}_{\epsilon}^{1}} \left(\frac{f}{|\det DS_{\epsilon}|} \circ S_{\epsilon|Z}^{-1} \right) \cdot 1_{S_{\epsilon}Z}$$

where Z_{ϵ}^{n} denotes for each $n \geq 1$ the partition of X into pieces on which S_{ϵ}^{n} is C^{2} . As $S_{\epsilon} = \Phi_{\epsilon} \circ S_{0}$ we have $Z_{\epsilon}^{1} = Z_{0}^{1}$ is a rectangular partition, namely the |L|-fold direct product of the monotonicity partition of τ . Observe however that this is not true for n > 1.

We want to argue that S_{ϵ}^{*} leaves actually the space BV(X) invariant. More precisely: Given τ and a_1, a_2 as in Theorem 1, there are constants $C_1, C_2 > 0$ and $\epsilon_0 > 0$ such that for each $\epsilon \in [0, \epsilon_0]$ and for each $f \in BV(X)$ holds

$$\operatorname{var}\left(S_{\epsilon}^{*}f\right) \leq \left(\frac{2}{\kappa_{1}} + C_{1}\epsilon\right) \cdot \operatorname{var}\left(f\right) + C_{2} \cdot \|f\|_{L^{1}} .$$

$$(8)$$

(Here as in the sequel we write var (f) instead of var ${}^{L}(f)$.) This type of inequality was first derived for piecewise expanding maps like τ in [13]. Generalizations to higher dimensional maps are numerous, see e.g. [10, 2, 3]. As these approaches use euclidean variation or some variant of it, they do not yield dimension independent constants C_1, C_2 if applied to coupled map lattices. (This will be explained later.) There is a slightly different notion of variation introduced in [1] which leads to similar conclusions as the ones discussed here.

If the constants κ_1 and C_1 are such that $\alpha := (\frac{2}{\kappa_1} + C_1\epsilon) < 1$, a simple inductive argument shows that $\limsup_{n\to\infty} \operatorname{var}((S_{\epsilon}^*)^n f) \leq \frac{C_2}{1-\alpha}$ for each probability density $f \in$ $\operatorname{BV}(X)$, and because of the compact embedding property (5) the Kakutani/Yoshida theorem yields the L^1 -convergence of the sequence $(\frac{1}{n}\sum_{k=0}^{n-1}(S_{\epsilon}^*)^k f)_{n>0}$ to an S_{ϵ} invariant probability density (cf. [13]) thus proving the first part of Theorem 1. But even more is true. The Ionescu-Tulcea/Marinescu theorem can be applied and results in the following **Theorem 2** There is $\epsilon_{\max} > 0$ independent of L such that for each $\epsilon \in [0, \epsilon_{\max}]$ holds: The transfer operator S_{ϵ}^* , canonically extended to the complexification of BV(X), has a spectral decomposition

$$(S_{\epsilon}^{\star})^n = \sum_{i=1}^p \lambda_i^n P_i + (S_{\epsilon}^{\star})^n \circ P$$

where $\lambda_1 = 1$, $|\lambda_i| = 1$ (i = 1, ..., p) and where P and the P_i are mutually orthogonal finite-dimensional projections commuting with S^* and such that $P + \sum_i P_i = \text{Id}$. Furthermore there are M > 0 and $q \in (0, 1)$ such that

$$\|(S^*_{\epsilon})^n \circ P\|_{\mathsf{BV}} \leq M \cdot q^n \quad \forall n \in \mathbb{N} .$$

Remarks: a) The numbers p, rank (P_i) , M and q may depend heavily on the dimension d = |L| of the phase space X.

b) The assumption $\alpha < 1$ is rather restrictive, because it requires $\inf |\tau'| = \kappa_1 > 2$, which excludes *e.g.* the tent maps τ . It can be avoided by deriving inequality (8) directly for $(S_{\epsilon}^{*})^{M}$, in which case κ_1 is replaced by $\kappa_M > 2$. However, while this is easy for $\epsilon = 0$ because Z_0^{M} is a rectangular partition, it is much more delicate if $\epsilon > 0$. We discuss the difficulties of this case, which was treated in the thesis [12], below.

c) For transfer operators of piecewise expanding maps such a theorem was first proved in [10].

Next we discuss the role expansion plays for the derivation of inequality (8). The following lemma from [11] is basic:

Lemma 1 Let $U, V \subset \mathbb{R}^d$ be open and suppose $T \in C^2(U; V)$ is such that DT has full rank. Let $A := (DT)^{-1}$. Then

$$\operatorname{var}_{\mathbb{R}^d}(T^*f \cdot 1_V) \leq \sup_{x \in U} \|A(x)\|_{\infty} \cdot \operatorname{var}_{\mathbb{R}^d}(f \cdot 1_U) + \frac{1}{d} \cdot \sup_{x \in U} |\nabla \cdot A(x)|_1 \cdot \int_U |f(x)| \, dx$$

for $f \in L^1(U)$. (Here $\nabla \cdot A$ denotes formal matrix multiplication of the row vector ∇ with the matrix A.) If T extends continuously to ∂U with $T(\partial U) = \partial V$ then also

$$\operatorname{var}_V(T^*f) \leq \sup_{x \in U} \|A(x)\|_\infty \cdot \operatorname{var}_U(f) + \frac{1}{d} \cdot \sup_{x \in U} |\nabla \cdot A(x)|_1 \cdot \int_U |f(x)| \, dx \, .$$

Remarks: a) The estimate of this lemma is sharp in the sense that it is a direct consequence of the identity

$$\operatorname{div}(\psi) \circ T = \operatorname{div}(A \cdot (\psi \circ T)) - (\nabla \cdot A) \cdot (\psi \circ T)$$

valid for any test function $\psi \in C^1(V; \mathbb{R}^{d_2})$.

b) The factor $\sup_{x \in U} ||A(x)||_{\infty}$ is less than 1 if DT increases the $| . |_{\infty}$ -norm of each vector in \mathbb{R}^d . Also $\frac{1}{d} \cdot \sup_{x \in U} |\nabla \cdot A(x)|_1 \leq \sup_{1 \leq i \leq d} \sup_{x \in U} ||D_iA(x)||_{\infty}$.

c) If one works with euclidean variation, $\sup_{x \in U} ||A(x)||_{\infty}$ in Lemma 1 is replaced by $\sup_{x \in U} ||A(x)||_2$, which may lead to sharper estimates in some situations.

d) The lemma remains true, if $U \subseteq \mathbb{R}^{d_1}$, $V \subseteq \mathbb{R}^{d_2}$, $d_1 > d_2$, and if A denotes the Moore-Penrose inverse of DT.

In order to derive (8), Lemma 1 must be applied to each "branch" of S_{ϵ} separately. As $DS_{\epsilon}(x) = D\Phi_{\epsilon}(S_0x) \cdot DS_0(x)$, we have

$$\begin{split} \sup_{x} \|(DS_{\epsilon})^{-1}\|_{\infty} &\leq \sup_{x} \|DS_{0}(x)\|_{\infty} \cdot \sup_{y} \|D\Phi_{\epsilon}(y)\|_{\infty} \leq \frac{1}{\kappa_{1}} \sup_{y} \|E + DA_{\epsilon}(y)\|_{\infty} \\ &\leq \frac{1}{\kappa_{1}} (1 + \operatorname{const} \cdot \epsilon) \end{split}$$

and

$$\sup_{x} |\nabla \cdot (DS_{\epsilon})^{-1}(x)|_{1} \le \text{const}$$

with constants independent of the dimension, see (2). Summing over all branches $S_{\epsilon|Z}$ yields

$$\operatorname{var}\left(S_{\epsilon}^{\star}f\right) \leq \frac{1}{\kappa_{1}}\left(1 + \operatorname{const} \cdot \epsilon\right) - \sum_{Z \in \mathbb{Z}_{\epsilon}^{1}} \operatorname{var}_{\mathbb{R}^{d}}(f \cdot 1_{Z}) + \operatorname{const} \cdot \|f\|_{L^{1}} .$$
(9)

The crucial step is now to pass from (9) to (8), i.e. to show that

$$\operatorname{var}_{\mathbb{R}^d}(f \cdot 1_Z) \le (2 + \operatorname{const} \cdot \epsilon) \cdot \operatorname{var}_Z(f) + \operatorname{const} \cdot \int_Z |f(x)| \, dx \tag{10}$$

for each $Z \in \mathbb{Z}^1_{\epsilon}$. In fact, any factor ρ replacing $(2 + \text{const} \cdot \epsilon)$ in front of $\text{var}_Z(f)$ that neither depends on the dimension d = |L| of Z nor on $\epsilon \leq \epsilon_{\max}$ would be useful. We discuss some classical cases of this inequality:

- If d = 1 and Z = [u, v] one simply has (see [13])

$$\operatorname{var}_{\mathbb{R}}(f \cdot 1_{Z}) = |f(u)| + |f(v)| + \operatorname{var}_{Z}(f) \le 2 \cdot \operatorname{var}_{Z}(f) + \frac{2}{|v-u|} \int_{Z} |f(x)| \, dx \; .$$

- If $Z = [u_1, v_1] \times \ldots \times [u_d, v_d]$ is rectangular (our situation!), then the trivial estimate for d = 1 extends easily to the general case, if one uses the variation based on the $| \cdot |_1$ -norm as introduced above. Namely:

$$\operatorname{var}_{\mathbb{R}^{d}}(f \cdot 1_{Z}) \leq 2 \cdot \operatorname{var}_{Z}(f) + 2 \sum_{i=1}^{d} \frac{1}{|v_{i} - u_{i}|} \int_{Z} |f(x)| \, dx \tag{11}$$

- If ∂Z is piecewise smooth and satisfies a cone condition (our situation!) and if one works with euclidean variation, then there are $\rho > 1$ and C > 0 such that $\int_{\partial Z} |f(s)| ds \leq \rho \cdot \operatorname{var}_{Z}(f) + C \cdot \int_{Z} |f(x)| dx$. Here ρ depends essentially on the angle ω of the widest cone that can be attached to ∂Z at any of its points, namely $\rho \approx (\sin \frac{\omega}{2})^{-1}$. However, even for rectangular Z the value of $(\sin \frac{\omega}{2})^{-1} = \sqrt{d}$ depends heavily on the dimension d of Z. This is the main reason why we do not use euclidean variation. What remains is the case where Z is not rectangular but only close to that. This situation is encountered if $\kappa_1 \leq 2$ such that $\operatorname{var}((S^*_{\epsilon})^M f)$ with M > 1 as in (1) must be estimated directly. The partition \mathcal{Z}^M_{ϵ} , although not rectangular, is very close to a rectangular one in the following sense:

Lemma 2 [12, Satz 2.26] Suppose $\kappa_M > 2$. Then there is $\epsilon_1 > 0$ such that for all $\epsilon \in (0, \epsilon_1)$ holds: The partitions Z_0^M and Z_{ϵ}^M have the same cardinality and their elements $Z_{0,\ell}$ and $Z_{\epsilon,\ell}$, respectively, can be labeled such that $Z_{0,\ell}$ is diffeomorphic to $Z_{\epsilon,\ell}$ with a diffeomorphism $\Psi_{\epsilon,\ell}: Z_{\epsilon,\ell} \to Z_{0,\ell}$ which is C^1 -close to the identity in the following sense:

$$\|\Psi_{\epsilon,\ell}(x) - x\|_{\infty}, \ \|D\Psi_{\epsilon,\ell}(x) - E\|_{\infty}, \ \|D_i D\Psi_{\epsilon,\ell}(x)\|_{\infty} \leq \text{const} \cdot \epsilon$$

for all $i \in L$ and $x \in Z_{\epsilon,\ell}$ with constants which are independent of the size of L. The same is true for $\Psi_{\epsilon,\ell}^{-1}$.

Let $\Psi = \Psi_{\epsilon,\ell}$. With the aid of of Lemma 2, Lemma 1 and Remark b) thereafter we prove (10) for $Z = Z_{\epsilon,\ell}$ as in [12, Lemma 1.40]:

$$\begin{aligned} \operatorname{var}_{\mathbb{R}^d}(f \cdot 1_{Z_{\epsilon,\ell}}) &= \operatorname{var}_{\mathbb{R}^d}((\Psi^{-1})^*\Psi^*f \cdot 1_{Z_{\epsilon,\ell}}) \\ &\leq (1 + \operatorname{const} \cdot \epsilon) \cdot \operatorname{var}_{\mathbb{R}^d}(\Psi^*f \cdot 1_{Z_{0,\ell}}) + \operatorname{const} \cdot \epsilon \cdot \int_{Z_{0,\ell}} |\Psi^*f(x)| \, dx \\ &\leq (2 + \operatorname{const} \cdot \epsilon) \cdot \operatorname{var}_{Z_{0,\ell}}(\Psi^*f) + \operatorname{const} \cdot \int_{Z_{\epsilon,\ell}} |f(x)| \, dx \\ &\leq (2 + \operatorname{const} \cdot \epsilon) \cdot \operatorname{var}_{Z_{\epsilon,\ell}}(f) + \operatorname{const} \cdot \int_{Z_{\epsilon,\ell}} |f(x)| \, dx \; .\end{aligned}$$

As the other steps of the estimate are essentially the same for S_{ϵ}^{M} as for S_{ϵ} , we obtain the basic inequality (8) for $(S_{\epsilon}^{*})^{M}$ with κ_{1} replaced by κ_{M} , and Theorem 2 follows as before.

3.2 Infinite lattices

The way var (f) is defined in case $L = \mathbb{Z}^r$ allows an immediate extension of the basic inequality (8) from the finite to the infinite case. In [11] the estimate is obtained directly from the " $d_1 > d_2$ " version of Lemma 1 (see Remark d) thereafter). Alternatively, in [12] the dynamics on $X = [0, 1]^L$ are approximated by those on finite periodic lattice systems. For the easy details we refer to the original sources.

Unfortunately I do not see how classical ergodic theorems could be applied to S_{ϵ}^{*} in the infinite lattice case just on the basis of the compactness property (7) and inequality (8). For S_{ϵ}^{*} acting on $(L^{1}(X), \| \cdot \|_{L^{1}})$ property (7) does not guarantee the weak compactness of sequences $(\frac{1}{n}\sum_{k=0}^{n-1}(S_{\epsilon}^{*})^{k}f)_{n>0}$ which is needed for the Kakutani/Yoshida theorem. On the other hand, I am not able to apply a topological vector space version of this theorem that one might try for S_{ϵ}^{*} acting on $(L^{1}(X), \| \cdot \|_{J}\}_{J \in \mathcal{F}(L)})$ or on $L^{1}(X)$ equipped with a similar topology (see the end of section 2.2), because I

cannot prove uniform continuity of the iterates $(S_{\epsilon}^*)^n$. However, properties (7) and (8) are of course sufficient for the existence of weak accumulation points of sequences $(\frac{1}{n}\sum_{k=0}^{n-1}(S_{\epsilon}^*)^k f)_{n>0}$ and thus for S_{ϵ} -invariant measures in BV(X).

4 Relations to other approaches

There are a few other mathematical approaches to chaotic coupled map lattices in the literature of which I know.

- Bunimovich and Sinai [6] consider piecewise onto maps $\tau : [0,1] \rightarrow [0,1]$ and particular interaction operators Φ_{ϵ} which allow them to construct Markov partitions, to represent a CML as a 2-dimensional shift system and to identify the invariant measures with absolutely continuous marginals as Gibbs measures for a suitable family of conditional probabilities. Referring to results from statistical mechanics they prove this way existence, uniqueness and exponential mixing properties of these measures.² Volevich [15] extends this approach from a pure equilibrium theory to a more kinematic theory by characterizing the class of measures that is attracted under the dynamics to the unique invariant one.³ (The corresponding class in our approach is $BV([0, 1]^{Z^r})$). Analogous results for coupled axiom-A-systems are proved in [30].
- In a series of papers Gundlach and Rand [8] study CMLs with piecewise onto τ : [0, 1] → [0, 1] but with much more general couplings than Bunimovich and Sinai. Using a "bundle system approach" they construct suitable Markov partitions also for these more general couplings. In this way they obtain results similar to those of Bunimovich and Sinai. ⁴ In addition they describe the dynamics of the CML by means of a "bundle transfer operator" which gives further insight into the mixing properties.
- Bricmont and Kupiainen [4] study systems where both the map $\tau: S^1 \to S^1$ and the interaction operator Φ_{ϵ} are real analytic. Using a so called cluster expansion for S^*_{ϵ} when L is finite they obtain a spectral decomposition of S^*_{ϵ} acting on a suitable space of smooth functions where the involved constants are estimated directly. (Technically they use that the transfer operator τ^* of τ has 1 as a simple eigenvalue and the rest of its spectrum is contained in a disc of radius less than 1.) This is in sharp contrast to our Theorem 2 where the constants result from more abstract spectral theory and no explicit dependence on the size of L is known, even under the same spectral assumptions on τ^* as in [4]. It is not clear whether cluster expansion is applicable in our context.

²The result of Dobrushin referred to in [6, 30] does not exactly apply to the setting of these papers. Bricmont and Kupiainen [5], however, provided recently a result of this type which is exactly tailored to the needs of the statistical mechanics approach.

³Also this result is rederived in [5].

⁴Instead of their reference to a result by Campbell and Rand, which is not correct, one has to use Theorem 1 of [5]. In the same paper this point is discussed in some more detail.

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Dynamics of networks: Features which persist from the uncoupled limit

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Abstract

The theme of these notes is to look for aspects of the dynamics of a network of units which can be continued from the uncoupled case, uniformly in the size of the system. Some answers are given, and particularly interesting answers are found in the case of conservative systems.

1 Introduction

Many systems are well described as a network of dynamically interacting units. As examples, consider:

- electricity production, distribution and consumption networks
- Josephson junction arrays
- optical computer memory
- crystals and quasicrystals
- multicellular organisms
- nervous systems
- economies

The issue I wish to address is how much can be learned from the uncoupled case. One might think the answer is "very little", and indeed there are many phenomena, like waves, pattern formation, and synchronisation, which depend heavily on the coupling. Nonetheless, a lot can be learned from the uncoupled limit. In particular, many results can be obtained which are uniform in the size of the network. In fact they also apply to infinite networks; from the physical point of view, infinite networks do not exist, but they are convenient mathematical idealisations.

By a *network* let us understand for present purposes a system of ordinary differential equations (ODEs) of the form

$$\dot{x}_s = F_s(x_s) + K_s(x,\epsilon), \tag{1}$$

where s belongs to a countable index set S labelling units of the network, x_s belongs to some finite-dimensional manifold M_s , x denotes the whole configuration $(x_s)_{s\in S}$, and ϵ belongs to a finite-dimensional manifold P (parameter space). We might as well think of P as \mathbb{R}^p , some $p \in \mathbb{N}$, because my analysis will be local to a neighbourhood of a point 0 of P, where

$$K_s(x,0) = 0, \forall s \in S.$$
⁽²⁾

Thus x is a point of $M = \times_{s \in S} M_s$, and the equations can be written as

$$\dot{x} = F(x) + K(x,\epsilon). \tag{3}$$

Let us call F_s the local dynamics of unit s and K the coupling. Suppose that each M_s and P are endowed with Finsler metrics, meaning a metric induced by a norm |.| on tangent vectors, and for the norm of a tangent vector to M we take the supremum over $s \in S$ of the norms of its components on the M_s . Furthermore, I suppose that F is C^1 (with respect to the sup norm) and K is jointly C^1 in (x, ϵ) .

A prime example of coupling is diffusive coupling on a graph. Here S is the set of nodes of a graph, $M_s = \mathbb{R}^N$ for some $N, P = \mathbb{R}$, and

$$K_s(x,\epsilon) = \frac{\epsilon}{k_s} \sum_{r \in N_s} (x_r - x_s), \qquad (4)$$

where N_s is the set of nodes neighbouring to s in the graph, and k_s is the number of neighbours. Note that our definition of a network does not require the coupling to be local in any sense, though we will in due course examine the effects of locality of the coupling if it exists.

Extensions of the definition of network, and variations on the theme, are possible. For ex.mple, there is the much studied discrete-time analogue, *coupled map lattices*. Many of our considerations can be translated directly to that context, but I prefer to concentrate on the continuous-time case as being closer to most applications, using coupled map lattices only as a simplifying pedagogical tool in Section 6. An extension which deserves serious attention is to couplings that are not described as perturbations to the vector field on the product manifold, for example time-delayed coupling, or coupling via a convolution in time, or via a capacitor or inductor or a bistable system (as in some cell membranes), or even via a partial differential equation (PDE) representing a transmission line. I have not yet addressed these generalisations, though I learnt recently that Jack Hale has looked at the transmission line case. Indeed, I learnt from Hale that in addition to the references that I cite here there are some other precursors to several of the issues I will address. I have not yet had the time to study them, however, and I apologise to both the authors and the readers for this incompleteness.

The lectures were given in two parts. In the first lecture, persistence of equilibria, stability, the effects of locality of the coupling, periodic orbits, uniformly hyperbolic sets, normally hyperbolic manifolds, and structural stability for networks were discussed. In the second lecture, I specialised to the Hamiltonian and time-reversible cases, which I refer to collectively as *conservative*. The notes follow the same outline. I will not touch on the important area of ergodic theory of networks (interested readers are referred to [30], for example), though recently I think I have found a beautiful approach to understanding the statistical behaviour of networks of chaotic units. Neither will I touch on the interesting and I believe potentially very useful concept of the rotation set for the chain-recurrent set; for information about that see [22]. I would like the notes to be seen as partly a survey of established results, and partly as an invitation to join an interesting ongoing research programme. Dynamics of networks

2 Equilibria

Let us begin by studying to what extent equilibria of the uncoupled network persist to the coupled case. This section is based on [27]. From Eq. (1), it is a question of solving

$$G(x,\epsilon) := F(x) + K(x,\epsilon) = 0.$$
(5)

Suppose x^0 is an equilibrium for $\epsilon = 0$, i.e. for all $s \in S$

$$F_s(x_s^0) = 0, (6)$$

and suppose it is uniformly non-degenerate¹, meaning that there exists $B \in \mathbb{R}$ such that for all $s \in S$

$$|DF_s(x_s^0)^{-1}| \le B.$$
(7)

Theorem 1 There exists $\epsilon_0 > 0$, depending only on the suprema of ||DF||, $||DF^{-1}||$, $||\frac{\partial K}{\partial \epsilon}||$ and $||DK||/|\epsilon|$ in a neighbourhood U of $(x^0, 0) \in M \times P$, such that x^0 has a unique continuation $X(\epsilon)$ for $|\epsilon| < \epsilon_0$ (with $X(0) = x^0$).

Here and elsewhere, when applied to functions on $M \times P$, D denotes derivative with respect to $x \in M$ and $\frac{\partial}{\partial \epsilon}$ denotes derivative with respect to $\epsilon \in P$.

Theorem 1 is proved by application of the implicit function theorem (e.g. [12]) to Eq. (5). Furthermore, it follows from the proof that the function X is C^1 and satisfies

$$\frac{\partial X}{\partial \epsilon} = -DG(X(\epsilon), \epsilon))^{-1} \frac{\partial K}{\partial \epsilon}(X(\epsilon), \epsilon), \tag{8}$$

as long as DG remains invertible.

We can use this to estimate an explicit ϵ_0 for Theorem 1. For example, taking norms of both sides of Eq. (8) and using Eq. (5),

$$\left|\frac{\partial X}{\partial \epsilon}\right| \le \frac{\left|\left|\frac{\partial K}{\partial \epsilon}(X(\epsilon), \epsilon)\right|\right|}{\left|\left|DF^{-1}(X(\epsilon))\right|\right|^{-1} - \left|\left|DK(X(\epsilon), \epsilon)\right|\right|\right|}.$$
(9)

Suppose

$$||DF(x)^{-1}|| \geq a - b\tau,$$
 (10)

$$||DK(x,\epsilon)|| \leq c\eta, \tag{11}$$

$$\left\|\frac{\partial K}{\partial \epsilon}(x,\epsilon)\right\| \leq d + e\tau + f\eta, \qquad (12)$$

in some neighbourhood U of $(x^0, 0)$, where

$$\tau = |x - x^0|, \qquad (13)$$

$$\eta = |\epsilon|. \tag{14}$$

¹Actually it is not necessary to insist on uniformity as this is automatic under the C^1 hypothesis on F: if DF is bounded and invertible then the inverse is bounded. See [13], for example.

Then

$$\left|\frac{\partial\tau}{\partial\epsilon}\right| \le \frac{d+e\tau+f\eta}{a-b\tau-c\eta},\tag{15}$$

as long as x remains in U and the denominator remains positive. It follows that the continuation can be performed at least up to ϵ_0 given by the value of η at the first time that the solution of

$$\frac{d\tau}{d\eta} = \frac{d + e\tau + j\eta}{a - b\tau - c\eta} \tag{16}$$

reaches either the boundary of U or the line $a - b\tau - c\eta = 0$.

Here is a concrete example, which we call coupled bistability. Suppose all the $F_s = f$, a C^1 "bistable" function of one variable, possessing attracting zeroes at x = 0 and 1 with f'(0), f'(1) < 0, and f' is monotone on intervals $[0, c_0]$ and $[c_1, 1]$, with $f'(c_0) = f'(c_1) = 0$. Suppose K is diffusive coupling on a graph as in Eq. (4), and $\epsilon \in \mathbb{R}_+$. Then we can estimate $||DG^{-1}||$ as in Eq. (9), or better by

$$||DG^{-1}|| \le \frac{1}{||\Lambda^{-1}||^{-1} - ||\Delta||},\tag{17}$$

where Λ is the diagonal part of DG and Δ its off-diagonal part. Hence

$$||DG^{-1}|| \leq \frac{1}{\inf_{s \in S} |f'(x_s) - \epsilon| - |\epsilon|},\tag{18}$$

as long as the denominator remains positive. But the $f'(x_s)$ all start negative and $\epsilon \geq 0$, so it follows that

$$||DG^{-1}|| \le \frac{1}{\inf_{s \in S}(-f'(x_s))},\tag{19}$$

as long as the denominator remains positive.

We could estimate $|\frac{\partial K}{\partial \epsilon}|$ by a formula like Eq. (12) but we can do better. All solutions of Eq. (5) which are continuations of $x^0 \in \{0,1\}^S$ have $x \in [0,1]^S$ for $\epsilon \ge 0$. This is because if x_s is the leftmost value then $K_s \ge 0$, so to solve Eq. (5) we require $f(x_s) \le 0$. Since f(0) = 0 and f'(0) < 0, the solution can not cross 0. Similarly, it can not cross $x_s = 1$. In the case of an infinite network the above argument needs modifying by taking the limit of x_s near $\inf_{s \in S}(x_s)$, but the same conclusion holds. Hence

$$\left|\frac{\partial K}{\partial \epsilon}\right| \le \sup_{x \in [0,1]^S, s \in S} \frac{1}{k_s} \left|\sum_{r \in N_s} (x_r - x_s)\right| = 1,\tag{20}$$

Putting Eqs (8), (19) and (20) together,

$$\frac{d\tau}{d\epsilon} \le \frac{1}{\inf_{s \in S}(-f'(x_s))} \le \frac{1}{\min(-f'(\tau), -f'(1-\tau))},\tag{21}$$

by the monotonicity of f'. Hence, the equilibria continue at least up to

$$\epsilon_0 = \int_0^{\min(c_0, 1-c_1)} \min(-f'(\tau), -f'(1-\tau)) d\tau.$$
(22)

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Note that if the minimum in the integrand is always attained by the first term then this gives simply $-f(c_0)$. If it is always attained by the second term then it gives $f(c_1)$. Consequently, if either one or the other is true, as for cubic f, then we obtain the very simple explicit bound

$$\epsilon_0 = \min(-f(c_0), f(c_1)).$$
 (23)

In conclusion, for $0 \leq \epsilon < \epsilon_0$ there is an injection from $\{0,1\}^S$ into the set of equilibria. We can say that "computer memory survives weak coupling".

By the same method, we can continue unstable equilibria of the uncoupled system, using for one or more $s \in S$, $x_s^0 = u$, an unstable zero of f, provided f'(u) > 0. By continuity of f at least one unstable zero must exist between 0 and 1, and generically it satisfies f'(u) > 0. But note that we will not be able to obtain quite as good a bound ϵ_0 for these unstable equilibria because the neat cancellation of ϵ in the denominator of Eq. (18) will no longer occur. Nonetheless the resulting differential inequality is easily solved explicitly, and gives an explicit ϵ_0 .

The method can even be applied to problems where the uncoupled system possesses only one equilibrium, but on sufficient coupling gains many equilibria. An example is the type of system with negative diffusion discussed by Mallet-Paret in this Colloquium. The way the method can be applied is to start from a different uncoupled limit, which includes the diagonal part of the negative diffusion and hence exhibits bistability at each site once the diffusion parameter exceeds a certain value, and then show that in suitable parameter regimes one can continue the resulting stable equilibria with respect to the off-diagonal part of the diffusion. I will write up the details separately.

The coupled bistability example raises two questions. Firstly, do the equilibria keep the same stability-type as ϵ grows? Secondly, how do we know that no new equilibria are created as ϵ grows? We will address the first question immediately, and the second question later.

3 Stability

In this section it is proved (following [27] again, but improving on it) that subject to a strengthening of the condition of uniform non-degeneracy to uniform hyperbolicity, the equilibria obtained in Theorem 1 preserve their stability-type for at least $|\epsilon| < \epsilon_1$, for some $\epsilon_1 > 0$ but not necessarily as large as ϵ_0 . By preserve their stabilitytype I mean that there is a continuous (with respect to ϵ) splitting of the tangent space into contracting and expanding subspaces for the linearised dynamics about the equilibrium $X(\epsilon)$; in particular their dimensions do not change. Here, "expanding" means "contracting in negative time". Let us say that an equilibrium x^0 of the uncoupled system Eq. (1) is uniformly hyperbolic² if there exists $B \in \mathbb{R}$ such that for

²As in Section 2, one does not need to insist on the uniformity: uniformity with respect to $s \in S$ follows from $F \in C^1$, and uniformity with respect to λ is automatic because for $|\lambda| > ||DF||$ we have $||(\lambda I - DF)^{-1}|| \leq \frac{1}{|\lambda| - ||DF||}$, and it is continuous with respect to $\lambda \notin \text{spec } DF$.

all $s \in S$ and λ on the imaginary axis,

$$||(\lambda I - DF_s(x_s^0))^{-1}|| \le B,$$
 (24)

where I denotes the identity matrix.

Theorem 2 There exists $\epsilon_1 > 0$, depending only on the suprema of $\sup_{\Re \lambda = 0} ||(\lambda I - DF)^{-1}||$, ||DF||, $||\frac{\partial K}{\partial \epsilon}||$ and $||DK||/|\epsilon|$ in a neighbourhood U of $(x^0, 0) \in M \times P$, such that the continuation $X(\epsilon)$ of $(x^0, 0)$ keeps the same stability type for $|\epsilon| < \epsilon_1$.

To prove this, the linearised dynamics is given by

$$\xi = DG(X(\epsilon), \epsilon)\xi := M(\epsilon)\xi.$$
(25)

For $\lambda \notin \text{spec } M$, define the resolvent operator

$$R_{\lambda}(M) = (\lambda I - M)^{-1}. \tag{26}$$

Then if there is no spectrum on the imaginary axis, the desired splitting is given by the complementary projections

$$\Pi_c = \frac{1}{2\pi i} \int_{\Gamma_c} R_\lambda d\lambda, \qquad (27)$$

$$\Pi_e = \frac{1}{2\pi i} \int_{\Gamma_e} R_\lambda d\lambda, \qquad (28)$$

where Γ_c and Γ_e are closed anticlockwise contours in the complex λ -plane enclosing respectively all the spectrum in the left half-plane and all the spectrum in the right half-plane.

To prove that no spectrum reaches the imaginary axis for ϵ small enough and that the projections are continuous with respect to ϵ , we note firstly that if

$$||M' - M|| < ||R_{\lambda}(M)||^{-1},$$
(29)

then $R_{\lambda}(M')$ exists, so $\lambda \notin \text{spec } M'$. Let

$$r = \sup_{\Re \lambda = 0} ||R_{\lambda}(M(0))||, \tag{30}$$

which is finite, by the hypothesis Eq. (24). Then there is no spectrum on the imaginary axis as long as

$$||M(\epsilon) - M(0)|| < \frac{1}{r},$$
 (31)

and by continuity of M on ϵ (in fact uniformly in the system size), we deduce that there is $\epsilon_1 > 0$ such that no spectrum reaches the imaginary axis for $|\epsilon| < \epsilon_1$. Secondly, we note that $R_{\lambda}(M)$ is continuous with respect to M, for $\lambda \notin$ spec M. Indeed, if Eq.(29) holds then

$$R_{\lambda}(M') - R_{\lambda}(M) = R_{\lambda}(M)(M - M')R_{\lambda}(M').$$
(32)

So in particular we have

$$||R_{\lambda}(M') - R_{\lambda}(M)|| \le \frac{||R_{\lambda}(M)||^{2}||M' - M||}{1 - ||R_{\lambda}(M)||||M' - M||}$$
(33)

The continuity of the projections with respect to ϵ (as long as no spectrum reaches the imaginary axis) follows from this.

As an illustration, for the equilibria of the example of the previous section, obtained by continuation from $\{0,1\}^S$,

$$r = \frac{1}{\min(|f'(0)|, |f'(1)|)},\tag{34}$$

and

$$||M(\epsilon) - M(0)|| \le \sup_{s \in S} |f'(x_s) - f'(x_s^0) - \epsilon| + \epsilon.$$
(35)

So we deduce that $X(\epsilon)$ is stable as long as

$$\max(2\epsilon, |f'(0) - f'(\tau) + \epsilon| + \epsilon, |f'(1) - f'(1 - \tau) + \epsilon| + \epsilon) < \min(|f'(0)|, |f'(1)|).$$
(36)

This can be translated into a bound on ϵ by using Eq. (21).

In fact, for this example if every unit has the same number of neighbours then we can do better, because it becomes a gradient flow. *Gradient flows* are dynamical systems of the form:

$$\dot{x} = -\nabla W(x) \tag{37}$$

for some "energy function" W, where the gradient is taken with respect to some inner product. For gradient flows, the stability type of an equilibrium is preserved as long as it continues to be *non-degenerate*, meaning DG (in this case D^2W) remains invertible. Thus in this case, the bounds for continuation and preservation of stability-type can be taken identical. This is because the spectrum is purely real, so the only point of the imaginary axis it can approach is 0, and that corresponds to losing non-degeneracy, whereas in the general case, Poincaré-Andronov-Hopf bifurcation can also occur. So the equilibria of the coupled bistability example remain stable as long as they remain non-degenerate, in particular at least up to ϵ_0 .

In the case of *attracting* stability type (i.e. hyperbolic with trivial expanding subspace) one could ask the question whether the equilibrium is attracting for the full (nonlinear) system (with respect to sup-norm). This is almost certainly true, but I did not yet check it. If so, one could further ask whether uniform stability estimates can be found with respect to the size of the system. For example, are there $\kappa < 1, \delta_0 > 0, \mu > 0$ independent of system size, such that for all $\delta < \delta_0$, the orbits of all initial conditions within $\kappa\delta$ of the equilibrium lie within $\delta e^{-\mu t}$ for all positive time t? Again, this is almost certainly true, but I have not yet done the estimates.

4 Spatial structure

Next, we address the question of what additional statements we can deduce about the equilibria we have continued, if the coupling is local in some sense. Let us suppose a metric d on S. For example, for a connected graph, d(r, s) could be the shortest number of edges joining the nodes r and s, and this is our default metric if we refer to the network as a graph.

There are several interesting types of local coupling. The conditions all apply to the combination

$$L_{rs} = \frac{1}{\epsilon} \frac{\partial K_s}{\partial x_r}.$$
(38)

The simplest is nearest neighbour coupling in a graph:

$$|L_{rs}| = 0 \text{ for } d(r, s) > 1.$$
(39)

Another is exponentially decaying coupling, though this needs careful formulation in cases where the number of units at distance ρ grows exponentially with ρ .

If the coupling is local we expect the resulting solutions $X(\epsilon)$ to have some special spatial features. For instance, in the example of Section 2, if $x_s^0 = 1$ for one unit, say s = o, and 0 elsewhere, then does $X_s(\epsilon)$ decay exponentially with d(s, o)? More generally in this example, if two equilibria x^0 and \tilde{x}^0 at $\epsilon = 0$ differ only at one site, o, then does the difference $X_s(\epsilon) - \tilde{X}_s(\epsilon)$ decay exponentially with d(s, o)?

We have proved this for the example of Section 2 and in a number of other situations. The key step is to derive exponential decay estimates for the norms of the matrix elements of DG^{-1} . We call this property *finite coherence length*. First we describe some finite coherence length results and then we will return to how to deduce exponential decay results of the type of the previous paragraph. These results were derived in a different context but apply here nonetheless. Note that cases 1 and 3 do not require any smallness assumption on the off-diagonal part of DG.

Case 1: One-dimensional chains with nearest neighbour coupling only, though not necessarily symmetric nor translation invariant. This was done in [24]. Write

$$DG = \Lambda + L_+ + L_-, \tag{40}$$

where Λ is the (block-)diagonal part of DG, and L_{\pm} are the super- and sub- (block-) diagonals. Supposing DG is invertible, let

$$\eta = ||DG^{-1}||\max(||L_{+}||, ||L_{-}||), \tag{41}$$

and

$$\kappa = \frac{1}{2\eta} + \sqrt{\frac{1}{4\eta^2} + 1} > 1.$$
(42)

Then for all $\lambda \in (\kappa^{-1}, 1)$ there exists $K \in \mathbb{R}$ (see [24] for an explicit way to obtain K) such that

$$|(DG^{-1})_{rs}| \le K\lambda^{d(r,s)}.$$
(43)

Case 2: One-dimensional chains with not too large exponentially decaying coupling, again not necessarily symmetric nor translation invariant. This was done in [25]. Write

$$DG = \Lambda + \Delta, \tag{44}$$

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with Λ being the (block-)diagonal part and Δ the rest. Supposing Λ is invertible, put

$$J = -\Lambda^{-1}\Delta,\tag{45}$$

so

$$DG = \Lambda(I - J). \tag{46}$$

Suppose that Δ decays exponentially in such a way that

$$|J_{rs}| \le C_{d(r,s)},\tag{47}$$

for some sequence C_k with

$$0 \le C_k \le K\lambda^k, \lambda < 1, \tag{48}$$

and

$$\sum_{k\geq 1} C_k < 1. \tag{49}$$

Then the action of I - C decomposes into Bloch spaces $B_{\theta}, \theta \in \mathbb{R}/2\pi\mathbb{Z}$, where the dependence on site number $s \in \mathbb{Z}$ is proportional to $e^{is\theta}$. Let

$$A(\theta) = (I - C)|_{B(\theta)}, \tag{50}$$

which is analytic in the strip $|\Im \theta| < \log \lambda^{-1}$ and invertible on the real axis. So $A(\theta)^{-1}$ is analytic in the strip

$$|\Im\theta| < \mu := \min(\log \lambda^{-1}, \Im\theta), \tag{51}$$

where θ is the nearest degeneracy of A to the real axis. Thus

$$\limsup_{|r-s| \to \infty} \frac{\log |((I-C)^{-1})_{rs}|}{|r-s|} \le -\mu.$$
(52)

Using the formula

$$((I-J)^{-1})_{rs} = \sum_{\gamma \in \Gamma} \prod_{i} J_{s_i, s_{i+1}},$$
(53)

where Γ is the set of paths $\gamma = (s_i)$ from r to s, and Eq. (47), we deduce that Eq. (52) also applies to $(I - J)^{-1}$.

This case has a generalisation (though with less explicit decay rate) to exponentially decaying coupling on all "non-exponential" graphs under hypotheses Eq. (47) and Eq. (49); see section IV-3 of [5].

Case 3: Graphs for which DG is symmetric. This is satisfied for gradient flows, or if the coupling is symmetric and the on-site dynamics is locally a gradient flow (in particular, one-dimensional on-site dynamics suffices). We suppose DG is invertible, but we will use the ℓ_2 norm, denoted by subscript 2, in order to establish exponential decay estimates. By the hypothesis of symmetry,

$$||DG^{-1}||_2 \le ||DG^{-1}||_2 \tag{54}$$

Choose a site $o \in S$, and for $n \ge 1$, let

$$P_n = \sum_{s:d(o,s) \ge n} |(DG^{-1})_{os}|^2.$$
(55)

Let

$$A_{pq}^{(n)} = \sum_{s:d(s,o)=n-1} DG_{ps}^* DG_{sq} \text{ for } d(p,o) = d(q,o) = n,$$
(56)

$$B_{pq}^{(n)} = \sum_{s:d(s,o)=n} DG_{ps}^* DG_{sq} \text{ for } d(p,o) = d(q,o) = n-1,$$
(57)

and

$$T = \sup_{n \ge 1} (||A^{(n)}||_2, ||B^{(n)}||_2) \le ||DK||_2^2 \le ||DK||^2.$$
(58)

Then it is proved in [8], using a result from [6], that

$$P_n \le C\lambda^{n-1} ||DG^{-1}||^2, (59)$$

where

$$C = ||DG^{-1}||^2 T, (60)$$

$$\Lambda = \frac{2K}{1 + \sqrt{1 + 4K^2}} < 1.$$
(61)

I expect that there is a general result which would encompass all three of these cases and many more. It would have the form " A_{rs} exponentially decaying and A invertible implies $(A^{-1})_{rs}$ exponentially decaying", but I have not yet found it. Note that many people (e.g. [30, 11]) consider weighted spaces which force exponential decay, and then prove that the solution lies in these spaces. I prefer not to do this.

Finally, I discuss some of the consequences of finite coherence length results. Firstly, the reason for the name is that the matrix DG^{-1} governs the response to a small external force distribution $h = (h_s)_{s \in S}$. The problem

$$\dot{x} = G(x,\epsilon) + \eta h \tag{62}$$

has a unique equilibrium solution near each non-degenerate equilibrium $X(\epsilon)$ of the undisturbed system, given by integrating

$$\frac{\partial x}{\partial \eta} = -DG^{-1}h\tag{63}$$

from $\eta = 0$ to 1 starting at $x = X(\epsilon)$. So if the matrix elements of DG^{-1} decay exponentially with distance between units then the response to a localised external force h decays exponentially from that location.

Secondly, if two equilibria at the uncoupled limit differ only at one site, say $o \in S$, then the difference between their continuations $X(\epsilon)$ and $\tilde{X}(\epsilon)$ decays exponentially from that site, at least for ϵ small enough. To prove this let us adapt an idea of [5]. Replace the equation $G_o(x) = 0$ for the unit o by the equation

$$x_o = \lambda \tilde{x}_o(\epsilon) + (1 - \lambda) x_o(\epsilon), \tag{64}$$

where λ will range from 0 to 1. Denote the corresponding system of equations by

$$\bar{G}(x,\lambda) = 0. \tag{65}$$

Now for $\lambda = 0$ we have a solution $X(\epsilon)$ and for $\lambda = 1$ we have a solution $\overline{X}(\epsilon)$. For ϵ small these are continuations of each other with respect to λ via a solution $X(\epsilon, \lambda)$ of Eq. (65), because this is true at $\epsilon = 0$. As long as they remain continuations of each other with respect to λ , we have

$$\frac{\partial X}{\partial \lambda} = -D\bar{G}^{-1}\frac{\partial \bar{G}}{\partial \lambda},\tag{66}$$

and exponential decay of the elements of $D\bar{G}^{-1}$. By integrating this equation from $\lambda = 0$ to 1, we deduce exponential decay for $\tilde{X}_s(\epsilon) - X_s(\epsilon)$ with respect to d(s, o). The argument can be extended to initial equilibria differing at more than one site.

5 Periodic Orbits

So far we have addressed only the simplest type of dynamics: equilibria. What can be said about persistence of periodic orbits of the uncoupled network?

Aubry and I tackled this problem in the conservative context [24], and I will discuss that case in Section 10, but it can also be studied in the general context, as I will now outline. The details are being written up in a paper with Sepulchre.

Periodic orbits of a dynamical system

$$\dot{x} = G(x, \epsilon) \tag{67}$$

on a manifold M can be seen as zeroes of the following map:

$$\Phi: (\hat{x}, T) \mapsto T\hat{x} - G(\hat{x}, \epsilon), \tag{68}$$

where \hat{x} belongs to a space of periodic functions of period 1, and $T \in \mathbb{R}_+$ represents the period. The object on the right is then also a periodic function of period 1. The aim is to make it be the zero function, because then $x(t) = \hat{x}(t/T)$ is a periodic orbit of Eq. (67). There are many choices for the spaces of periodic functions, which we call *loop spaces*. Perhaps the simplest is that $\hat{x} \in C^1(S^1, M)$ and the righthand side belongs to $C^0(S^1, TM)$, where S^1 denotes the circle of length 1 and TM the tangent bundle to M. If G is C^1 then so is Φ .

Then, with a view to applying the implicit function theorem again, we can ask for which periodic orbits of the uncoupled system is $D\Phi$ invertible? Unfortunately, the answer is "none". The problem is that (for an autonomous system) the infinitesimal phase shift $(\hat{x}, 0)$ is always in the kernel of $D\Phi$. But Φ is covariant with respect to phase shifts, so this is not a real problem. It can be tackled by using Fredholm theory, which is the extension of the implicit function theorem when some non-invertibility is inevitable.

Now let us apply the above to a network system. Suppose the local dynamics on one site $o \in S$ has a non-degenerate periodic orbit (i.e. no normal Floquet multiplier +1), and a hyperbolic equilibrium at all the other sites. Then the resulting periodic orbit for the network is non-degenerate in the above sense and hence persists for some range of ϵ , uniformly in the size of the network. Again one can address the questions of stability and finite coherence length. We find analogous results to those for equilibria.

What happens if we start from periodic orbits on two or more sites, with equilibria at the others? If the periods are in rational ratio, i.e. integer multiples of some common super-period T, then the full system has periodic orbits of period T, and one might hope to continue them to non-zero ϵ . But this is false, because in addition to (overall) phase-shift degeneracy there are relative phase shift degeneracies in this case. In fact, the product of N periodic orbits and arbitrarily many equilibria is an Ntorus. If the periods are in rational ratio, the N-torus is foliated into an (N-1)-torus of periodic orbits of the same period. Hence there are automatically N - 1 relative phase-shift degeneracies. It is easy to create couplings which destroy all these periodic orbits, for example by making the frequency ratio incommensurate. Nonetheless, we do expect persistence of the invariant N-torus, though the dynamics on the torus may become more complicated than periodic. This will be addressed in Section 8.

6 Uniformly Hyperbolic Sets

The persistence results for equilibria and periodic orbits have a powerful generalisation to aperiodic orbits, under an analogous condition of uniform hyperbolicity. It is simplest here to make an excursion into discrete-time, which avoids technical problems due to the continuous time-translation symmetry of autonomous ODEs. Thus we consider *coupled map lattices*³ of the general form:

$$x_s^{t+1} = F_s(x_s^t) + K_s(x^t, \epsilon), s \in S, t \in \mathbb{Z},$$

$$(69)$$

which we condense to the general form for a parametrised family of discrete-time dynamical systems:

$$x^{t+1} = G(x^t, \epsilon), x^t \in M.$$
(70)

It is clear that the problem of persistence of fixed points of Eq. (70) is virtually identical to the problem of persistence of equilibria of networks, with the only change being from a zero-finding problem to a fixed point problem. Thus the key condition of invertibility of DG should be replaced by invertibility of I - DG. The problem of persistence of periodic orbits, of period q say, of a coupled map lattice also reduces to

³Note that the word "lattice" is used in a weaker sense than the pure mathematicians' sense: there is no need for S to be closed under an operation of subtraction.

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the same sort of problem, either by considering the q^{th} iterate of G or more simply by writing a system of q equations for x^0, \ldots, x^{q-1} .

The standard definition of uniform hyperbolicity for dynamical systems involves a splitting of the tangent space into the direct sum of invariant expanding and contracting bundles, with uniform exponential estimates. I prefer to give a functionalanalytic definition of uniform hyperbolicity, which can be proved to be equivalent to the usual one (see below), but is much more useful and allows generalisation to nondynamical problems like elliptic PDEs⁴, for example [1]. To lead into the definition, note that orbits of Eq. (70) (fixing ϵ for the moment) are fixed points of the operator $H: M^{\mathbb{Z}} \to M^{\mathbb{Z}}$ defined by

$$H(x)^{t} = G(x^{t-1}).$$
(71)

In the case of a coupled map lattice, M is already a product of manifolds, one for each unit of the lattice, so $M^{\mathbb{Z}}$ is a product of manifolds, one for each point in space-time. For norm on $M^{\mathbb{Z}}$, use the supremum over the \mathbb{Z} -direction of the norms on M.

An orbit $x \in M^{\mathbb{Z}}$ of Eq. (70) is said to be uniformly hyperbolic if I - DH is invertible. An invariant set Σ is uniformly hyperbolic if its orbits are uniformly hyperbolic with a common bound on $||(I - DH)^{-1}||$ (and if Σ is non-compact, a common module of continuity for DH is required). This definition is not so new, in fact, as it is essentially Mather's characterisation of Anosov systems, presented to the Dutch Academy of Sciences in 1968, perhaps in this very room. Furthermore, its continuous-time analogue, named *exponential dichotomy*, goes back to 1958 or so (see [28])! For an introductory article which explains many aspects of the equivalence between this definition and the usual one, see [20], and for more see [32]. For the particular case of symplectic twist maps, see [6].

With this definition, persistence of uniformly hyperbolic orbits, uniformly in the size of the lattice, becomes immediate. It is just the same as for non-degenerate fixed points of a coupled map lattice, but with the lattice replaced by the grand lattice, and G replaced by H. The mapping between the perturbed and the unperturbed orbits of uniformly hyperbolic sets is easily shown to be a homeomorphism. Alternative, but closely related, proofs were given for one-dimensional chains by [30] and [11].

The way the persistence results are applied to coupled map lattices differ from that in Section 2, however, as one would not usually start from a grand lattice with no coupling in time. Mind you, this latter concept, named the "anti-integrable limit" by Aubry [4], has proved extremely fruitful, and I will say a few words about it in Section 9. Instead one would start from the limit with no coupling in "space". If the dynamics of the individual units is uniformly hyperbolic, and uniformly so over the whole lattice, then the resulting orbits are uniformly hyperbolic and hence persist uniformly with respect to the coupling. For example, one could take a coupled map lattice with a Plykin attractor at one site and attracting fixed points at the others; this would result in an attractor with spatially localised chaos for weak coupling.

The continuous-time case is analogous, but complicated slightly by the fact that there is always time-translation degeneracy. This means that the definition of uniform

⁴Note the unfortunate clash of terminology which renders many elliptic PDE problems uniformly hyperbolic!

hyperbolicity needs to be adapted and to establish a persistence result we have to allow the time-parametrisation of the orbits to change with ϵ .

One aspect of uniform hyperbolicity which is important for applications is the robustness of uniformly hyperbolic orbits to small time-dependent perturbations. In fact, the notion of uniform hyperbolicity (using the above definition) is not at all limited to autonomous dynamical systems. In particular, if a system with a uniformly hyperbolic orbit is subjected to small forcing then the orbit has a unique continuation to a solution of the forced problem. In the most interesting case for applications, namely where the orbit is attracting, this solution represents the response for all initial conditions close to the original orbit. The solution can be found by continuation, as throughout these notes, and bounds can be deduced on the size of forcing for which one can be sure that the response remains within desired safety limits. Bishnani and I are in the process of developing such estimates, in continuous-time. We are particularly interested in adapting the measures of size of the forcing function. This technique should have a uniform extension to network problems.

Next I give the promised construction of the stable-unstable splitting for the tangent bundle on uniformly hyperbolic sets (in the discrete-time case). The construction of the splitting is the same for networks as for single dynamical systems; the only difference is that to deduce exponential decay estimates in time for a network we need to suppose suitable spatial structure for the coupling. Under this condition, we also obtain a finite coherence length property for the splitting.

If I - DH is invertible then given a tangent vector ξ at a point $x \in M$, define the tangent vector $\Xi \in TM^{\mathbb{Z}}$ along the orbit of x by

$$\Xi^0 = \xi, \tag{72}$$

and all other components zero. Define the tangent vectors

$$\xi^{-} = -DG_{G^{-1}x}\pi^{(-1)}(I - DH)^{-1}\Xi$$
(73)

$$\xi^+ = \pi^0 (I - DH)^{-1} \Xi, \tag{74}$$

at $x \in M$, where $\pi^t : M^{\mathbb{Z}} \to M$ is the component at time $t \in \mathbb{Z}$. Then ξ^- has bounded backwards orbit, ξ^+ has bounded forward orbit, and

$$\xi^{+} + \xi^{-} = \xi. \tag{75}$$

This is the desired splitting of ξ .

To show that the forwards, respectively backwards, orbits of ξ^{\pm} decay exponentially, note that for a single dynamical system or finite network we can use Case 1 of Section 4, where the one dimension is taken to be time. Thus $(I - DH)^{-1}\Xi$ decays exponentially in both directions of time, and its forward and backward parts are in fact the forward and backward orbits of ξ^{\pm} respectively. For an infinite network, or to obtain uniform results with respect to the size of the network, one has to impose hypotheses on the coupling which guarantee exponential decay of the matrix elements of $(I - DH)^{-1}$ in space-time. For example, the hypotheses Eq. (47) and (49) suffice for an arbitrary graph, as explained at the end of Case 2. Then summing over the t = constant sets in the space-time graph gives the desired exponential decay in time.

To complete the treatment of the splitting, we must show that the union E_x^+ of the ξ^+ over all tangent vectors ξ at a given point $x \in M$, and the union E_x^- of the ξ^- , are linear spaces forming a direct sum decomposition of TM_x . They are linear spaces because if ξ_1^+ and $\xi_2^+ \in E_x^+$ and $\alpha_1, \alpha_2 \in \mathbb{R}$, then let $\xi_\alpha = \alpha_1 \xi_1^+ + \alpha_2 \xi_2^+$ and apply Eq. (74), to deduce that $\xi_\alpha \in E_x^+$. Similarly E_x^- is a linear subspace. We already proved that every $\xi \in TM_x$ can be split into a sum of vectors in E_x^\pm . It is clear that $E_x^+ \cap E_x^- = 0$, because the orbit Ξ of any tangent vector ξ in the intersection is bounded in both directions of time and hence is a solution of $(I - DH)\Xi = 0$, so $\Xi = 0$ by the invertibility of I - DH.

Continuity of the splitting follows from the exponential decay. In particular, the dimensions (in the finite dimensional case) of E_x^{\pm} are constant over chain-transitive components of uniformly hyperbolic sets.

The spaces E^{\pm} are traditionally called "stable" and "unstable" subspaces, respectively, but this is confusing terminology, as the stable subspace is unstable with respect to the dynamics and the unstable one is stable. I prefer to call E_x^{\pm} the forward and backward contracting subspaces, respectively. Note again that some people use "expanding" for E_x^- , but the forward orbits of all vectors of $TM_x \backslash E_x^+$ are also eventually expanding.

For coupling with suitable spatial structure, the splitting can be shown to have a finite coherence length property, i.e. the matrix elements of the induced projections depends exponentially weakly on the distance between sites.

Forward and backward contracting manifolds can also be constructed from this point of view. They are the sets of points in M whose forward, respectively backwards, orbits converge together, and the content of the "stable manifold theorem" is that they are the images of injective differentiable immersions from the forward and backward contracting subspaces, respectively into M. Note again that I avoid the terms "stable", "unstable" and "expanding". "Expanding" is additionally dangerous here because it can happen (e.g. the separatrix for a frictionless pendulum, and in general any homoclinic tangency) that tangent vectors to a backward contracting manifold also contract in forwards time! It would be interesting to obtain uniform estimates on the sizes of the contracting manifolds, especially in the case of attractors, where the union of the stable manifolds is the basin of attraction.

7 Structural Stability

The persistence results of the previous Sections are very nice, but leave open an important question: how do we know that new equilibria, or periodic orbits, or other forms of recurrent motion are not created on adding small coupling? More strongly, is the uncoupled system structurally stable, uniformly in the size of the network?

A C^r -dynamical system ($r \ge 1$ throughout this section) is said to be C^r -structurally stable if all C^r -small enough perturbations are topologically equivalent to it. Two flows $\phi_i : M_i \times \mathbb{R} \to M_i, i = 1, 2$ are topologically equivalent if there is a homeomorphism $\Theta: M_1 \to M_2$ and a time-reparametrisation map $\tau: M_1 \times \mathbb{R} \to \mathbb{R}$ which is an orientation-preserving homeomorphism of \mathbb{R} for each $x \in M_1$, such that

$$\tau(\phi_1(x,t),t') = \tau(x,t+t') - \tau(x,t), \tag{76}$$

$$\phi_2(\Theta(x),\tau(x,t)) = \Theta(\phi_1(x,t)). \tag{77}$$

The broadest notion of recurrence is "chain recurrence". The chain-recurrent set R for a dynamical system $\dot{x} = G(x)$ is the set of points x which, for all $\eta > 0$, lie on a periodic solution of the differential inclusion

$$\dot{x} \in B(G(x), \eta), \tag{78}$$

the ball of radius η around G(x).

The basic result of finite-dimensional structural stability theory is that the chainrecurrent set is C^r -structurally stable if it is uniformly hyperbolic (and the converse is proved for r = 1). So under this condition, no new chain recurrent behaviour is generated under perturbation.

If one wants structural stability of transient behaviour too, it is necessary to strengthen the hypotheses. An AS system⁵ is one for which the chain recurrent set R is uniformly hyperbolic and for all $x, y \in R$, the stable manifold of x is transverse to the unstable manifold of y. Every AS system is C^r -structurally stable, and this is also proved to go both ways for r = 1. For an up-to-date introduction, see [31].

The question to ask here is whether structural stability can be proved with uniform estimates on the size of the network. This is almost certainly true. Hence we would deduce that in the example of Section 2, for instance, no new equilibria are created for $|\epsilon| < \epsilon_2$, some $\epsilon_2 > 0$, and in this range the dynamics is topologically equivalent to the uncoupled case. In particular, for this range of ϵ , no travelling front solutions would exist, i.e. solutions with a region of units essentially in the 0-state and a region of units essentially in the 1-state, separated by a front which moves. This is known as "propagation failure" [16].

8 Normally Hyperbolic Sets

Let us now return to the question of what happens if several (say N) units, each with an attracting periodic orbit are coupled together weakly, the remaining units having attracting equilibria. The product system then has an attracting invariant torus of dimension N. I believe that this N-torus persists for small coupling, uniformly in the system size, subject to some uniformity in the attraction rates and periods of the periodic orbits. The dynamics on the N-torus, however, can and indeed typically will, become more complicated than the uncoupled case (for which the flow is conjugate to a uniform translation).

To justify this, consider the more general problem of persistence of normally hyperbolic sets. Roughly speaking, these are invariant subsets with a tangent bundle T (e.g. a submanifold, but solenoids are also allowed, for instance), such that expansion

⁵Following [32], "AS" stands for "Axiom A and Strong Transversality Condition".

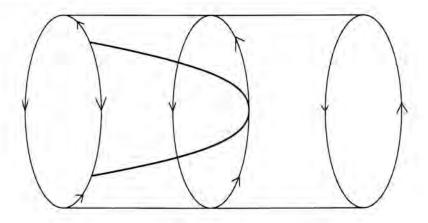


Figure 1: The attracting invariant cylinder for an uncoupled neuron.

and contraction in T is weaker than expansion and contraction in the normal bundle N (i.e. the total tangent space modulo T). There is a well established theory of persistence of normally hyperbolic sets for finite dimensional systems (e.g. [36]). The issue I wish to address is whether for a network the persistence results can be made uniform in its size.

The discrete-time case of this question was investigated by [11]. It would be interesting to check that everything works for the continuous-time case also. This would, for example, justify the reduction of a system of weakly coupled oscillators with attracting periodic orbits to a system of phase equations

$$\dot{\theta} = F(\theta), \theta \in (S^1)^S. \tag{79}$$

In the case that the motion is close to a rational rotation, averaging could then be used to reduce to phase-difference equations as proposed by [19], up to a small remainder term.

Another very interesting problem to study, which would be greatly helped by such a result on persistence of normally hyperbolic sets for networks, is a model that I wish to propose for (physiological) neural networks. Think of a neuron as a dynamical system given by the unfolding of a saddle-node on a cycle together with slow evolution in the "parameter", depending on the inputs (and its own state, but I will regard that as a coupling effect too). Thus the uncoupled neuron has a normally hyperbolic attracting invariant cylinder in its phase space, as sketched in Figure 1.

An uncoupled network of N such units has a normally hyperbolic N-cylinder (i.e. product of N cylinders). Assume that the effect of neuron s going round the cylinder is to cause a slight parameter increase or decrease (depending whether the coupling is excitatory or inhibitory) on all neurons to which it outputs, including possibly itself. Then, provided the coupling is integrable in some sense, we expect the product system to continue to have a normally hyperbolic N-cylinder on which the motion is close to the uncoupled case, but with more interesting dynamics. The question is what sort of dynamics can it exhibit? In particular, can it exhibit "intelligence"?

9 Conservative case: equilibria

For Sections 9 and 10, I specialise to the case of Hamiltonian systems and their close relatives: time-reversible systems. A system is *Hamiltonian* if it can be written in the form

$$\dot{z} = JDH(z),\tag{80}$$

where J is the isomorphism from 1-forms to tangent vectors induced by a symplectic form ω , by

$$\omega(J\eta,\xi) = \eta(\xi), \forall \xi. \tag{81}$$

It is time-reversible if

$$\dot{z} = F(z) = -DR^{-1}F \circ R(z),$$
(82)

for some involution R, which shall be required to reverse precisely half the dimensions. The intersection of the two categories is especially relevant, in particular with the added condition that R be anti-symplectic, i.e.

$$DR^{-1}JDR = -J. \tag{83}$$

A basic example which we shall treat is

$$\ddot{x}_s + V'(x_s) = \epsilon \sum_{r \in N_s} g_{rs}(x_r - x_s), \tag{84}$$

where N_s is the set of neighbours of site s in a graph S, g_{rs} is symmetric, and $x_s \in \mathbb{R}$. This is Hamiltonian with

$$H(x,p) = \sum_{s \in S} \left(\frac{1}{2}p_s^2 + V(x_s)\right) + \frac{\epsilon}{2} \sum_{d(r,s)=1} g_{rs}(x_r - x_s)^2, \tag{85}$$

where the second sum is over unordered pairs (r, s), and time-reversible with (antisymplectic) involution

$$R(x,p) = (x,-p).$$
 (86)

Persistence of equilibria for such systems is a special case of persistence of equilibria for general networks, so does not require special treatment. Nonetheless, there is a slight improvement which can be made using the Hamiltonian structure. Instead of solving JDH(z) = 0 one can solve G(z) := DH(z) = 0, and so DG is symmetric, which can improve estimates, particularly on the exponential decay. This approach has been powerful in deducing interesting results for symplectic twist maps, because their orbits are equivalent to the equilibria of an associated one-dimensional translation-invariant nearest neighbour chain. The uncoupled case is a singular limit from the symplectic map point of view, christened the "anti-integrable limit" by Aubry. The ideas were first developed by [4] and [35], and subsequently used to construct many interesting types of orbit for symplectic twist maps, e.g. cantori of various types [7, 26], and bifurcations [3, 17].

Note that one special feature of the Hamiltonian case is that the signature of the second variation D^2H of the Hamiltonian can not change as long as D^2H remains

non-degenerate. This does not prevent stability change, but limits the possibilities. In particular, if it starts definite it must remain definite and the equilibrium remains stable as long as it can be continued (in fact, fully so with respect to ℓ_2 -norm, not just linearly, though in general not with respect to sup-norm). If D^2H starts indefinite then we can nonetheless deduce a range of ϵ for which the stability type of the equilibrium remains unchanged, as in Section 3, provided some additional hypotheses are satisfied (separation of spectrum with opposite signatures). The notion of stability type has to be refined in the conservative case to allow a central component in the splitting and to take account of the Krein signature of pure imaginary spectrum (e.g. [21]).

10 Conservative case: periodic orbits

In contrast to the case of equilibria, continuation of periodic orbits of conservative systems requires special treatment. This is because for an autonomous Hamiltonian system every periodic orbit is degenerate, owing to energy conservation. Of course, this is easily dealt with by restricting the vector field to an energy surface, giving a family of systems with one extra parameter, namely the energy. But it can be dealt with in other ways and I shall discuss one.

Similarly, symmetric periodic orbits of time-reversible systems, that is orbits which are sent to their time-reverse by the involution R, are automatically degenerate, because denoting the total dimension by 2N, symmetric periodic orbits correspond to intersections of the orbit ((N + 1)-dimensional) of a reflection surface with the reflection surface (N-dimensional), which is 1-dimensional if transverse. This problem is not as easily dealt with as the autonomous Hamiltonian case, and thus the method I will sketch is particularly useful.

The method that Aubry and I proposed for these two classes of problems is to assume anharmonicity and to continue at constant period [24]. Anharmonicity means that the period of the orbit varies non-trivially with respect to energy (or appropriate parameter) along the family of periodic orbits. Of course, anharmonicity is not always present, and then other approaches are required, but it is a common case.

This method allows us to construct "self-localised vibrations" [24, 23], discovered numerically by [33], and named "discrete breathers" by [10] and "nonlinear localised excitations" by [15].

As I ran out of time to write up these notes, my treatment of this problem will be regrettably brief. The reader is referred to [24] for more details and to [23] for some suggestions for directions for future work.

I begin with the simplest case, namely "1-site breathers". Each unit of the uncoupled network is assumed to be a Hamiltonian or time-reversible system and to possess a one-parameter family of periodic orbits. We parametrise the family by the *action* $I = \int p.dq$ in the Hamiltonian case, and some analogous measure of its size in the time-reversible case (if not also Hamiltonian). Denote its period by T(I). For $\epsilon = 0$, choose a periodic orbit of the local system on one unit $o \in S$ and put all other units on equilibrium points. This gives a periodic orbit γ of the product system.

Hypotheses 1. Anharmonicity: $dT/dI \neq 0$ for the chosen periodic orbit of unit o. 2. Non-resonance: $d(\{\omega_s : s \in S \setminus \{o\}\}, \omega\mathbb{Z}) > 0$, where $\omega = 2\pi/T$ and ω_s is the frequency of infinitesimal vibrations about the equilibrium on site s.

3. Uniformity: The vector field is C^1 with respect to sup norm over sites, with uniform bounds with respect to the size of the network.

Theorem 3 Under hypotheses 1, 2 and 3, γ has a unique (up to phase shift) continuation $\gamma(\epsilon)$ as a periodic orbit of the same period T for $|\epsilon| < \epsilon_0$, for some $\epsilon_0 > 0$, uniformly in the size of the network.

Our proof is by the implicit function theorem for a C^1 function Φ from a space of C^1 loops to a space of C^0 loops, as in Section 5, but here we work with fixed period T and impose some restrictions related to the Hamiltonian or time-reversible structure. The point of the above hypotheses is to make $D\Phi$ invertible; physically, they allow the breather to detune from the phonons and avoid harmonics of the frequency falling in the phonon band. It should be possible to do a proof in a space of Fourier coefficients too; indeed this was our original approach but we ran into technical problems making sure that Φ was C^1 . I have subsequently found out how to prove this and intend to write up the proof soon.

In [24] we also prove finite coherence length for breathers in one-dimensional nearest neighbour chains. This can easily be generalised to other forms of network with suitable spatial structure, e.g. any which fit cases 1,2 or 3 of Section 4.

One question is what estimates on the continuation we can obtain. We did not yet obtain any explicit estimates, as one step in our proof was to transform to actionangle variables at the excited site, and the continuation estimates will depend on the size of the derivative of this transformation and its inverse, which in general are not explicitly calculable. However, they are calculable for certain potentials and estimable for many others, and it would be very interesting to do this and work out some explicit estimates for the continuation of breathers. Once the Fourier coefficient proof is available, I believe that it would be the best one to use, as I think it is better adapted to the problem.

Another question is about stability of the resulting breathers. One can not expect them to be linearly stable uniformly in the system size, because of the possibility of constructive interference of phonons. I believe, however, that the 1-site breathers obtained above are linearly stable in ℓ_2 for $\epsilon < \epsilon_1$, for some $\epsilon_1 > 0$ uniform in the system size, provided that the non-resonance condition is strengthened to the following:

Stability condition There exists r > 0 such that $d(\{e^{i\omega_s T} : s \neq o\}, \{e^{-i\omega_s T} : s \neq o\} \ge r$, where ω_s is the frequency of infinitesimal vibrations about the equilibrium for site s, with sign chosen according to the signature of the second variation of the Hamiltonian there (positive for the minima of V in the example of Eq. (84)).

In particular, ω must avoid $2|\omega_s|/n$ for all $n \in \mathcal{N}$, $s \in S$. The reason for the stability condition is that it ensures that no collisions of Floquet multipliers of opposite Krein signature can occur, which implies spectral stability is preserved (e.g. [2]). As

before, it should be true that the spectrum moves controllably with respect to ϵ and hence the existence of ϵ_1 will follow.

It is unlikely that the breathers would be fully stable, as the usual arguments about the set of KAM tori not dividing phase space apply as soon as the number of sites exceeds two. However, they are Nekhoroshev stable, meaning that if you start close (in ℓ_2 -norm) then you stay close for an exponentially long time [9].

The next issue is existence of multi-site breathers. Here again, the interested reader is referred to [24], where we construct them for time-reversible systems subject to two conditions on the solution in the uncoupled case: firstly, there must be a common period, satisfying the non-resonance condition, and secondly, there must be an origin of time with respect to which the solution is time-symmetric. In that paper, we also suggested a method for proving existence of multisite breathers without using timereversal invariance. I have subsequently come up with what I believe will be a better approach, a Melnikov-type method, which I hope to write up soon. N-site breathers will correspond to critical points of a function on an (N - 1)-torus. There should be relations between the spectral stability type of the breather and the index of the critical point. The (N - 1)-torus should give a non-invariant but Nekhoroshev-stable N-torus in the phase space.

It should not be necessary to have an "uncoupled" case from which to continue breathers. Any starting point possessing non-degenerate breathers would suffice; this is probably the case for Flach's breathers in homogeneous Fermi-Pasta-Ulam chains [14], for example. Furthermore, the anharmonicity condition is probably not really required: one could continue at constant energy rather than constant period. This would allow one to prove existence of impurity modes for nonlinear systems, by continuation from the linear case.

Another question is about existence of quasiperiodic breathers. There are works (e.g.[18]) which prove existence of invariant N-tori of quasiperiodic motions for N = 2, 3, ... in large and infinite-dimensional Hamiltonian systems, but it is not clear whether they can be applied here. Also, in some numerics (e.g. [34]) travelling breathers are observed, and it is a challenge to try to prove or disprove their existence.

The real issue with discrete breathers is to explain why typical initial conditions seem to be "attracted" to a distribution of breathers. My guess [23] is that it is a similar phenomenon to the stickiness of elliptic islands for area-preserving maps, but this merits much investigation. Then it would be very interesting to develop their physical significance and investigate their role for statistical mechanics.

11 Limits to continuation

I conclude by raising two questions which I am not yet in a position to answer: what are the limits to continuation, and what happens beyond?

Firstly, how are equilibria or periodic orbits or uniformly hyperbolic sets or normally hyperbolic sets of a network lost (if at all) as coupling increases? It is clear that they can undergo bifurcations just as for finite-dimensional systems, but are there new possibilities for infinite networks? Aubry and Marin are investigating this numerically for the case of discrete breathers.

A simpler setting in which quite a lot can be understood is the bifurcations of the set of equilibria for 1D nearest neighbour chains of particles in a cubic potential, because this reduces to studying orbits of the area-preserving Hénon map. The analogues of the breathers are the orbits whose symbol sequence has all but finitely many 0s in the uncoupled case (0 labelling the potential well and 1 labelling the local maximum). In particular, the first bifurcation is known to be the annihilation of the symbol sequences $0^{\infty}1010^{\infty}$ and $0^{\infty}1110^{\infty}$ (Smillie), which occurs without loss of finite coherence length, but the symbol sequences $0^{\infty}10^{\infty}$ and $0^{\infty}110^{\infty}$ almost certainly are lost by annihilation together with 0^{∞} and 1^{∞} , and the coherence length goes to infinity there.

Secondly, what new phenomena lie beyond the regime of continuation from the uncoupled limit? This is a particularly interesting question in the case of loss of a uniformly hyperbolic attractor.

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Spatial patterns, spatial chaos, and traveling waves in lattice differential equations

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Abstract

We survey recent results in the theory of lattice differential equations. Such equations yield continuous-time, usually infinite-dimensional, dynamical systems, which possess a discrete spatial structure modeled on a lattice. The systems we consider, generally over a higher-dimensional lattice such as $\mathbb{Z}^D \subseteq \mathbb{R}^D$, are the simplest nontrivial ones which incorporate both local nonlinear dynamics and short range interactions. Of particular interest are stable equilibria, and the regular patterns, or lack thereof, that are displayed. Traveling wave solutions in such systems are also discussed.

1 Introduction

By a lattice differential equation or LDE we mean a system of ordinary differential equations, often of infinite order, in which the state vector $u = \{u_\eta\}_{\eta \in \Lambda}$ is coordinatized by a set Λ , the lattice, which possesses some underlying spatial structure. Typical choices of $\Lambda \subseteq \mathbb{R}^D$ are the *D*-dimensional integer lattices \mathbb{Z}^D , the hexagonal lattice in the plane, and the crystallographic lattices in three dimensions. When numerical simulations of such systems are performed, one takes a finite, usually large, subset of the infinite lattice.

A general autonomous LDE on a lattice Λ can be written as

$$\dot{u}_{\eta} = g_{\eta}(u), \qquad \eta \in \Lambda,$$
 (1.1)

where each $u_{\eta} \in \mathbb{R}^{N}$ is a finite-dimensional variable, and $u = \{u_{\eta}\}_{\eta \in \Lambda}$ is the state vector. Of course, the nonlinearities g_{η} should reflect the geometry of the lattice. For example, for a so-called *short range interaction* each g_{η} depends only on those coordinates u_{ξ} with $d(\xi, \eta) \leq \nu$ for some ν , where $d(\cdot, \cdot)$ denotes the metric on Λ . It is also typical to impose some growth or boundedness condition on u_{η} (as a function of η) in order that the initial value problem for Eq. (1.1) be well-posed. This restricts u to some Banach space X, for example $u \in X = l^{p}(\Lambda)$, where

$$l^{p}(\Lambda) = \{ u : \Lambda \to \mathbb{R}^{N} \mid ||u||_{p} < \infty \},$$
$$||u||_{p} = \left(\sum_{\eta \in \Lambda} |u_{\eta}|^{p} \right)^{1/p} \text{for } p < \infty, \qquad ||u||_{\infty} = \sup_{\eta \in \Lambda} |u_{\eta}|,$$

(see, for example, [1]), and so $g_{\eta} : X \to \mathbb{R}^N$ for each $\eta \in \Lambda$. We shall generally take $X = l^{\infty}(\Lambda)$, meaning that $\eta \in \Lambda \to u_{\eta}$ is bounded in η for each state vector $u = \{u_{\eta}\}_{\eta \in \Lambda}$.

If the g_{η} are such that $g: X \to X$ is locally Lipschitz with respect to the norm in X, and where we denote $g = \{g_{\eta}\}_{\eta \in \Lambda}$, then for any $u^{0} \in X$ the initial value problem

$$u_{\eta}(0) = u_{\eta}^{0}$$

is well-posed for Eq. (1.1), and yields a unique solution u(t) for $t \in I$, that is, $u: I \to X$, on some open interval I containing t = 0. The proof of this fact is essentially the same as the proof of the corresponding result for ODE's.

Lattice differential equations are of particular interest in modeling a wide variety of applications in which spatial structure plays a role, particularly when the spatial structure has a discrete character. Many models are to be found in chemical reaction theory [32, 44], image processing and pattern recognition [22, 23, 24, 34, 59], material science [10, 25, 38], and biology [7, 8, 29, 30, 39, 40, 42, 64]. Much has been done on chains of coupled oscillators, usually arising in biology or electronics (Josephson junctions); see for example [4, 5, 29, 30, 32, 41, 42, 43, 52, 54, 56, 57], and the references therein. See also the papers [46, 49, 50, 51]. Coupled-map lattices, namely lattice systems with discrete time, is a closely related subject; see, for example, [2, 3], and [21].

The numerical and experimental work of Leon Chua and his collaborators, and Martin Hasler and his collaborators, are strong motivations for our work. They consider equations (the so-called CNN, or *Cellular Neural Network* systems) very similar to (2.1) below, and are developing algorithms based on these equations which identify various prescribed patterns, for example edges, or corners, in a digitized image. The CNN equations are more complicated than Eq. (2.1), as they contain a separate coupling coefficient for each of the eight neighbors in the 3×3 square in \mathbb{Z}^2 centered at (i, j), instead of our two coefficients α^+ and α^{\times} . In part, our motivation in studying Eq. (2.1) is to attempt to provide a theoretical framework for understanding these more complicated systems. Besides numerical investigations, Chua has constructed an electrical circuit on a chip which simulates the CNN system. See, for example, [22], [23], [24], [59], [63], and the references therein.

Of course partial differential equations are extensively used to model spatial structures in systems, and one naturally obtains an LDE upon making a spatial discretization of the PDE. For example, let $f : \mathbb{R} \to \mathbb{R}$ and $\alpha \in \mathbb{R}$, and consider the system

$$\dot{u}_i = \alpha (u_{i+1} + u_{i-1} - 2u_i) - f(u_i), \qquad i \in \mathbb{Z}, \tag{1.2}$$

on the integer lattice $\Lambda = \mathbb{Z}$. For large α , the system (1.2) arises as a discretization of the so-called Allen-Cahn, or Chafee-Infante, or Nagumo equation,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - f(u), \qquad x \in \mathbb{R},$$
(1.3)

where $\alpha = h^{-2}$, with $0 < h \ll 1$ the grid size. On the other hand, much theoretical work in lattice differential equations concerns one-dimensional lattices with weak coupling $0 < \alpha \ll 1$, between lattice sites. In [45], for example, an uncountable set of stable equilibria were obtained for (1.2), via a perturbation from $\alpha = 0$. Our interest here, by contrast, is with lattice systems in arbitrary dimensions, with coupling coefficients varying throughout a broad range which includes both weak and strong couplings. This is certainly the case in the pattern recognition and material science models above, and as well in the cardiac model [64]. In many models, LDE's do not necessarily arise from PDE's, but rather occur as systems in their own right, and as such need not be "near" a continuum limit PDE. We note that the initial value problem for Eq. (1.2) is mathematically well-posed (in $l^{\infty}(\mathbb{Z})$) for any choice of α , including $\alpha < 0$, as long as f is locally Lipschitz. Equation (1.2) can be considered, and indeed does arise in the above models, for essentially any value of α . Some of the most interesting phenomena are to be found for ranges of α , including $\alpha < 0$, far away from the PDE limit.

Some phenomena of particular interest which we shall discuss in this article are pattern formation, spatial chaos, and traveling waves. The first two, pattern formation and spatial chaos, pertain to equilibrium solutions, specifically to stable equilibrium solutions, of Eq. (1.1). An equilibrium $u \in X$ of Eq. (1.1) is a time-independent solution, that is, a solution to g(u) = 0. By a stable equilibrium we mean stability in the usual Lyapunov sense in the phase space X. Traveling waves, on the other hand, are solutions which vary in time, assuming a fixed spatial profile which moves at constant speed in a given direction. Such solutions have been much studied for PDE's, but their theory for LDE's is considerably more complicated, and still in its infancy.

Much of the work we describe herein is given more fully in [11], [18], and [19], for pattern formation and spatial chaos, and in [13], [17], and [47], for traveling waves. The numerical results [12] provided a strong initial stimulus for our theoretical studies. We finally mention the survey articles [16], [48], and the tutorial article [20] which discuss various aspects of this subject.

2 Pattern formation via bifurcations

In Section 4 we shall give precise definitions of pattern formation and spatial chaos, at least for a particular class of LDE's. To understand one mechanism which can generate patterns, let us consider a two-dimensional version

$$\bar{u}_{i,j} = \alpha^+ (\Delta^+ u)_{i,j} + \alpha^\times (\Delta^\times u)_{i,j} - f(u_{i,j}), \qquad (i,j) \in \mathbb{Z}^2,$$
(2.1)

of (1.2) on the lattice $\Lambda = \mathbb{Z}^2$. Here Δ^+ and Δ^{\times} correspond to discrete Laplace operators based on +- and \times -shaped stencils, given by

$$(\Delta^+ u)_{i,j} = \left(\sum_{|a-i|+|b-j|=1} u_{a,b}\right) - 4u_{i,j}, \qquad (\Delta^\times u)_{i,j} = \left(\sum_{|a-i|=|b-j|=1} u_{a,b}\right) - 4u_{i,j},$$

respectively. The parameters $\alpha^+, \alpha^{\times} \in \mathbb{R}$ are the so-called *coupling coefficients*, and they can be of either sign or of any magnitude. Typical choices of f have the form

$$f_{1}(z) = (z^{2} - 1)(z - a), \qquad -1 < a < 1,$$

$$f_{2}(z) = \gamma z + cz^{3}, \qquad \gamma \in \mathbb{R}, \quad c > 0, \qquad (2.2)$$

$$f_{3}(z) = (\gamma - 2)z + \log((1 + z)/(1 - z)), \qquad \gamma \in \mathbb{R}, \quad -1 < z < 1.$$

For such f the ODE $\dot{z} = -f(z)$ has either a globally stable equilibrium, or exhibits bistable behavior. We may think of Eq. (2.1) as one of the simplest nontrivial lattice differential equation which combines both short range interaction in a higher-dimensional lattice, with nonlinear dynamics.

For the bifurcation analysis of this section, we shall assume (for simplicity) that f is odd and sufficiently smooth. We seek two types of equilibrium solutions: stripes (horizontal or vertical), and checks. We are in part motivated by the numerical simulations of [12], in which a system very similar to (2.1), namely the discrete Cahn-Hilliard equation

$$\dot{u}_{i,j} = -(\Delta^+ + \Delta^\times) \left(\alpha^+ (\Delta^+ u)_{i,j} + \alpha^\times (\Delta^\times u)_{i,j} - f(u_{i,j}) \right), \quad (i,j) \in \mathbb{Z}^2, \quad (2.3)$$

with $f = f_3$, was studied. In these numerical simulations, a wide variety of patterns, including stripes and checks, were observed. Beginning with a random choice of values $u_{i,j}^0 \in (-1,1)$ for the initial condition, on a large rectangular sublattice of \mathbb{Z}^2 with standard (periodic or Neumann) boundary conditions, Eq. (2.3) was solved numerically. It was observed that an initial rapid coarsening (as with the corresponding PDE) first occurred, in which spatial patterns sometimes emerged. Often different patterns, separated by interfaces, appeared in different regions of the lattice. Figure 1 depicts several such solutions at this stage. Then, in many cases, the interfaces slowly moved as the solution u(t) tended toward an equilibrium state.

Let us return to Eq. (2.1). A pattern of vertical stripes takes the form $u_{i,j} = (-1)^i k$ for some $k \in \mathbb{R}$, and for such u we have $(\Delta^+ u)_{i,j} = -4(-1)^i k$ and $(\Delta^\times u)_{i,j} = -8(-1)^i k$ by a simple calculation. One sees that such u is an equilibrium of Eq. (2.1) if and only if

$$0 = -(4\alpha^{+} + 8\alpha^{\times})k - f(k)$$
(2.4)

(note the oddness of f is used here). The same condition (2.4) holds for horizontal stripes $u_{i,j} = (-1)^{j}k$. A checkerboard, on the other hand, is given by $u_{i,j} = (-1)^{i+j}k$ for some k. For this we have $(\Delta^{+}u)_{i,j} = -8(-1)^{i+j}k$ and $(\Delta^{\times}u)_{i,j} = 0$, so u is an equilibrium of (2.1) if and only if

$$0 = -8\alpha^{+}k - f(k).$$
 (2.5)

We see that both Eqs. (2.4) and (2.5) take the form

$$0 = \lambda k - f(k), \tag{2.6}$$

Spatial patterns, spatial chaos, and traveling waves

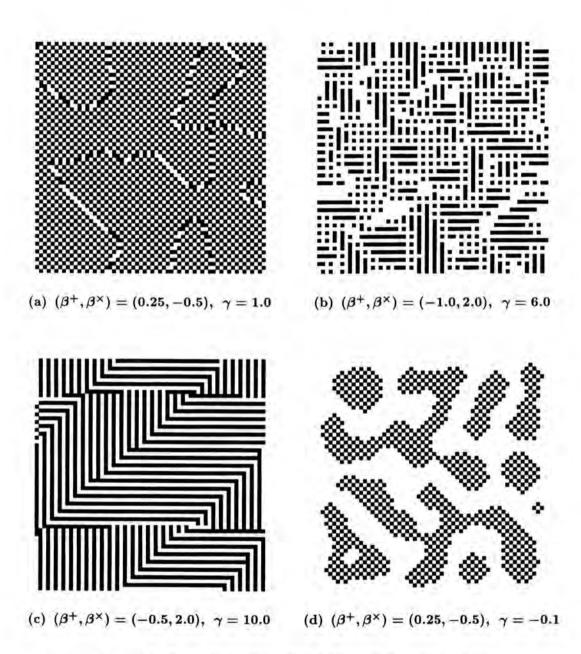


Figure 1: Some Numerical Simulations of Equation (2.3)

where $\lambda = -(4\alpha^+ + 8\alpha^*)$, respectively, $\lambda = -8\alpha^+$, in (2.4) and (2.5). Equation (2.6) can be analyzed by elementary methods, and one sees that this equation undergoes a simple bifurcation (generically a pitchfork) at $\lambda = f'(0)$.

To be specific, let us suppose that $f'(0) = \gamma > 0$ and f'''(0) = 6c > 0, such as for $f = f_2$ or f_3 with $\gamma > 0$, for example. Then Eq. (2.6) possesses the nontrivial solutions $k \sim \pm ((\lambda - \gamma)c^{-1})^{1/2}$ for $\lambda > \gamma$ and λ near γ , arising from the origin as a supercritical pitchfork bifurcation. For convenience let us also write

$$\beta^+ = -\alpha^+, \qquad \beta^\times = -\alpha^\times \tag{2.7}$$

(we shall use the notation (2.7) throughout this article), so that Eq. (2.1) becomes

$$\dot{u}_{i,j} = -\beta^+ (\Delta^+ u)_{i,j} - \beta^\times (\Delta^\times u)_{i,j} - f(u_{i,j}), \qquad (i,j) \in \mathbb{Z}^2.$$
(2.8)

Then with our assumptions on f, the local bifurcation of stripes, respectively, checks, occurs on and to the right of the lines

$$4\beta^+ + 8\beta^{\times} = \gamma, \qquad 8\beta^+ = \gamma, \tag{2.9}$$

respectively, in the $(\beta^+, \beta^{\times})$ -plane.

To study the interaction of the above stripe and check solutions, one needs to consider a higher dimensional bifurcation problem. Consider states u which are of (spatial) period 2 in both the horizontal and vertical directions, so $u_{i+2,j} = u_{i,j+2} = u_{i,j}$ for all $(i, j) \in \mathbb{Z}^2$. The set of all such u forms a four-dimensional vector space which is invariant under the dynamics of Eq. (2.8), and any such u can be written uniquely as

$$u_{i,j} = (-1)^{i} v + (-1)^{j} w + (-1)^{i+j} x + y, \qquad (2.10)$$

for $(v, w, x, y) \in \mathbb{R}^4$. One sees that the coordinates v, w, x, y represent, respectively, vertical stripes, horizontal stripes, checks, and a solid pattern. With respect to the coordinate system (2.10), one sees after a calculation that Eq. (2.8) becomes

$$\begin{split} \dot{v} &= (4\beta^{+} + 8\beta^{\times} - \gamma)v - g_{1}(v, w, x, y), \\ \dot{w} &= (4\beta^{+} + 8\beta^{\times} - \gamma)w - g_{2}(v, w, x, y), \\ \dot{x} &= (8\beta^{+} - \gamma)x - g_{3}(v, w, x, y), \\ \dot{y} &= -\gamma y + g_{4}(v, w, x, y), \end{split}$$
(2.11)

Here we have separated the linear part of the vector field from the higher order terms $g_i : \mathbb{R}^4 \to \mathbb{R}$. Each g_i depends only on f, and satisfies

$$g_i(v, w, x, y) = O(|v|^3 + |w|^3 + |x|^3 + |y|^3)$$

near the origin. A number of symmetries, which in fact form a group of order 16, are also present in the system (2.11); for example, the vector field in (2.11) commutes with

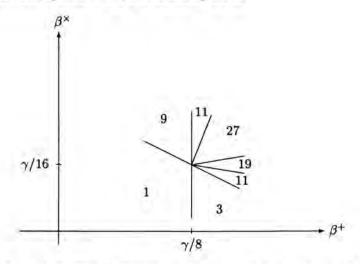


Figure 2: The Bifurcation Diagram for Equation (2.11)

the transformations $(v, w, x, y) \rightarrow (w, v, x, y)$ which exchange vertical and horizontal stripes.

The two bifurcation lines (2.9) intersect at the point $(\beta^+, \beta^{\times}) = (\gamma/8, \gamma/16)$ in parameter space, and one sees at that point that the linearization of (2.11) at the origin has a three-dimensional kernel, with one negative eigenvalue $-\gamma < 0$ in the y direction. Therefore, there exists a center manifold

$$y = \Phi(v, w, x, \beta^+, \beta^\times) \tag{2.12}$$

for (β^+, β^\times) near $(\gamma/8, \gamma/16)$, which passes through the origin (v, w, x, y) = (0, 0, 0, 0)and is tangent to the (v, w, x)-subspace at that point. Substitution of (2.12) into the system (2.11) yields a reduced three-dimensional system. With the techniques of bifurcation theory, all the (local) equilibria of (2.11), along with their stability, can be determined. This analysis yields the bifurcation diagram in Fig. 2, which depicts the number of such equilibria in terms of the parameters (β^+, β^\times) near $(\gamma/8, \gamma/16)$ (we continue here to assume that $f'(0) = \gamma > 0$ and f'''(0) > 0, with f odd). In addition to the stripe and check solutions noted above, various other equilibria which are hybrids of stripes and checks also occur, however, none of these hybrids are stable for the system (2.11). In fact, the stripe and check solutions are only stable over a portion of the parameter space, and are unstable for other parameter values, even some of those near the bifurcation point.

In addition to the equilibria, the dynamics of (2.11) can be studied. Equation (2.11) possesses a global Lyapunov function; in fact, the system (2.8) on the finite $m \times n$ lattice

$$F_{m,n} = \{0, 1, 2, \dots, m-1\} \times \{0, 1, 2, \dots, n-1\}$$
(2.13)

with periodic boundary conditions possesses the Lyapunov function

$$\begin{split} V(u) &= -\sum_{i=1}^{m} \sum_{i=1}^{n} \left(\frac{\beta^{+}}{2} \left((u_{i+1,j} - u_{i,j})^{2} + (u_{i,j+1} - u_{i,j})^{2} \right) \\ &+ \frac{\beta^{\times}}{2} \left((u_{i+1,j+1} - u_{i,j})^{2} + (u_{i+1,j-1} - u_{i,j})^{2} \right) - F(u_{i,j}) \right), \\ F'(z) &= f(z), \end{split}$$

If $F(z) \to \infty$ at a rate faster than quadratic as $z \to \pm \infty$, then $V(u) \to \infty$ as $|u| \to \infty$. In this case the system (2.8) on $F_{m,n}$ is dissipative, and so possesses a maximal compact attractor $A \subseteq \mathbb{R}^{mn}$. The set A contains all equilibria of (2.8), and every solution u(t) of (2.8) tends to an equilibrium (or a connected set of equilibria) as $t \to \infty$. Solutions lying on the attractor A are precisely those for which u(t) is bounded as $t \to \pm \infty$. Equivalently, A consists of the set of all equilibria together with their center-unstable manifolds. Various topological tools, such as the Conley index and the Conley connection matrix, can be used to study the structure of A in terms of solutions connecting various equilibria. If in particular m = n = 2, we obtain the system (2.11), and even here we obtain a very intricate picture of connecting orbits and their bifurcations.

3 Mosaic solutions: existence and stability

In contrast to the above bifurcation analysis, which is local and is restricted to the 2×2 -periodic problem, one seeks a more global picture of the equilibria of the full system (2.8). One approach, taken in [27] and [55], is to consider (2.8) with the so-called "double-obstacle" nonlinearity given by a set-valued function

$$f(z) = \begin{cases} \gamma z \text{ if } |z| < 1, & f(1) = [\gamma, \infty), \\ \emptyset & \text{if } |z| > 1, & f(-1) = (-\infty, -\gamma]. \end{cases}$$
(3.1)

Here one interprets the system (2.8) with this set-valued f as a differential inclusion. Observe that the graph of f consists of a linear piece in |z| < 1, together with vertical lines at $z = \pm 1$, and in a sense is a cartoon of the logarithmic function f_3 in (2.2), or even of the cubic function f_2 . It is the case, proved in [18], that for any (β^+, β^\times) and γ , any initial value problem

$$u_{i,j}(0) = u_{i,j}^0, \quad (i,j) \in \mathbb{Z}^2,$$

for (2.8) possesses a unique solution u(t) in the forward direction $t \ge 0$, provided that $|u_{i,j}^0| \le 1$ for each (i, j). (By definition, one requires for any such solution that $|u_{i,j}(t)| \le 1$ for all (i, j) and t, as $f(z) = \phi$ for |z| > 1.) The system (2.8), with (3.1), in fact generates a semiflow in the phase space $[-1, 1]^{\mathbb{Z}^2} \subseteq l^{\infty}(\mathbb{Z}^2)$, consisting of all $u = \{u_{i,j}\}_{(i,j)\in\mathbb{Z}^2}$ with $|u_{i,j}| \leq 1$ for all (i, j), with the l^{∞} topology. (In general, if Y and Z are any two sets, we let Y^Z denote the set of all functions $u : Z \to Y$.) Also, in light of the above existence and uniqueness result, it makes sense to talk about stable (in the usual Lyapunov sense) equilibria.

An equilibrium of (2.8), (3.1), is an element $u \in [-1, 1]^{\mathbb{Z}^2}$ for which the inclusion

$$0 \in -\beta^{+} (\Delta^{+} u)_{i,j} - \beta^{\times} (\Delta^{\times} u)_{i,j} - f(u_{i,j}), \qquad (i,j) \in \mathbb{Z}^{2},$$
(3.2)

holds. In many cases, one has that $u_{i,j} \in \{-1, 0, 1\}$ for all (i, j), for such equilibria; for example, the search for stripes $u_{i,j} = (-1)^i k$ or $(-1)^j k$, and checks $u_{i,j} = (-1)^{i+j} k$, leads to the problem $0 \in \lambda k - f(k)$, which is analogous to (2.6). If $\lambda < \gamma$ then the only solution to this is k = 0, while if $\lambda > \gamma$ we have k = 0 and $k = \pm 1$ as solutions. Motivated by this, we make the following definitions.

Definition 1 A mosaic is a function $u : \mathbb{Z}^2 \to \{-1, 0, 1\}$, that is, a doubly-indexed sequence $\{u_{i,j}\}_{(i,j)\in\mathbb{Z}^2}$ with $u_{i,j} \in \{-1, 0, 1\}$ for all $(i, j) \in \mathbb{Z}^2$. We let $\mathcal{M} = \{-1, 0, 1\}^{\mathbb{Z}^2}$ denote the set of all mosaics.

Definition 2 A mosaic solution of (2.8), with (3.1), is a mosaic $u \in \mathcal{M}$ which is an equilibrium solution, that is, which satisfies (3.2).

It is not hard to rewrite the condition (3.2), for mosaics, as follows. For any $u \in \mathcal{M}$, define the quantities

$$\begin{aligned} \sigma_{i,j}^+ &= \sum_{|a-i|+|b-j|=1} u_{a,b}, & \sigma_{i,j}^\times &= \sum_{|a-i|=|b-j|=1} u_{a,b}, \\ \tau_{i,j}^+ &= 4 - u_{i,j}\sigma_{i,j}^+, & \tau_{i,j}^\times &= 4 - u_{i,j}\sigma_{i,j}^\times. \end{aligned}$$

Then (3.2), for any $u \in \mathcal{M}$, is equivalent to

$$\beta^{+}\tau_{i,j}^{+} + \beta^{\times}\tau_{i,j}^{\times} \geq \gamma \text{ whenever } u_{i,j} = \pm 1,$$

$$\beta^{+}\sigma_{i,j}^{+} + \beta^{\times}\sigma_{i,j}^{\times} = 0 \text{ whenever } u_{i,j} = 0.$$

$$(3.3)$$

Observe that the quantities $\sigma_{i,j}^{\bullet}$ and $\tau_{i,j}^{\bullet}$ (with \bullet denoting either + or ×, here and elsewhere) are integers in the range

$$-4 \le \sigma_{i,j}^{\bullet} \le 4, \qquad 0 \le \tau_{i,j}^{\bullet} \le 8, \tag{3.4}$$

and so there is only a finite number of possibilities for the equations in (3.3). Thus the space of parameters $(\beta^+, \beta^*, \gamma) \in \mathbb{R}^3$ is divided into only finitely many regions, corresponding to the finite number of cases that must be considered.

It is possible to give sufficient conditions for a mosaic solution to be stable. Specifically, we have [18] the following theorem. **Theorem 1** Suppose u is a mosaic solution of Eq. (2.8) with (3.1), that is, a mosaic satisfying (3.3). Then if the inequality in (3.3) is strict,

$$\beta^{+}\tau_{i,j}^{+} + \beta^{\times}\tau_{i,j}^{\times} > \gamma \text{ whenever } u_{i,j} = \pm 1, \qquad (3.5)$$

and if it also holds that

$$(4 + z_{i,j}^{+} \operatorname{sgn}(\beta^{+}))\beta^{+} + (4 + z_{i,j}^{\times} \operatorname{sgn}(\beta^{\times}))\beta^{\times} < \gamma \text{ whenever } u_{i,j} = 0, \qquad (3.6)$$

Z where

$$z_{i,j}^{+} = \operatorname{card}\{(a,b) \in \mathbb{Z}^2 \mid u_{a,b} = 0 \text{ and } |a-i|+|b-j|=1\},$$

$$z_{i,j}^{\times} = \operatorname{card}\{(a,b) \in \mathbb{Z}^2 \mid u_{a,b} = 0 \text{ and } |a-i| = |b-j|=1\},$$

then u is asymptotically stable.

The proof of Theorem 1, which is not obvious, involves construction of a neighborhood

$$\mathcal{N}(u,\theta,\delta) = \{ v \in [-1,1]^{\mathbb{Z}^2} \mid |v_{i,j} - u_{i,j}| \le \delta \text{ whenever} \\ u_{i,j} = \pm 1, \text{ and } |v_{i,j}| \le \theta \text{ whenever } u_{i,j} = 0 \}$$

of u in the phase space $[-1,1]^{\mathbb{Z}^2}$, such that $\mathcal{N}(u,\theta,\delta)$ is positively invariant, and such that all solutions of $\mathcal{N}(u,\theta,\delta)$ are attracted to u as $t \to \infty$. In fact, the proof of the invariance of $\mathcal{N}(u,\theta,\delta)$ yields explicit lower bounds on the quantities θ and δ , so the size of the basin of attraction of u can be estimated. Moreover, Theorem 1 is robust with respect to f, in the sense that the same techniques in the proof yield analogous stability results for smooth nonlinearities f, such as those in (2.2).

We may consider the set

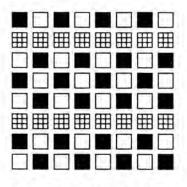
 $\mathcal{S}(\beta^+, \beta^{\times}, \gamma) = \{ u \in \mathcal{M} \mid \text{conditions (3.3), (3.5), and (3.6) all hold} \}$ (3.7)

of all mosaics satisfying the conditions of Theorem 1. We formalize this with the following definition.

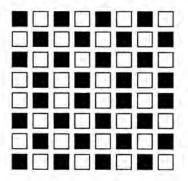
Definition 3 An S-solution of (2.8), (3.1), is an element $u \in S(\beta^+, \beta^{\times}, \gamma)$.

Let us remark that the conditions of Theorem 1 are sufficient, but not in general necessary, for a mosaic solution to be stable, as was noted in [18]. We also note that in general there can exist other equilibria which are not mosaics; see [63]. Nevertheless, the S-solutions provide a rich supply of stable equilibria, some of which exhibit regular, or almost regular spatial patterns, while others display a disordered appearance.

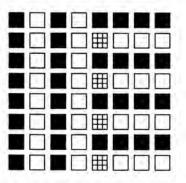
A number of S-solutions were presented in [18]. In the case of stripes, say $u_{i,j} = (-1)^i$ for all (i, j), one has that $(\tau_{i,j}^+, \tau_{i,j}^\times) = (4, 8)$ for all (i, j), and so such u is a



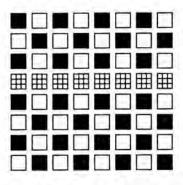
(a) Checkerboard with Horizontal Interfaces



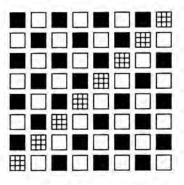
(c) Checkerboard with Thin Horizontal Interface



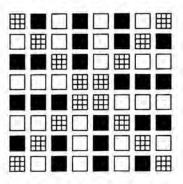
(e) Vertical and Horizontal Stripes with Vertical Interface



(b) An Impossible S-Solution



(d) Checkerboard with Diagonal Interface



- (f) Quad Junction

Figure 3: Some Stable Mosaic Solutions

stable equilibrium provided that $4\beta^+ + 8\beta^* > \gamma$. For checks $u_{i,j} = (-1)^{i+j}$ one has $(\tau_{i,j}^+, \tau_{i,j}^*) = (8,0)$ for all (i, j) and so this is a stable equilibrium provided $8\beta^+ > \gamma$. In contrast to the bifurcation results of the previous section, which are only local, here we have solutions existing for a large range of the (β^+, β^*) -plane. Figure 3 depicts portions of several mosaics composed of stripes or checks separated by interfaces, where we denote

$$\blacksquare = 1 \qquad \blacksquare = 0 \qquad \Box = -1.$$

With the exception of Figure 3(b), each of these mosaics occurs as an S-solution for a nonempty open set of parameters $(\beta^+, \beta^\times, \gamma)$ which can be determined by Theorem 1. Consider, for example, Figure 3(a), the checkerboard with interfaces of zeros. We assume here that the rows of zeros (the interfaces) are separated by at least two rows of checkerboard. In addition to the values $(\tau_{i,j}^+, \tau_{i,j}^\times) = (8,0)$ which occur at those checkerboard points $u_{i,j} = \pm 1$ which are not adjacent to a zero-row, one sees that $(\tau_{i,j}^+, \tau_{i,j}^\times) = (7,2)$ when $u_{i,j} = \pm 1$ is adjacent to a zero-row. Also, when $u_{i,j} = 0$ then $\sigma_{i,j}^+ = \sigma_{i,j}^\times = 0$ (so the second condition of (3.3) is satisfied), and we also see that $(z_{i,j}^+, z_{i,j}^\times) = (2,0)$. It follows from Theorem 1 that such a mosaic is an S-solution, and therefore is a stable equilibrium of (2.8), (3.1), if

$$8\beta^+ > \gamma, \qquad 7\beta^+ + 2\beta^\times > \gamma, \qquad (4 + 2\operatorname{sgn}(\beta^+))\beta^+ + 4\beta^\times < \gamma, \qquad (3.8)$$

all hold. If $\gamma \neq 0$, there is a nonempty open set of $(\beta^+, \beta^{\times})$ satisfying (3.8).

Observe that in Figure 3(b) the checkerboard "changes its phase" across the interface in a manner different from that in Figure 3(a). In particular, we have either $(\sigma_{i,j}^+, \sigma_{i,j}^{\times}) = (2, -4)$ or (-2, 4) whenever $u_{i,j} = 0$ in Figure 3(b), and it can be shown that this mosaic can never be an S-solution.

For a given choice of parameters $(\beta^+, \beta^{\times})$ and γ , the conditions (3.3), (3.5), (3.6), for an S-solution can be thought of as combinatorial conditions on the mosaic u. Also, as above, as these parameters vary one encounters only a finite number of possibilities, or cases, for the sets $S(\beta^+, \beta^{\times}, \gamma)$. More precisely, let $\gamma \neq 0$ be fixed and let L(a, b)and $L_0(a, b)$ denote the lines in the $(\beta^+, \beta^{\times})$ -plane

$$L(a,b) = \{(\beta^+, \beta^\times) \mid a\beta^+ + b\beta^\times = \gamma\},$$

$$L_0(a,b) = \{(\beta^+, \beta^\times) \mid a\beta^+ + b\beta^\times = 0\},$$

for $(a, b) \in \mathbb{R}^2$. In particular, consider the sets

$$\mathcal{L} = \bigcup_{\substack{0 \le a, b \le 8\\(a,b) \neq (0,0)}} L(a,b), \qquad \mathcal{L}_0 = \bigcup_{\substack{-4 \le a, b \le 4\\(a,b) \neq (0,0)}} L_0(a,b),$$

which are unions of $9^2 - 1 = 80$ lines, and 25 lines, respectively. Let us restrict $(\beta^+, \beta^{\times})$ to lie in the complement $\mathbb{R}^2 \setminus \mathcal{L}$ of the set \mathcal{L} , noting that this complement is an open dense subset of the plane. Then, the set of those pairs $(\tau_{i,j}^+, \tau_{i,j}^{\times})$ and $(z_{i,j}^+, z_{i,j}^{\times})$ for which the inequalities in (3.5) and (3.6) hold depends only on which

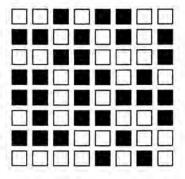


Figure 4: A Spatially Disordered Mosaic in S_1

connected component of the set $\mathbb{R}^2 \setminus \mathcal{L}$ that (β^+, β^\times) belongs to. If we further restrict (β^+, β^\times) to lie in the open dense set $\mathbb{R}^2 \setminus \mathcal{L}_0$, then the equality on the second line of (3.3) forces $\sigma_{i,j}^+ = \sigma_{i,j}^\times = 0$, in light of the range (3.4) of $\sigma_{i,j}^\bullet$. Thus, we may think of each connected component $\mathcal{O} \subseteq \mathbb{R} \setminus \mathcal{L}$ as yielding as particular case, in the sense that the set $\mathcal{S}(\beta^+, \beta^\times, \gamma)$ remains unchanged for $(\beta^+, \beta^\times) \in \mathcal{O} \setminus \mathcal{L}_0$. The number of such cases, that is, the number of connected components of $\mathbb{R} \setminus \mathcal{L}$, is finite but large, as the following result shows.

Theorem 2 The set $\mathbb{R}^2 \setminus \mathcal{L}$ has precisely 2,041 connected components.

Given any connected component \mathcal{O} of $\mathbb{R} \setminus \mathcal{L}$, and fixing γ , one might hope to characterize or describe the set $S(\beta^+, \beta^\times, \gamma)$ of all S-solutions for $(\beta^+, \beta^\times) \in \mathcal{O} \setminus \mathcal{L}_0$. This can be done in some cases, but is in general quite difficult. For example, let $\gamma = 1$, and let \mathcal{O}_k , for $1 \leq k \leq 9$, denote the component of $\mathbb{R} \setminus \mathcal{L}$ which contains the point $(\beta^+, \beta^\times) = ((k-0.5)^{-1}, 0)$. In [18] the set $S_k = S(\beta^+, \beta^\times, \gamma)$, for $(\beta^+, \beta^\times) \in \mathcal{O}_k \setminus \mathcal{L}_0$, was studied. It was determined there that S_9 contains only the trivial (zero) solution $u_{i,j} = 0$, that S_8 contains only the checkerboard mosaic $u_{i,j} = (-1)^{i+j}$ and its negative $u_{i,j} = (-1)^{i+j+1}$, and that S_7 contains only those mosaics of Figure 3(a), comprised of checkerboards with horizontal interfaces, as well as analogous interfaces with vertical interfaces. The set S_6 is comprised only of checkerboards with thin horizontal interfaces (as in Figure 3(c)), checkerboards with diagonal interfaces (as in Figure 3(d)), and rotations and reflections of these. Thus, for $k \geq 6$ we have that the mosaics of S_k exhibit a fairly regular pattern.

By contrast, this is not the case for the elements of S_k for $1 \le k \le 5$. It was shown in [18] that the mosaics u in these S_k typically possess a chaotic display. Mathematically, it was shown that the spatial entropy $h(S_k)$ (discussed in the next section) is zero $h(S_k) = 0$ for $6 \le k \le 9$, and positive $h(S_k) > 0$ for $1 \le k \le 5$.

Consider in particular the set S_1 . With $(\beta^+, \beta^{\times}) = (2,0) \in \mathcal{O}_1$, we have (recall

that $\gamma = 1$) that (3.5) is equivalent to

 $\tau_{i,j}^+ \neq 0$ whenever $u_{i,j} = \pm 1$.

The inequality in condition (3.6) can never hold, as $4\beta^+ = 8 > \gamma = 1$, and so $u_{i,j} \neq 0$ for all $u \in S_1$. Thus S_1 consists precisely of those mosaics $u \in \mathcal{M}$ such that $u_{i,j} = \pm 1$ for all $(i, j) \in \mathbb{Z}^2$, and such that $\tau_{i,j}^+ \neq 0$ for all $(i, j) \in \mathbb{Z}^2$, equivalently, such that the arrays



occur nowhere in u. Figure 4 depicts a portion of such a mosaic $u \in S_1$, and one sees that this u exhibits no regular pattern.

4 Pattern formation and spatial chaos

The mathematical notion which distinguishes pattern formation from spatial chaos is the concept of spatial entropy. In the context of S-solutions above, the spatial entropy is a nonnegative quantity $h = h(S(\beta^+, \beta^{\times}, \gamma)) \ge 0$ which measures the complexity of the set of S-solutions, the larger values of h corresponding to more disordered, or chaotic, spatial presentations.

Before specifically considering S-solutions, let us define the spatial entropy in a more general setting. We work here with the D-dimensional lattice \mathbb{Z}^D . Let \mathcal{A} be a finite set of d elements (an alphabet), let $D \geq 1$, and consider the set $\mathcal{A}^{\mathbb{Z}^D}$ of all functions $u : \mathbb{Z}^D \to \mathcal{A}$. Note that in the previous section $\mathcal{M} = \mathcal{A}^{\mathbb{Z}^2}$, where $\mathcal{A} = \{-1, 0, 1\}$. We say that a subset $\mathcal{B} \subseteq \mathcal{A}^{\mathbb{Z}^D}$ is translation invariant in case $S_k u \in \mathcal{B}$ whenever $u \in \mathcal{B}$, for $1 \leq k \leq D$, where $S_k : \mathcal{A}^{\mathbb{Z}^D} \to \mathcal{A}^{\mathbb{Z}^D}$ denotes the translation operator

$$(S_k u)_\eta = u_{\eta + e_k}, \quad \eta \in \mathbb{Z}^D,$$

in the direction $e_k \in \mathbb{Z}^D$, with $\{e_k\}_{k=1}^D$ denoting the standard basis in \mathbb{R}^D .

Consider now any nonempty translation invariant set $\mathcal{B} \subseteq \mathcal{A}^{\mathbb{Z}^D}$. For simplicity of notation, we shall take D = 2, although the following construction extends to arbitrary D in an obvious fashion. Recall, for any $m \ge 1$ and $n \ge 1$, the finite lattice $F_{m,n} \subseteq \mathbb{Z}^2$ given by Eq. (2.13). Any $u \in \mathcal{A}^{\mathbb{Z}^2}$, that is, $u : \mathbb{Z}^2 \to \mathcal{A}$, can be restricted to $u : F_{m,n} \to \mathcal{A}$, thereby yielding an element of $\mathcal{A}^{F_{m,n}}$. Thus we have a map

$$\pi_{m,n}:\mathcal{A}^{\mathbb{Z}^2}\to\mathcal{A}^{F_{m,n}},$$

given by this restriction. As $F_{m,n}$ and \mathcal{A} are finite sets with mn and d elements respectively, the set $\mathcal{A}^{F_{m,n}}$ is also finite and has d^{mn} elements. For a nonempty, translation invariant set $\mathcal{B} \subseteq \mathcal{A}^{\mathbb{Z}^{D}}$, consider the image $\pi_{m,n}(\mathcal{B}) \subseteq \mathcal{A}^{F_{m,n}}$, and let

$$b_{m,n} = \operatorname{card}(\pi_{m,n}(\mathcal{B})), \tag{4.1}$$

Spatial patterns, spatial chaos, and traveling waves

the cardinality of this set.

Definition 4 The spatial entropy of the translation invariant set $\mathcal{B} \subseteq \mathcal{A}^{\mathbb{Z}^2}$ is the quantity

$$h(\mathcal{B}) = \lim_{m,n\to\infty} \frac{1}{mn} \log b_{m,n}.$$
(4.2)

It is a consequence of the translation invariance of \mathcal{B} that the limit (4.2) always exists. In fact, each of the terms in the right-hand side of Eq. (4.2) is an upper bound for the spatial entropy, so

$$h(\mathcal{B}) = \inf_{m,n \ge 1} \frac{1}{mn} \log b_{m,n} \tag{4.3}$$

also holds. Clearly $1 \leq b_{m,n} \leq d^{mn}$, and so $0 \leq h(\mathcal{B}) \leq \log d$. Roughly, the quantities $b_{m,n}$ count the number of different patterns one observes among the elements of \mathcal{B} through a window of size $m \times n$ in the lattice \mathbb{Z}^2 . The translation invariance of \mathcal{B} implies that without loss we may take this window to be $F_{m,n}$, with the lower left point at the origin. Thus, larger values of $h(\mathcal{B})$ correspond to a richer variety of patterns observable among the elements of \mathcal{B} .

One easily sees that the set $S(\beta^+, \beta^{\times}, \gamma) \subseteq \mathcal{M}$ is translation invariant, and so one can calculate its spatial entropy $h(S(\beta^+, \beta^{\times}, \gamma))$. With this, we make a fundamental definition.

Definition 5 We say that Eq. (2.8), with (3.1), exhibits pattern formation in case $h(S(\beta^+, \beta^{\times}, \gamma)) = 0$. We say this system exhibits spatial chaos if $h(S(\beta^+, \beta^{\times}, \gamma)) > 0$.

In general, there is no method for calculating the entropy of a set \mathcal{B} , or even for determining whether the entropy is zero or positive, at least for higher-dimensional $D \geq 2$ lattices. While Eq. (4.3) supplies explicit upper bounds, these bounds are generally positive even when $h(\mathcal{B}) = 0$. Sufficient conditions on \mathcal{B} for $h(\mathcal{B}) = 0$ to hold, or positive lower bounds for $h(\mathcal{B})$ when $h(\mathcal{B}) > 0$, generally are difficult to obtain. We note that in the case of the one-dimensional lattice \mathbb{Z} , it is possible to calculate $h(\mathcal{B})$ in case \mathcal{B} is a Markov shift, or a subshift of finite type. Taking the alphabet $\mathcal{A} = \{1, 2, 3, \ldots, d\}$, one defines a Markov shift by means of a $d \times d$ Boolean matrix M, the so-called transfer matrix. Here $u \in \mathcal{B} \subseteq \mathcal{A}^{\mathbb{Z}}$ if and only if we have $m_{u_i,u_{i+1}} = 1$ for the (u_i, u_{i+1}) entry of M. For such \mathcal{B} , there is the well-known formula (see, for example, [58])

$$h(\mathcal{B}) = \log \lambda, \qquad \lambda = \text{the largest eigenvalue of } M.$$
 (4.4)

It is possible to define higher-dimensional Markov shifts, that is, analogs of the above on the lattice \mathbb{Z}^{D} . However, there is no analog of the formula (4.4) in this case [62]. Indeed, it has been shown [9] that there is no universal algorithm for determining whether \mathcal{B} is empty or not.

In [18], we are nevertheless able to obtain conditions under which $h(\mathcal{B}) = 0$, and also obtain positive lower bounds for $h(\mathcal{B})$ when $h(\mathcal{B}) > 0$, for the set $\mathcal{B} = \mathcal{S}(\beta^+, \beta^\times, \gamma)$ of S-solutions, over a wide range of the (β^+, β^\times) -plane. We have already noted such results for the sets \mathcal{S}_k , for $1 \leq k \leq 9$, in Section 3. The conclusion $h(\mathcal{S}_k) = 0$, obtained for $6 \leq k \leq 9$, is essentially a matter of providing a precise description of the elements $u \in \mathcal{S}_k$ (for example, as checkerboards with certain types of interfaces), and then obtaining upper bounds on $b_{m,n}$ in a more or less straightforward fashion. Positive lower bounds on $h(\mathcal{S}(\beta^+, \beta^\times, \gamma))$, on the other hand, can be obtained by explicitly constructing subsets $\widetilde{\mathcal{B}} \subseteq \mathcal{S}(\beta^+, \beta^\times, \gamma)$ of mosaics for which the limit (4.2), with $\widetilde{\mathcal{B}}$ in place of \mathcal{B} in (4.1), is positive.

To illustrate the latter approach, let \mathcal{B} denote the set of all mosaics $u \in \mathcal{M}$ such that $u_{i,j} = \pm 1$ for all $(i,j) \in \mathbb{Z}^2$, and such that $u_{2\alpha,j} = -u_{2\alpha+1,j}$ for all integers a and j. Roughly, elements of $\widetilde{\mathcal{B}}$ are obtained by "paving" the lattice \mathbb{Z}^2 with 2×1 "bricks," each of the form either

selecting these bricks arbitrarily to cover the sites (2a, j), $(2a+1, j) \in \mathbb{Z}^2$. (This set \mathcal{B} is not translation invariant, however, that property is not needed for our argument.) Denote $\tilde{b}_{m,n} = \operatorname{card}(\pi_{m,n}(\widetilde{\mathcal{B}}))$, and let $b_{m,n}$ be as in (4.1) with $\mathcal{B} = \mathcal{S}(\beta^+, \beta^{\times}, \gamma)$. Then if

$$\mathcal{B} \subseteq \mathcal{B} = \mathcal{S}(\beta^+, \beta^\times, \gamma), \tag{4.6}$$

it follows that $\tilde{b}_{m,n} \leq b_{m,n}$, and so

$$\limsup_{m,n\to\infty}\frac{1}{mn}\log\widetilde{b}_{m,n} \leq \lim_{m,n\to\infty}\frac{1}{mn}\log b_{m,n} = h(\mathcal{S}(\beta^+,\beta^\times,\gamma)).$$

However, we see that $\tilde{b}_{m,n} \geq 2^{mn/2}$, since the sublattice $F_{m,n}$ intersects at least mn/2 (in fact exactly this many if m is even) of the 2×1 sites on which the bricks covering \mathbb{Z}^2 are placed, and we have a choice of the two possible bricks (4.5). Thus,

$$h(\mathcal{S}(\beta^+, \beta^{\times}, \gamma)) \geq \limsup_{m, n \to \infty} \frac{1}{mn} \log 2^{mn/2} = \frac{\log 2}{2}, \tag{4.7}$$

whenever the inclusion (4.6) holds.

We must next determine those (β^+, β^\times) and γ for which (4.6) holds. To do this, we determine all possible pairs $(\tau_{i,j}^+, \tau_{i,j}^\times)$ which can occur among the mosaics in $\widetilde{\mathcal{B}}$. It can be seen that without loss we may take (i, j) = (0, 0), with $u_{0,0} = 1$. Then the 3×3 block in such u, centered at (0, 0), has the form

$$\begin{pmatrix} u_{-1,1} & u_{0,1} & u_{1,1} \\ u_{-1,0} & u_{0,0} & u_{1,0} \\ u_{-1,-1} & u_{0,-1} & u_{1,-1} \end{pmatrix} = \begin{pmatrix} c & a & -a \\ d & 1 & -1 \\ e & b & -b \end{pmatrix},$$

where $a, b, c, d, e \in \{-1, 1\}$, but are otherwise arbitrary. Thus $\sigma_{0,0}^+ = a + b + d - 1$ and $\sigma_{0,0}^{\times} = -a - b + c + e$, and so

$$(\tau_{0,0}^+, \tau_{0,0}^\times) = (5 - a - b - d, 4 + a + b - c - e).$$

By considering all possible values of a, b, c, d, and e, one can enumerate the possible pairs $(\tau_{0,0}^+, \tau_{0,0}^\times)$ (or in fact $(\tau_{i,j}^+, \tau_{i,j}^\times)$ for any (i, j)) as

It follows immediately from the definition (3.7) of $S(\beta^+, \beta^\times, \gamma)$, in particular using (3.5), that the inclusion (4.6) holds if and only if $a\beta^+ + b\beta^\times > \gamma$ for all pairs (a, b) in (4.8). In fact, one only need take the extreme points (2,4), (2,8), (4,8), (6,0), (8,0), and (8,4), in the set of pairs (4.8), so this condition is in fact equivalent to

$$2\beta^{+} + 4\beta^{\times} > \gamma, \qquad 2\beta^{+} + 8\beta^{\times} > \gamma, \qquad 4\beta^{+} + 8\beta^{\times} > \gamma,$$

$$6\beta^{+} > \gamma, \qquad 8\beta^{+} > \gamma, \qquad 8\beta^{+} + 4\beta^{\times} > \gamma,$$
(4.9)

all holding.

We conclude, therefore, that when (β^+, β^\times) and γ satisfy (4.9), then the lower bound (4.7) on the spatial entropy holds, and we have spatial chaos. Observe in particular that this is the case for the regions S_1 and S_2 discussed in Section 3. A similar argument, with different sets $\tilde{\mathcal{B}}$, yields positive lower bounds for the entropy of S_k , for k = 3, 4, and 5.

Numerical calculations of $h(S(\beta^+, \beta^\times, \gamma))$ were given in [19]. Equation (2.8), but on the lattice $\{0, 1, 2, \ldots, m-1\} \times \mathbb{Z}$ of finite width m, was considered by imposing "*m*-corkscrew" boundary conditions $u_{i+m,j} = u_{i,j+1}$ on the full lattice \mathbb{Z}^2 . With this, the stability conditions of Theorem 1 were interpreted as a one-dimensional Markov shift with the alphabet $\mathcal{A} = \{-1, 0, 1\}^{2m+2}$ of all sequences

$$U_i = (u_{i,0}, u_{i+1,0}, u_{i+2,0}, \dots, u_{i+2m+1,0})$$

of length 2m + 2. A transfer matrix M expressing the transition from U_i to U_{i+1} was constructed and its largest eigenvalue $\lambda = \lambda_m$ numerically found. Following (4.4), the quantity $\log \lambda_m$ was taken as an approximation to $h(\mathcal{S}(\beta^+, \beta^{\times}, \gamma))$. As \mathcal{A} has 3^{2m+2} elements, the matrix M is enormous even for moderate m, having size $3^{2m+2} \times 3^{2m+2}$. Nevertheless, M is very sparse, and calculation of λ_m was accomplished efficiently.

5 Traveling waves

While there is a vast literature on traveling wave solutions of PDE's, very little is known for LDE's. For the PDE (1.3), a traveling wave solution takes the form $u(t, x) = \varphi(x - ct)$ for some function $\varphi : \mathbb{R} \to \mathbb{R}$ and quantity $c \in \mathbb{R}$ (the wave speed), where substitution into (1.3) yields the equation

$$-c\varphi'(\xi) = \varphi''(\xi) - f(\varphi(\xi)), \quad \xi \in \mathbb{R}.$$
(5.1)

One typically imposes boundary conditions for φ , of the form

$$\varphi(-\infty) = q_{-}, \qquad \varphi(\infty) = q_{+}, \tag{5.2}$$

where $f(q_{\pm}) = 0$, generally with $z = q_{\pm}$ as stable equilibria for the associated ODE $\dot{z} = -f(z)$. Both φ as well as c are unknown, and must be sought as part of the solution, that is, a solution to (5.1), (5.2), is a pair (φ , c) as above.

One often views the boundary conditions (5.2) as prescribing a heteroclinic orbit joining the equilibria $\xi = q_{\pm}$ of Eq. (5.1). As such, many of the tools of dynamical systems, for example the Mel'nikov function, find use in this problem.

We take a class of nonlinearities f of which the cubic f_1 in (2.2) is representative (note that $q_{\pm} = \pm 1$ here). The so-called *detuning parameter* a, as in f_1 , plays a prominent role in what follows. Then with such f there is [33] a unique solution $(\varphi, c) = (\varphi(\xi, a), c(a))$, which depends smoothly on a, and moreover, the monotonicity properties

$$\frac{\partial \varphi(\xi, a)}{\partial \xi} > 0, \qquad c'(a) > 0, \tag{5.3}$$

both hold.

For an LDE, say (1.2) on the one-dimensional lattice \mathbb{Z} , a traveling wave solution takes the form

$$u_i(t) = \varphi(i - ct), \qquad i \in \mathbb{Z}, \tag{5.4}$$

for some $c \in \mathbb{R}$. If $c \neq 0$ then $\varphi : \mathbb{R} \to \mathbb{R}$, while if c = 0 we have $\varphi : \mathbb{Z} \to \mathbb{R}$. In either case, substitution of (5.4) into Eq. (1.2) yields the equation

$$-c\varphi'(\xi) = \alpha \left(\varphi(\xi+1) + \varphi(\xi-1) - 2\varphi(\xi)\right) - f(\varphi(\xi)), \qquad \xi \in \mathbb{R} \text{ or } \mathbb{Z}, \quad (5.5)$$

which is a differential-difference equation if $c \neq 0$, and is a difference equation if c = 0. As in the case of a PDE, the wave speed c is unknown, being determined as part of the solution, and the boundary conditions (5.2) are typically imposed.

Equation (5.5) is a much more difficult system to analyze than the ODE (5.1), particularly if $c \neq 0$. In this case (5.5) does not generate a dynamical system, as does (5.1), and it is inherently infinite dimensional. While there is a very large literature for functional differential equations (see [36]), with the exception of [60], [61], this almost exclusively concerns time-delay (retarded) problems, as opposed to Eq. (5.5) where both forward and backward shifts in the argument ξ appear. The first results on Eq. (5.5), with (5.2), were given in [37] (see also [65], [66], and [67]) for a class of nonlinearities including f_1 in (2.2), where existence of a solution (φ, c) when $\alpha > 0$ was established. This existence proof was based on degree theory arguments, so unfortunately gave no indication of the global structure (such as uniqueness, or smooth dependence on parameters) of the set of all solutions. More recently [47], we have been able to establish uniqueness of the wave speed c, and if $c \neq 0$ then we also have uniqueness of the solution φ , smooth dependence of φ and con parameters (such as a and α), as well as the monotonicity conditions (5.3), at least for a class of f which includes f_1 in (2.2). The proof of these results relies on a global continuation method (in the spirit of proofs in [6], [14], [15], and [31]) via a Mel'nikov function, together with comparison arguments. A key feature is the development of a Fredholm alternative, and adjoint theory, in the spirit of [35], for asymptotically autonomous linear equations of the form

$$\psi'(\xi) = \sum_{k=1}^{m} A_k(\xi)\psi(\xi + r_k), \qquad \xi \in \mathbb{R},$$
(5.6)

with hyperbolic spectrum for the limiting equations at $\xi = \pm \infty$ (the quantities r_k in (5.6) are given constants). Such equations (5.6) occur as the linearization of (5.5) about solutions φ , when $c \neq 0$, and one needs the Fredholm theory in order to use Lyapunov-Schmidt techniques to construct the Mel'nikov function for Eq. (5.5).

If c = 0, on the other hand, then typically φ is not unique. In addition, the phenomenon of propagation failure generally occurs, wherein the wave speed vanishes identically $c \equiv 0$ as the parameters a and α vary throughout an open set. Propagation failure is a hallmark of spatially discrete systems and does not generally occur for PDE's such as (1.3). In the above example it is perhaps most easily seen upon observing that when c = 0, then Eq. (5.5) takes the form of a planar map $(u, v) \rightarrow$ $(2u - v + \alpha^{-1} f(u), u)$ for which the two equilibria (u, v) = (1, 1) and (-1, -1) are saddles. Typically, heteroclinic orbits of such a map are transverse intersections of stable and unstable manifolds, and so persist throughout a range of parameters. One now concludes from (5.3) when $c(a) \neq 0$, and with propagation failure on an interval $(a^-, a^+) \subseteq (-1, 1)$, that

$$c(a) \begin{cases} > 0 & \text{for} \quad a \in (a^+, 1), \\ = 0 & \text{for} \quad a \in [a^-, a^+], \\ < 0 & \text{for} \quad a \in (-1, a^-), \end{cases}$$

where generally $a^- < a^+$. Early work on propagation failure was given in [39], [40]. See also [44] for its significance in other applications.

For the PDE (1.3), stability issues can be addressed by introducing the moving coordinate $\xi = x - ct$ into the time-dependent problem. For the LDE (1.2), it is possible [17], with some effort, to construct a continuously moving coordinate system in an analogous fashion. While the details are too lengthy to present here, we mention that a key point involves passing from the identity operator I on $l^{\infty}(\mathbb{Z})$ to other linear

isomorphisms (for example, the shift operator) on this space, moving continuously through the space of linear isomorphisms. That this can be done is a consequence of the connectedness of the space $GL(l^{\infty}(\mathbb{Z}))$, proved in [26].

The results of [47] are in fact quite general, and extend to higher dimensional lattices. In such cases one must also prescribe the direction of motion, in the lattice, in which the wave travels. Consider, for example, Eq. (2.1), with $\alpha^{\times} = 0$. We write

$$\dot{u}_{i,j} = \alpha(\Delta^+ u)_{i,j} - f(u_{i,j}), \qquad (i,j) \in \mathbb{Z}^2, \tag{5.7}$$

denoting $\alpha = \alpha^+$. Given any $\theta \in \mathbb{R}$, then by a traveling wave solution of (5.7) in the direction θ we mean a solution of the form

$$u_{i,j}(t) = \varphi(i\cos\theta + j\sin\theta - ct).$$

We see that φ must satisfy

$$-c\varphi'(\xi) = \alpha \big(\varphi(\xi + \sigma) + \varphi(\xi - \sigma) + \varphi(\xi + \kappa) + \varphi(\xi - \kappa) - 4\varphi(\xi)\big) - f(\varphi(\xi)),$$

$$\sigma = \sin\theta, \qquad \kappa = \cos\theta,$$

(5.8)

for $\xi \in \mathbb{R}$ if $c \neq 0$, or for $\xi \in \mathbb{D}$ if c = 0, where we denote $\mathbb{D} = \{i\sigma + j\kappa \mid (i, j) \in \mathbb{Z}^2\}$. Observe that \mathbb{D} is a discrete set if $\tan \theta$ is rational (regarding ∞ here as rational), and is a dense set if $\tan \theta$ is irrational.

In order better to understand the dependence of c on the parameter a, as well as on the direction θ , the traveling wave equation (5.8) was studied [13] with the choice of a piecewise linear nonlinearity

$$f(z,a) = \begin{cases} z+1 \text{ if } z < a, \\ z-1 \text{ if } z > a, \end{cases}$$
(5.9)

where -1 < a < 1. This f is a cartoon of the smooth function f_1 in (2.2), and was used previously by McKean [53] for the associated PDE. The advantage of the nonlinearity (5.9) is that with it one can explicitly solve Eq. (5.8) by Fourier transform methods. Perhaps the most striking outcome of this study was the discovery of the pathological behavior of the critical value $a^+ = a^+(\theta)$ on the direction parameter θ (here one has $a^- = -a^+$). The function $\theta \to a^+(\theta)$ was shown to be continuous precisely at those $\theta \in \mathbb{R}$ for which $\tan \theta$ is irrational, with points of discontinuity, specifically with $a^+(\theta \pm 0) > a^+(\theta)$, when $\tan \theta$ is rational. Roughly, this means that propagation failure is more likely to occur for wavefronts with rational slopes, than with irrational slopes. Moreover, preliminary evidence indicates that this phenomenon holds quite generally for smooth f, and is not an artifact of the discontinuity in (5.9). See [28] for numerical simulations of this problem with (5.9).

More generally, one would like to understand traveling waves which join more complex patterns. For example, again with $f = f_1$ in (2.2), consider such a solution of Eq. (1.2) which joins an asymmetric one-dimensional checkerboard

$$u_{2i} = k_e, \qquad u_{2i+1} = k_o,$$

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as $i \to -\infty$, with the homogeneous solution $u_i = 1$ as $i \to \infty$. Setting

$$u_{2i}=\varphi(i-ct), \qquad u_{2i+1}=\psi(i-ct),$$

yields the system

$$-c\varphi'(\xi) = lpha \left(\psi(\xi) + \psi(\xi - 1) - 2\varphi(\xi)\right) - f(\varphi(\xi)),$$

 $-c\psi'(\xi) = lpha \left(\varphi(\xi + 1) + \varphi(\xi) - 2\psi(\xi)\right) - f(\psi(\xi)),$

with the boundary conditions

$$(\varphi(-\infty),\psi(-\infty))=(k_e,k_o),\qquad (\varphi(\infty),\psi(\infty))=(1,1),$$

where the quantities k_e and k_o satisfy $2\alpha(k_e - k_o) = f(k_o) = -f(k_e)$.

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Part III: Random Differential Equations and Applications

Reaction telegraph equations and random walk systems

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Abstract

In reaction diffusion equations spatial spread is modeled by Brownian motion. If Brownian motion is replaced by a correlated random walk or related processes then semilinear random walk systems and reaction telegraph equations are obtained. We investigate these systems and discuss their relevance for modeling and applications in comparison with reaction diffusion equations.

1 Introduction

In all fields of science, economics and engineering, the interactions between several types or species have to be modeled. If the number of particles is large then one will describe the different types by their population sizes or densities and the reactions between them by (systems of) ordinary differential equations $\dot{u} = f(u)$. The right hand sides of these equations often assume the form of polynomials or rational functions (e.g. derived from stoichiometric laws) but in principle any type of nonlinearity can occur. It should be underlined that the description by differential equations is a most natural one since these equations describe nothing else than the law that connects the change of the system "in the immediate future" to the present state. Thus the concept of differential equation arises naturally from the proper choice of the state and the assumption of causality. The usefulness of the differential equations approach is thus limited only by the assumption of large numbers. Of course it is tacitly assumed that the nonlinearity of the equation describes the underlying process correctly. That may not always be taken for granted if one thinks of complicated chemical molecules that react only in specified geometric configurations.

Modelling spatial spread seems less straightforward. In general one will either start from deterministic balance considerations or from stochastic processes such as Brownian motion. Both approaches lead, with certain assumptions that are both intuitively plausible and supported by experiment, to the diffusion equation or, in another physical context, to the heat equation.

Assuming that reaction and diffusion act together one arrives at a type of system that has become known as reaction diffusion equation ([17, 38, 62, 68]). These systems have the form

$$\frac{\partial u_i}{\partial t} = D_i \Delta u_i + f_i(u_1, \dots, u_m), \quad i = 1, \dots, m, \quad x \in \Omega \subset \mathbb{R}^n,$$

or, in condensed notation,

$$u_t = D\Delta u + f(u). \tag{1}$$

The fact that the Laplacian and the reaction term appear as a sum is worth noticing. The most important example is the scalar reaction diffusion equation, m = n = 1,

$$u_t = Du_{xx} + f(u). \tag{2}$$

The diffusion equation can be justified a *posteriori* since many stochastic processes can be approximated by diffusion processes. Nevertheless, the diffusion equation has several deficiencies. The Laplace operator is strictly local, i.e. long distance effects are not taken into account. The diffusion equation shows the phenomenon of infinite propagation, i.e. particles can move with arbitrarily high speed, quite in contrast to common laws of physics.

The question arises what type of equation is obtained if the underlying stochastic process is not Brownian motion and if a diffusion approximation is not made. There is a wide variety of stochastic processes which can be used to model spatial spread and that lead to other types of evolution equations.

It turns out that these equations are quite interesting and sometimes show features different from those of reaction diffusion equations. On the other hand they appear mathematically more difficult. Probably they are not difficult *per se* but only in comparison with the large body of analytical tools that are available for the diffusion equation.

A first candidate for a stochastic process different from Brownian motion is a correlated random walk. Whereas in Brownian motion the directions of motion in successive time intervals are uncorrelated, in the correlated random walk the particles have some inertia. The simplest case is a walk in one space dimension with constant speed. This process leads to a hyperbolic system on the line. Other processes lead to integral equations or again to hyperbolic systems in higher dimensions.

Even in the scalar case the reaction diffusion equation (2) can be and has been interpreted in various ways. In a probabilistic setting, solutions to the linear diffusion equation are seen as probability densities $(u(t,x) \ge 0, \int_{-\infty}^{\infty} u(t,x) = 1)$, or probability distributions $(\lim_{x\to-\infty} u(t,x) = 0, \lim_{x\to\infty} u(t,x) \to 1, u(t,x)$ nondecreasing in x). In the latter case u(t,x) is the probability that the position $x_1(t)$ of the moving particle satisfies $x_1(t) < x$.

Fisher [18], in what is probably the first paper on a reaction diffusion equation, considered the spread of a genetic trait. In his interpretation u(t, x) is the proportion of individuals that carry the trait at the point x at time t, in other words, the value u(t, x) is a probability and thus $u(t, x) \in [0, 1]$. Fisher studied the propagation of the trait in the form of a travelling wave solution of Eq. (2) which develops from an initial datum u(0, x) = 1 for x < 0, u(0, x) = 0 for x > 0. Shortly later, Kolmogorov, Petrovskij, Piskunov [48] see u(t, x) as the density of matter at the position x at time t. Hence $u(t, x) \ge 0$ but no upper bound for u is required. In McKean's [51] model for particles that undergo a branching process and perform Brownian motion, the function u(t, x) is again a probability distribution. We shall see that these distinctions carry over to random walk systems and reaction telegraph equations. The theory of vector valued reaction diffusion equations has been stimulated by biological models, e.g. for pattern formation (Turing models), nerve axon models (Hodgkin-Huxley

equations) and various problems in ecology. We shall discuss whether it is meaningful to consider extensions of these problems.

The organization of the paper is as follows. In Section 2 we introduce a general transport equation and derive as special cases or approximations the equations of a correlated random walk in one dimension and general random walk systems. We relate these equations to the telegraph equation for electromagnetic signals and to generalized heat equations. In Section 3 we couple these equations to reaction processes and thus derive semilinear hyperbolic systems that replace reaction diffusion equations. In Section 4 we study these systems on bounded domains, we find the appropriate boundary conditions and we study the corresponding eigenvalue problems, in particular the connection between domain size and stability. In Section 5 we recall the travelling front problem. In Section 6 we quote results on pattern formation, space dependent diffusion, free boundary value problems, and nerve axon equations.

2 Models for spatial spread

In Brownian motion the state of the particle is given by its position in space. The particle does not have an assigned speed. Brownian motion is well suited to describe processes where the position of the particle is determined by many independent effects. When the particle has some memory or, in particular, if it has a well-defined velocity, then Brownian motion may not be an appropriate model. Of course these considerations are subject to choice of scale, and Brownian motion will usually appear as a limit case. Selecting velocity, in addition to location, as the most important variable, is motivated by various applications from physics, chemistry, and biology.

The state of the particle is given by its position $x \in \mathbb{R}^n$ and its velocity $s \in \mathbb{R}^n$. Let u(t, x, s) be the density of particles at time t. If particles just move and do not change velocity then the evolution of this density is described by the equation

$$\frac{\partial u}{\partial t} + \nabla_x \cdot su = 0.$$

Here $\nabla_x = (\partial/\partial x_1, \ldots, \partial/\partial x_n)$, the \cdot denotes the formal inner product. In coordinate notation the equation reads

$$\frac{\partial u}{\partial t} + \sum_{j=1}^n s_j \frac{\partial u}{\partial x_j} = 0.$$

This equation says that each particle moves with "its" velocity along a straight line. Now assume that particles stop their motion at random times determined by a Poisson process with parameter $\tilde{\mu}$, and then select a new velocity. Let $K(\cdot, \tilde{s})$ be the density of the new velocity, given the previous velocity is \tilde{s} . Then K must have the properties $K(s, \tilde{s}) \geq 0$, $\int_{\mathbb{R}^n} K(s, \tilde{s}) ds = 1$, and the equation of motion is

$$\frac{\partial u}{\partial t} + \nabla_x \cdot su = -\tilde{\mu}u + \tilde{\mu} \int_{\mathbb{R}^n} K(s, \tilde{s}) u(t, x, \tilde{s}) d\tilde{s}.$$
 (3)

This equation describes pure motion. No particle is produced or deleted. The total number of particles $\int_{\mathbb{R}^n} \int_{\mathbb{R}^n} u(t, x, s) ds dx$ (in case it is bounded) is an invariant of motion. With respect to the space variable x the system is fully symmetric. So far no symmetry with respect to the variable s has been assumed. Eq. (3) and some nonlinear versions have been introduced by Othmer, Dunbar and Alt [58] as the "velocity jump process" (as opposed to a "position jump process"). The equation is formally close to a Boltzmann equation [9] or a Broadwell system [5], [66] with the difference that here particles turn spontaneously and not in response to collisions.

There are various special cases that are perhaps easier to study than the full problem. In those cases where the velocity ranges over a manifold of lower dimension it is practical to formulate these problems *ab initio* rather than as special cases or as limit cases of Eq. (3). If the speed is constant then u(t, x, s) is defined on $\mathbb{R} \times \mathbb{R}^n \times S^{n-1}$ where S^{n-1} is the unit sphere in \mathbb{R}^n .

One can specialize to a symmetric convolution kernel K on S^{n-1} . With the convolution kernel one can apply a Taylor expansion and replace the integral operator by the second moment term. Then one obtains the equation

$$\frac{\partial u}{\partial t} + \nabla_x \cdot su = \bar{\mu} \Delta_s u \tag{4}$$

where Δ_s is the Laplace-Beltrami-Operator on S^{n-1} . If the velocity assumes only finitely many values s_i , i = 1, ..., m, then Eq. (3) is conveniently written as a system of equations for the variables $u^i(t, x) = u(t, x, s_i)$ (as in [60]),

$$\frac{\partial u^i}{\partial t} + \sum_{j=1}^n s_{ij} \frac{\partial u^i}{x_j} = -\bar{\mu} u^i + \bar{\mu} \sum_{l=1}^m K_{il} u^l, \quad i = 1, \dots, m,$$
(5)

where the kernel in Eq. (3) is replaced by a matrix with $K_{il} \ge 0$, $\sum_{i=1}^{m} K_{il} = 1$, $l = 1, \ldots, m$. We shall further discuss the general case at the end of this section. The simplest case arises for one space dimension, n = 1, and only two velocities, m = 2. If the velocities and the matrix K are chosen in a symmetric way, $s_1 = \gamma > 0$, $s_2 = -\gamma$, $K_{11} = K_{22} = 1 - \tau$, $K_{12} = K_{21} = \tau$, and if the dependent variables are denoted by $u^1 = u^+$, $u^2 = u^-$, then the system assumes the form

$$u_t^+ + \gamma u_x^+ = -\tilde{\mu} u^+ + \tilde{\mu} ((1-\tau)u^+ + \tau u^-),$$

$$u_t^- - \gamma u_x^- = -\tilde{\mu} u^- + \tilde{\mu} (\tau u^+ + (1-\tau)u^-).$$

Redefining $\tilde{\mu}\tau$ as μ we arrive at the normalized problem

$$\begin{aligned} u_t^+ + \gamma u_x^+ &= \mu(u^- - u^+), \\ u_t^- - \gamma u_x^- &= \mu(u^+ - u^-). \end{aligned}$$
 (6)

This problem has a probabilistic interpretation: The function (u^+, u^-) is the probability density of a particle performing a correlated random walk on the real line with speed $\gamma > 0$ and turning rate $\mu > 0$. Notice that the parameter μ in Eq. (6) is the

rate at which the particle changes direction whereas in Eq. (3) the parameter $\tilde{\mu}$ is the rate at which the particle chooses a new direction.

In Eq. (6) introduce the total particle number and the flow

$$u = u^+ + u^-, \quad v = u^+ - u^-.$$
 (7)

In terms of these variables the system (6) can be written

$$u_t + \gamma v_x = 0,$$

$$v_t + \gamma u_x = -2\mu v.$$
(8)

Of course u^+ , u^- can be recovered as $u^+ = (u+v)/2$, $u^- = (u-v)/2$.

For later use we introduce one further reformulation. Define $\gamma v = \tilde{v}$. Then Eq. (8) becomes

$$u_t + \tilde{v}_x = 0,$$

$$\frac{1}{2\mu} \tilde{v}_t + \frac{\gamma^2}{2\mu} u_x + \tilde{v} = 0.$$
(9)

The system (6) or (8) is the starting point of the present paper. As we shall see in the sequel, this *random walk system* assumes the role of the one-dimensional diffusion equation when finite speed of propagation is required.

It seems that Taylor [69] and Fürth [20] were the first who considered a correlated random walk, and S.Goldstein [25] performed a detailed analysis of such systems in the discrete and in the continuous case, see also [47], [12] and the exposition in [74]. A particle moves on the real line with constant speed $\gamma > 0$. The direction of motion is governed by a Poisson process with parameter μ . Thus at any time (except when direction is changed) the state of the particle is given by its location $x \in \mathbb{R}$ and its direction of motion. The state space is $\mathbb{R} \cup \{\pm\}$. The probability density for the state of the particle at time t is a function on the state space which we write $(u^+(t, \cdot), u^-(t, \cdot))$. The evolution of this density is governed by the hyperbolic system (6). For smooth initial data the functions (u^+, u^-) form a classical solution. For non-smooth data Eq. (6) must be seen as shorthand notation for a related integral equation. For the stochastic interpretation of Eq. (6) or Eq. (8) the density satisfies $u^+(t,x) \ge 0, u^-(t,x) \ge 0, \int_{-\infty}^{\infty} (u^+(t,x) + u^-(t,x)) dx = 1$. If (u^+, u^-) is interpreted as particle density then it makes sense to consider non-integrable solutions.

The systems (6) and (8) are equivalent. If (u, v) is a C^2 solution of the system (8) then

$$u_{tt} + \gamma v_{xt} = 0, \quad \gamma v_{tx} + \gamma^2 u_{xx} = -2\mu\gamma v_x = 2\mu u_t,$$

and thus

$$u_{tt} + 2\mu u_t = \gamma^2 u_{xx}.\tag{10}$$

This transition has been found by Kac [45]: For any smooth solution of Eq. (8) the particle density u satisfies the telegraph equation (10). However, in this transition a constant is lost. If (u, v) is a solution of (8) then $(u, v + ce^{-2\mu t})$, c any constant, is

a one-parameter family of solutions of (8), and all these are mapped into the same solution of Eq. (10). Assume two solutions (u, v) and (u, \bar{v}) of (8) differ only in the second component. Then, by the first equation of (8), the difference $\bar{v} - v$ is a function of t only, and by the second equation, this function is $ce^{-2\mu t}$.

On the other hand, assume u is a C^2 solution of (10). Then define, with some constant c,

$$v_0(x) = -\gamma \int_0^x u_t(0, y) dy + c, \tag{11}$$

$$v(t,x) = v_0(x)e^{-2\mu t} - \gamma \int_0^t e^{-2\mu(t-s)} u_x(s,x)ds.$$
(12)

Then the second equation of (8) is satisfied, and with assistance of Eq. (10) it follows that

$$e^{2\mu t} \gamma v_x(t,x) = \gamma v_x(0,x) - \gamma^2 \int_0^t e^{2\mu s} u_{xx}(s,x) ds$$

= $\gamma v_x(0,x) - \int_0^t e^{2\mu s} [u_{tt}(s,x) + 2\mu u_t(s,x)] ds$
= $\gamma v_x(0,x) - e^{2\mu t} u_t(t,x) + u_t(0,x).$

Thus

$$[u_t + \gamma v_x](t, x) = e^{-2\mu t} [u_t + \gamma v_x](0, x) = 0.$$

Hence every C^2 solution u of (10) is part of a C^2 solution (u, v) of (8). Thus there is a one-to-one correspondence between the solutions of Eq. (10) and one-parameter families of solutions of Eq. (8). The true nature of the constant c will show up in the case of several space dimensions.

If the telegraph equation (10) is written in the form

$$\frac{1}{2\mu}u_{tt} + u_t = \frac{\gamma^2}{2\mu}u_{xx}$$
(13)

then one sees immediately its connection to the diffusion equation. For $\gamma \to \infty$, $\mu \to \infty$ such that $\gamma^2/(2\mu) \to D > 0$, Eq. (13) becomes formally the diffusion equation (2). Thus Brownian motion is obtained as the limit of a correlated random walk if the speed becomes large and the turning rate becomes large (the free path length becomes short) in such a way that the limit $\gamma^2/(2\mu)$ exists.

Here the telegraph equation has been compared to the extreme situation where the free path length becomes very small. One can also compare to the other extreme of very large free path length, i.e. to the wave equation

$$U_{tt} = \gamma^2 U_{xx}.\tag{14}$$

Kac [45] has found a principle to produce solutions of the telegraph equation from those of the wave equation. Kaplan [46] has given an elegant proof and he has outlined the scope of this principle. A Poisson process with intensity $\mu > 0$ is a random variable N(t) that counts events. Let N(0) = 0. The probability that an event occurs in $(t, t + \Delta t)$ is $\mu \Delta t + o(\Delta t)$. Then $Prob\{N(t) = k\} = (\mu t)^k e^{-\mu t}/k!$. Introduce the random variable T(t) by

$$T(t) = \int_0^t (-1)^{N(s)} ds.$$
 (15)

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Then $-t \leq T(t) \leq t$. Kaplan shows the following. Let $U \in C^2(\mathbb{R})$, U = U(t). Define

$$u(t) = Exp\{U(T(t))\}.$$
 (16)

Then

$$\ddot{u}(t) + 2\mu \, \dot{u}(t) = Exp\{\dot{U}(T(t))\},\tag{17}$$

in particular, for U(t) = t, $Exp\{T(t)\} = (1 - e^{-2\mu t})/(2\mu)$.

Introduce a space variable x. Let U = U(t, x) be in $C^2(\mathbb{R}^2)$ and satisfy Eq. (14). Then, since ∂_x^2 and Exp commute, the function

$$u(t,x) = Exp\{U(T(t),x)\}$$
(18)

satisfies Eq. (10) and $\lim_{t\to 0} u(t,x) = U(0,x)$, $\lim_{t\to 0} u_t(t,x) = U_t(0,x)$. Eq. (18) says that, for any fixed x, the value u(t,x) is an average of the values U(t,x) where the weight is independent of the solution. Furthermore Kaplan shows that $A(t,x) = Prob\{T(t) \le x/\gamma\}$ is a distribution function, and

$$u(t,x) = \int_{-\infty}^{\infty} U(s,x) d_s A(t,s).$$
(19)

The function A = A(t, x) is itself a solution of Eq. (10), with A(0, x) = H(x), $A_t(0, x) = -\delta(x)$, H and δ being the Heaviside and delta function, respectively. These ideas have been generalized to operator equations in [43], [42].

The telegraph equation appears in the work of Kirchhoff (1857) (according to [49]), it has been derived from Maxwell's equations by Lord Kelvin and O.Heaviside (1876), it has been studied by Heaviside, Du Bois-Reymond [13], Poincaré [61], Picard [59], and many others. The book by Lieberstein [49] gives an excellent historical account of the physical applications, in particular on the idea to balance large leakage in long cables by introducing additional self-induction. Many insights into the mathematical developments can be gained from Riemann-Weber [72], § 125. Consider a transmission line of two parallel wires of length l. Let R be the Ohm resistance, L the self-induction, C the capacity, and A the loss of isolation (leakage), each per unit of length. Let vbe the voltage and i the cross current. These variables satisfy the equations

$$\frac{\partial v}{\partial x} + L\frac{\partial i}{\partial t} + Ri = 0, \quad \frac{\partial i}{\partial x} + C\frac{\partial v}{\partial t} + Av = 0.$$

Differentiate the first equation with respect to x and the second with respect to t, then eliminate the mixed derivatives and obtain the second order equation

$$LCv_{tt} + (AL + RC)v_t = v_{xx} - RAv.$$
⁽²⁰⁾

This equation is the telegraph equation or, as it is called in the earlier literature, the telegrapher's equation or telegraphist's equation. The function i satisfies the same equation.

As has been indicated above, the telegraph equation is in some sense between the wave equation and the diffusion equation. Assume R, C, A are given. If L is small

then the equation is essentially a heat equation with a decay term. Signals become flattened out. If L is large then (although AL + RC also increases) the equation is truly hyperbolic, sharp signals can be transmitted. For the corresponding initial value problems on the real axis, there is d'Alembert's formula for the wave equation and Poisson's formula for the diffusion equation. There is a similar well known formula for the telegraph equation where the kernel is a Bessel function with variable argument, see [67] for a detailed discussion.

Poincaré [61] derived this formula and considered it for initial data with compact support. He writes: " ... These results lead to various observations. First one sees that the head of the perturbation moves with a certain speed in such a way that the perturbation is zero in front of the head, in contrast to what happens in Fourier's theory and in agreement with the laws of propagation of light and sound by plane waves, derived from the equation of the vibrating string. But, with respect to the latter case, there is an important difference, because the perturbation, while propagating, leaves a nonzero remainder ... "

Poincaré's comments are interesting for several reasons. First he finds it remarkable that a model for the propagation of electric signals where no wave speed or particle speed has been introduced *a priori*, nevertheless produces a well-defined wave speed. This observation is trivial from what we presently know about hyperbolic systems, but it is not trivial looking at the physical problem. The second remarkable fact is that Poincaré relates the telegraph equation to Fourier's theory of heat. We shall follow this line of thought later in this section.

In the appropriate initial value problem for the system (6) the values of the functions u^+ , u^- are prescribed for t = 0,

$$u^+(0,x) = u_0^+(x), \quad u^-(0,x) = u_0^-(x).$$
 (21)

Then the initial data for Eq. (8) are

$$u(0,x) = u_0(x) = u_0^+(x) + u_0^-(x), \quad v(0,x) = v_0(x) = u_0^+(x) - u_0^-(x).$$
(22)

The usual initial data for the telegraph equation (10) are

$$u(0,x) = \phi(x), \quad u_t(0,x) = \psi(x).$$
 (23)

We follow the initial conditions in the transition from the random walk system (8) to the telegraph equation (10). Let (u, v) be a solution of Eq. (8) with initial data (22). Then u satisfies Eqs. (10) and (23) with

$$\phi(x) = u_0(x), \quad \psi(x) = -\gamma v'_0(x).$$
 (24)

Let u be a solution of Eq. (10) with initial data (23). Then define v by Eqs. (11)-(12) and (u, v) satisfies Eqs. (8), (22) with $v(0, x) = -\gamma \int_0^x \psi(y) dy + c$.

The classical formula (see, e.g. [67]) for the solution to the initial value problem (10) and (23) in terms of the Riemann function can be used to find a "Poisson formula" for the random walk problem (6) and (21).

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Let $I_{\nu}(x) = e^{\nu \pi i} J_{\nu}(ix)$ be the Bessel function of purely imaginary argument, in particular

$$I_0(x) = J_0(ix) = \sum_{k=0}^{\infty} \frac{1}{(k!)^2} (\frac{x}{2})^{2k},$$

 $I'_0(x) = I_1(x)$. The functions $I_0(x)$, $I_1(x)$ are positive for x > 0, and $I_1(x)/x$ is analytic. Define the kernels, for $x - \gamma t \le y \le x + \gamma t$,

$$K(t, x, y) = \frac{\mu e^{-\mu t}}{2\gamma} I_0(\frac{\mu}{\gamma} \sqrt{\gamma^2 t^2 - (y - x)^2}),$$
(25)

$$K_{\pm}(t,x,y) = \frac{\mu e^{-\mu t}}{2\gamma} \frac{I_1(\frac{\mu}{\gamma}\sqrt{\gamma^2 t^2 - (y-x)^2})}{\sqrt{\gamma^2 t^2 - (y-x)^2}} (\gamma t \mp (y-x)).$$
(26)

The solution to the initial value problem (6) and (21) reads

$$u^{+}(t,x) = u_{0}^{+}(x-\gamma t)e^{-\mu t} + \int_{x-\gamma t}^{x+\gamma t} K_{+}(t,x,y)u_{0}^{+}(y)dy + \int_{x-\gamma t}^{x+\gamma t} K(t,x,y)u_{0}^{-}(y)dy,$$

$$u^{-}(t,x) = u_{0}^{-}(x+\gamma t)e^{-\mu t} + \int_{x-\gamma t}^{x+\gamma t} K_{-}(t,x,y)u_{0}^{-}(y)dy + \int_{x-\gamma t}^{x+\gamma t} K(t,x,y)u_{0}^{+}(y)dy.$$
(27)

One sees immediately that the solution depends in a monotone way on the initial data and that u(t,x) depends only on data in $[x - \gamma t, x + \gamma t]$. Furthermore one sees how discontinuities of the initial data decay. In each equation the first term contains the discontinuity whereas the integral terms represent continuous functions. This formula is more symmetric than the corresponding formula for the telegraph equation. Of course it makes sense for any locally bounded and measurable initial data, thus extending the differential equation to an evolutionary system.

It is not evident how the concept of a random walk system (9) should be generalized to several space dimensions. One possible approach is guided by the theory of heat. The heat equation or Fourier's law (Fourier 1822) is the classical model for heat conduction. It is equivalent to the following two assumptions: A conservation law for the temperature u and the heat flow v,

$$\kappa \rho \, u_t + \operatorname{div} v = 0 \tag{28}$$

where ρ is the density and κ is the heat capacity. The heat flow v is proportional to the negative gradient of the temperature,

$$v = -k \operatorname{grad} u \tag{29}$$

where k is the heat conductivity. If Eq. (29) is introduced into Eq. (28) then the heat equation

$$u_t = \frac{k}{\kappa \rho} \Delta u \tag{30}$$

results.

The heat equation has the property that, contradicting other established physical laws, small amounts of heat are propagated with arbitrarily high speed. In their account of the history of the problem, Joseph and Preziosi [44] describe how, from the times of Maxwell, it was well understood, at least by some scientists in each generation, that the problem of infinite propagation is intimately connected with the fact that in Fourier's model the flow adapts instantaneously to the gradient whereas in real physical systems as well as in an appropriate microscopic description some time would be needed to observe the gradient and to adapt to it. The simplest model for an adaptation process is a linear feedback loop. Then Fourier's law is replaced by the equation

$$\tau v_t = -k \operatorname{grad} u - v. \tag{31}$$

Then Eqs. (28) and (31), i.e.

$$u_t + \frac{1}{\kappa\rho} \operatorname{div} v = 0, \qquad (32)$$
$$\tau v_t + k \operatorname{grad} u + v = 0.$$

becomes a hyperbolic system of n+1 equations that replaces the heat equation. There is a well defined finite propagation speed. In a physical context the time constant τ is so small that it can be neglected in most practical situations.

According to [44], the first formulation of the law (32) appears in a paper by Cattaneo [8]. Already the title of that paper indicates that the real problem is instantaneous propagation whereas infinite speed is only a consequence of Fourier's law. In [57] the system (32) appears as the linearization of some reaction equation.

As in Eq. (10) one can eliminate the function v and arrive at a damped wave equation or telegraph equation

$$\tau \, u_{tt} + u_t = \frac{k}{\kappa \rho} \Delta u. \tag{33}$$

In the formal limit $\tau \to 0$ we obtain the heat equation.

In the theory of diffusion we have an almost identical situation. The conservation law $u_t + \operatorname{div} v = 0$ for the concentration and the flow of some substance, and the first Fickian law (Fick 1855, see [10]) $v = -D\operatorname{grad} u$, with D being the diffusion coefficient, lead to the diffusion equation (the second Fickian law) $u_t = D\Delta u$. The same arguments as before lead to the system

$$u_t + \operatorname{div} v = 0, \qquad (34)$$

$$\tau v_t + D \operatorname{grad} u + v = 0.$$

Replacing the diffusion equation by the linear system (34) is one way to avoid the difficulties of infinite propagation. Quite another way leads to the so-called porous medium equation, i.e. a diffusion equation $u_t = \operatorname{div} (D(u)\operatorname{grad} u)$ where the diffusion coefficient depends on density and vanishes for u = 0, see e.g. [1].

Again the concentration u satisfies a telegraph equation

$$\tau \, u_{tt} + u_t = D\Delta u. \tag{35}$$

If w is any vector field with div w = 0 then $(u, v) = (0, w \exp\{-t/\tau\})$ is a solution of (34). These solutions are mapped into the zero solution of (35). The system (34) is a generalization of Eq. (9). The constant c in Eq. (11) is a vector field with divergence 0. For $\tau \to 0$ we formally obtain Eq. (1). When comparing the system (34) to a one-dimensional random walk (9) or to Brownian motion we shall identify

$$\tau = \frac{1}{2\mu}, \quad D = \frac{\gamma^2}{2\mu}.$$
(36)

Plane wave solutions of Eq. (34) satisfy a system of the form (9).

The work of S.Goldstein [25] has been extended to motions on multidimensional grids by Gillis [23], see also [37]. However there are difficulties to design random walks in the plane (and in \mathbb{R}^n for any $n \geq 2$) for which the probability density would satisfy a telegraph equation of the form (35) (see [56]).

We establish a connection between the velocity jump process (3) and the system (34). In Eq. (3) assume space dimension 2 and constant speed. Then, with φ being the coordinate on S^1 , the equation is

$$u_t(t, x, \varphi) + \gamma \cos \varphi \, u_{x_1}(t, x, \varphi) + \gamma \sin \varphi \, u_{x_2}(t, x, \varphi)$$

= $-\tilde{\mu} \, u(t, x, \varphi) + \tilde{\mu} \int_0^{2\pi} K(\varphi, \psi) u(t, x, \psi) d\psi.$ (37)

The total population size

$$U(t,x) = \int_0^{2\pi} u(t,x,\varphi) d\varphi$$
(38)

satisfies the conservation law

$$U_t(t,x) + \operatorname{div} W(t,x) = 0 \tag{39}$$

where $W = (W_1, W_2)^T$,

$$W_1(t,x) = \int_0^{2\pi} \gamma \cos \varphi \, u(t,x,\varphi) d\varphi, \quad W_2(t,x) = \int_0^{2\pi} \gamma \sin \varphi \, u(t,x,\varphi) d\varphi. \tag{40}$$

Assume $K \equiv 1/2\pi$. A simple calculation shows that

$$W_t + \gamma^2 \int_0^{2\pi} P(\varphi) \operatorname{grad}_x u(t, x, \varphi) d\varphi + \tilde{\mu} W = 0$$
(41)

where

$$P(\varphi) = \begin{pmatrix} \cos^2 \varphi & \sin \varphi \cos \varphi \\ \sin \varphi \cos \varphi & \sin^2 \varphi \end{pmatrix}, \tag{42}$$

for any given φ , is a projection that maps any given vector onto the span of $e_{\varphi} = (\cos \varphi, \sin \varphi)^T$. Eqs. (39)and (41) should be compared to Eq. (34) with $\tau = 1/\tilde{\mu}$ and $D = \gamma^2/\tilde{\mu}$. We see that formally the transition from the velocity jump process (37) to the system (34) is accomplished by replacing the projection by the identity. Thus the transition from Eq. (37), for functions $\mathbb{R}^2 \times S^1 \to \mathbb{R}$, to Eq. (34) for functions from $\mathbb{R}^2 \to \mathbb{R}^{n+1}$, relies on the assumption that, on the average, $\operatorname{grad}_x u(t, x, \varphi)$ is parallel to e_{φ} . Thus a smoothness property of the flow is assumed that should approximately be satisfied at least after long times. Notice, however, that in the heuristic argument no assumptions on γ or $\tilde{\mu}$ have been made.

3 Reaction random walk systems

The random walk system (8) replaces the diffusion equation in the case of a correlated random walk. The problem of defining meaningful generalizations of the scalar reaction diffusion equation can be approached in several ways. If we assume symmetry then the system should have the form

$$u_t^+ + \gamma u_x^+ = \mu(u^- - u^+) + F(u^+, u^-),$$

$$u_t^- - \gamma u_x^- = \mu(u^+ - u^-) + F(u^-, u^+).$$
(43)

If total production does not depend on the direction of motion then $F(u^+, u^-) + F(u^-, u^+)$ should be a function f(u) of $u = u^+ + u^-$. This requirement leaves still many possibilities for the form of the function F. In order to define specific problems we assume again the particle view. If the net production f(u) is distributed among the two directions then one has the simple system

$$u_t^+ + \gamma u_x^+ = \mu(u^- - u^+) + \frac{1}{2}f(u),$$

$$u_t^- - \gamma u_x^- = \mu(u^+ - u^-) + \frac{1}{2}f(u).$$
(44)

In many situations this assumption appears unrealistic: If particles disappear then they are removed from the appropriate class. Thus we introduce a birth rate m and a death rate g, both depending on the total population number u, and we assume that newly produced particles choose both directions with equal probability. Then we arrive at the following system,

$$u_t^+ + \gamma u_x^+ = \mu(u^- - u^+) + \frac{1}{2}m(u)u - g(u)u^+, u_t^- - \gamma u_x^- = \mu(u^+ - u^-) + \frac{1}{2}m(u)u - g(u)u^-.$$
(45)

Finally we can assume that the velocity of a "daughter" is correlated with that of the "mother". If the parameter $\tau \in [0, 1]$ determines the distribution of directions then

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$$u_t^+ + \gamma u_x^+ = \mu(u^- - u^+) + (\tau u^+ + (1 - \tau)u^-)m(u) - g(u)u^+, u_t^- - \gamma u_x^- = \mu(u^+ - u^-) + ((1 - \tau)u^+ + \tau u^-)m(u) - g(u)u^-.$$
(46)

The system (45) (the "uncorrelated case") is obtained for $\tau = 1/2$, and Eq. (44) is obtained with g = 0, f = m.

As in Eq. (8) we introduce the variables u and v. Then these three systems assume the form

$$u_t + \gamma v_x = f(u),$$

$$v_t + \gamma u_x = -h(u)v.$$
(47)

where

$$f(u) = m(u)u - g(u)u \tag{48}$$

and

$$h(u) = 2\mu, \tag{49a}$$

$$h(u) = 2\mu + g(u),$$
 (49b)

$$h(u) = 2\mu + (1 - 2\tau)m(u) + g(u)$$
(49c)

for Eqs. (44), (45), (46), respectively.

We call a system of the form (47) a reaction random walk system or simply a random walk system.

Since we do not have a microscopic description of the system (34), it is not obvious how to design specific models that would replace Eqs. (44-46) in the case of several space dimensions. We propose the system

$$u_t + \operatorname{div} v = f(u),$$

$$r v_t + D \operatorname{grad} u + v = 0$$
(50)

as the appropriate generalization of Eq. (44) or Eq. (47) and (49a), as a random walk system where the reaction is independent of the direction of motion or, more appropriate in the present context, where the feedback loop is independent of density. A generalization of Eqs. (47) and (49b,c) is

$$u_t + \operatorname{div} v = f(u),$$

$$\tau v_t + D \operatorname{grad} u + h(u)v = 0.$$
(51)

Holmes [41] has observed that, similar to Eqs. (8) and (10), some reaction random walk systems can be transformed into (nonlinear) telegraph equations. In Eq. (47) form second derivatives, eliminate mixed derivatives, and obtain

$$u_{tt} - f'(u)u_t = \gamma^2 u_{xx} + h(u)[f(u) - u_t] + h'(u)u_x \gamma v,$$

There is no way to get rid of the term containing v unless h is constant. In the latter case we arrive at the nonlinear telegraph equation

$$u_{tt} + (h - f'(u))u_t = \gamma^2 u_{xx} + hf(u).$$
(52)

Thus Eq. (44) and also Eq. (45), with g constant, can be carried into telegraph equations, but not the general system (47). The standard example is g = 0 which gives

$$u_{tt} + (2\mu - f'(u))u_t = \gamma^2 u_{xx} + 2\mu f(u).$$
(53)

This equation we call a reaction telegraph equation. As in the linear case, one can take the limit to Brownian motion. In Eq. (53) divide by 2μ , let $\mu \to \infty$, $\gamma \to \infty$ such that $\gamma^2/(2\mu) \to D$. Then formally one obtains the reaction diffusion equation (2).

The same idea can be applied to the system (50). From the initial value problem

$$u_t + \operatorname{div} v = f(u), \tag{54a}$$

$$\tau v_t + D \operatorname{grad} u + v = 0, \tag{54b}$$

$$u(0,x) = u_0(x), \quad v(0,x) = v_0(x).$$
 (54c)

one proceeds to the initial value problem of a reaction telegraph equation for the function \boldsymbol{u}

$$\tau \, u_{tt} + (1 - \tau \, f'(u))u_t = D\Delta u + f(u), \tag{55a}$$

$$u(0,x) = u_0(x), \quad u_t(0,x) = -\operatorname{div} v_0(x) + f(u_0(x)), \quad (55b)$$

and for the flow v

$$\tau v_{tt} + v_t = D \operatorname{grad} \operatorname{div} v - D \operatorname{grad} f(u), \tag{56a}$$

$$v(0,x) = v_0(x), \quad \tau v_t(0,x) = -D \operatorname{grad} u_0(x) - v_0(x).$$
 (56b)

Eq. (56a) can also be written in a form that is similar to Eq. (55a)

$$\tau v_{tt} + (1 - \tau f'(u))v_t = D \text{grad div} v - f'(u)v.$$
(57)

Now we see what really happens in Kac's transition Eqs. (8) and (10). The density u and the flow v both satisfy telegraph equations. The equation for u is nonlinear and independent of v, but the equation for v is linear with coefficients depending on u. Thus the equation for u separates. However the initial conditions do not separate, the condition for u_t depends also on v_0 . If a solution $(0, w \exp(-t/\tau))$, div w = 0, is added in Eq. (54) then this solution drops out in Eq. (55), it appears only in Eq. (56).

For $\tau \to 0$ the telegraph equation (55a) becomes the diffusion equation (1). Since τ is small in many (but not all) applications, one can consider (55a) as a singular perturbation of (1). The distance between the solutions has been discussed for the linear random walk case Eq. (10) by Griego and Hersh [28] (see also [26]) in a stochastic setting, and by Hale [36], Milani [53].

4 Bounded domains

If any of the reaction random walk systems are considered on compact domains then one has to specify boundary conditions that reflect the properties of the (supposed) underlying stochastic process similar to the Dirichlet, Neumann, and Robin boundary conditions for the reaction diffusion equation. The boundary conditions must respect the hyperbolic structure of the problem; data can only be prescribed along characteristics that are directed inwards.

We first consider the case n = 1. Then the domain is an interval [0, l]. We consider the standard system (44) or (47) and (49a) and the telegraph equation (53).

The homogeneous Dirichlet condition requires that any particles arriving at the boundary are absorbed. At x = 0 only particles of type u^- arrive, no particles of type u^+ emerge; similarly at x = l. Hence the homogeneous Dirichlet condition is

$$u^{+}(t,0) = 0, \quad u^{-}(t,l) = 0.$$
 (58)

In terms of the variables u and v this boundary condition reads

$$v(t,0) = -u(t,0), \quad v(t,l) = u(t,l).$$
 (59)

In the transition to the telegraph equation the boundary condition (59) for (u, v) becomes a time-dependent boundary condition for u alone

$$u_t(t,0) = \gamma u_x(t,0) - 2\mu u(t,0), \quad u_t(t,l) = -\gamma u_x(t,l) - 2\mu u(t,l).$$
(60)

As an intermediate problem one can study Eq. (53) with the stationary Robin condition

$$u(t,0) = \frac{\gamma}{2\mu} u_x(t,0), \quad u(t,l) = -\frac{\gamma}{2\mu} u_x(t,l).$$
(61)

Again we can consider the limit to Brownian motion. Then $\gamma/(2\mu)$ goes to zero, and formally we arrive at the usual homogeneous Dirichlet condition for the reaction diffusion equation. However, this limit is purely formal, the solutions behave rather differently, see (82) and (85).

The homogeneous Neumann condition describes reflection of particles at the boundary, hence

$$u^{+}(t,0) = u^{-}(t,0), \quad u^{-}(t,l) = u^{+}(t,l).$$
 (62)

In terms of the variables u and v the Neumann boundary condition is

$$v(t,0) = 0, \quad v(t,l) = 0.$$
 (63)

Again, for the telegraph equation we obtain formally

$$u_x(t,0) = 0, \quad u_x(t,l) = 0.$$
 (64)

Similarly one can formulate inhomogeneous boundary conditions.

Existence and uniqueness results for the Cauchy problems of the system (44) with boundary conditions (58), (62) are shown in [3], [40]. Of course there is a

vast literature on Cauchy problems for nonlinear wave equations (e.g. [52, 53, 55, 26]). It is an interesting question to what extent the solutions of the hyperbolic initial boundary value problems have properties similar to those of the corresponding reaction diffusion equations. Although there are maximum and comparison principles for hyperbolic equations (e.g. [73], [40]) such principles are not valid as generally as in the parabolic case. The system (6) preserves positivity, also with Dirichlet or Neumann conditions, and also (44) with f(0) = 0, f'(0) > 0. However, a comparison principle holds only under rather strong conditions on f'.

Next consider the case of several space dimensions, i.e. Eq. (50) on a bounded domain $\Omega \subset \mathbb{R}^n$. The boundary condition for the homogeneous Dirichlet problem requires that there should be no particles entering the domain along a characteristic direction which leads to

$$u(t,x) = \sqrt{\frac{\tau}{D}} \nu^T v(t,x) \quad \text{for} \quad x \in \partial\Omega$$
(65)

where ν is the outward normal at $x \in \partial \Omega$. The absorption boundary condition for the telegraph equation (55a) becomes a time dependent Robin condition,

$$\tau u_t = -\sqrt{\tau D} \frac{\partial u}{\partial \nu} - u \quad \text{for} \quad x \in \partial \Omega.$$
(66)

Again, one can study the intermediate problem Eq. (55a) with

$$u(t,x) = -\sqrt{\tau D} \frac{\partial u}{\partial \nu}$$
 for $x \in \partial \Omega$. (67)

The homogeneous Neumann condition for Eq. (50) is

$$\nu^T v(t, x) = 0 \quad \text{for} \quad x \in \partial \Omega \tag{68}$$

and

$$\frac{\partial u}{\partial \nu} = 0 \quad \text{for} \quad x \in \partial \Omega \tag{69}$$

for Eq. (55a).

The *u* components of stationary solutions of class C^2 of the Dirichlet or Neumann problems satisfy the differential equation

$$-D\Delta u = f(u) \tag{70}$$

and the appropriate boundary conditions Eq. (67) or (69), respectively. Hence known results on the existence of stationary solutions to boundary value problems of reaction diffusion equations (e.g. [63] for Robin boundary conditions) can be used in the hyperbolic case.

We discuss the case n = 1 in greater detail. We assume that the nonlinearity $f \in C^1(\mathbb{R})$ has the properties f(0) = f(1) = 0, f'(0) > 0, f'(1) < 0, f(u) > 0 for 0 < u < 1. We are mainly interested in solutions (u^+, u^-) with $u^+ \ge 0$, $u^- \ge 0$ or $0 \le u \le 1$. Stationary solutions of the Dirichlet problem (47) and (59) satisfy

$$\gamma u' = -h(u)v, \quad \gamma v' = f(u), \tag{71}$$

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$$v(0) = -u(0), \quad v(l) = u(l).$$
 (72)

For the moment we assume that h(u) > 0 for $u \in [0, l]$. Then we can rescale the independent variable (changing the length of the interval) and arrive at

$$\dot{u} = -v, \quad \dot{v} = f(u) \quad \text{where} \quad f(u) = f(u)/h(u).$$
 (73)

Eq. (73) is a Hamiltonian system with Hamiltonian

$$H(u,v) = \frac{1}{2}v^{2} + F(u), \quad F(u) = \int_{0}^{u} f(s)ds.$$
(74)

The stationary points are a center at (0,0) and a saddle point at (1,0). Solutions of Eqs. (71)-(72) correspond to (pieces of) trajectories that connect the line v = -uto the line v = u. There is a one-parameter family of such arcs parametrized by the value u(l/2) ranging from 0 to 1. To each value $\bar{u} \in (0,1)$ there is a unique solution to the boundary value problem for some l with $u(l/2) = \bar{u}$. For $\bar{u} \to 1$ we have $l \to \infty$, for $\bar{u} \to 0$ the length l converges to some well-defined positive number l^* that can be obtained from the linearization. However, l need not be a monotone function of \bar{u} .

The Hamiltonian system (73) describes also the stationary solutions of the Dirichlet problem of the reaction diffusion equation $u_t = u_{xx} + \tilde{f}(u)$, u(t,0) = u(t,l) = 0. Again, there is a branch of nonnegative solutions parametrized by $\bar{u} = u(l/2)$, with $l \to \infty$ for $\bar{u} \to 1$ and $l \to l_0$ for $\bar{u} \to 0$, with some $l_0 > 0$. But there is a marked difference in the two problems. In the parabolic case we look for an orbit that runs from u = 0 to u = 0, thus l_0 is one half of the period near (0,0), whereas l^* is usually considerably smaller. Thus the minimal length of an interval that supports a nontrivial stationary solution is considerably shorter in the hyperbolic case. This phenomenon has been discussed in detail in [58]. The difference will be quantitatively explored in terms of the eigenvalues of the linearization. The stationary solutions of the hyperbolic Dirichlet problem look quite different from those of the reaction diffusion equation. Even though particles are absorbed at the boundary, the function u does not vanish at the boundary.

For the stationary solutions of the homogeneous Neumann problem we have again the system (71). In the stationary situation the boundary conditions $u_x = 0$ and v = 0 are equivalent. Thus the situation is the same as in the parabolic case. In particular, (0,0) and (1,0) are the only nonnegative stationary solutions.

In the homogeneous Dirichlet problem of the scalar reaction diffusion equation (2) with f'(0) > 0 the stability of the zero solution is lost when the length l of the interval exceeds a certain threshold. This threshold can be obtained either by studying the period of the Hamiltonian system near the origin or by a discussion of the corresponding eigenvalue problem. In the hyperbolic case it is difficult to determine the critical length from the Hamiltonian system. The systematic approach to the spectral problem is simpler.

One can show ([55], [40]) that in standard function spaces $(L_p(0, l))^2$ the generators of the solution semigroups of the linearized problems (47), (59) or (63) have pure point spectrum and that the eigenvalues are the zeros of an analytic characteristic function. Here we derive this function explicitly and we extract some important quantities. Later we return to the case of several space dimensions. We start from the Dirichlet problem (47) and (59). We linearize at the zero solution and we put a = f'(0), b = h(0). The linearized system is

$$u_t + \gamma v_x = au, \tag{75}$$
$$v_t + \gamma v_x = -bv$$

with the same boundary condition. If $(u, v) \exp{\lambda t}$ is an exponential solution then u, v, λ satisfy

$$\gamma v' = (a - \lambda)u, \quad \gamma u' = -(b + \lambda)v, \tag{76}$$

$$u(0) + v(0) = 0, \quad u(l) - v(l) = 0.$$
 (77)

Put

$$\delta = (b+\lambda)/\gamma, \quad \kappa^2 = (b+\lambda)(\lambda-a)/\gamma^2. \tag{78}$$

Then $u'' = \kappa^2 u$. We are looking for solutions of the form $u(x) = c_1 e^{\kappa x} + c_2 e^{-\kappa x}$. Then $u'(x) = c_1 \kappa e^{\kappa x} - c_2 \kappa e^{-\kappa x}$, and the boundary conditions yield a linear system $\kappa(c_1 - c_2) = \delta(c_1 + c_2)$, $\kappa(e^{\kappa l}c_1 - e^{-\kappa l}c_2) = -\delta(e^{\kappa l}c_1 + e^{-\kappa l}c_2)$. The determinant vanishes if and only if $(\kappa - \delta)^2/(\kappa + \delta)^2 = e^{2\kappa l}$. Replacing κ and δ we find one form of the characteristic equation

$$\left(\frac{b+\lambda-\sqrt{(b+\lambda)(\lambda-a)}}{b+\lambda+\sqrt{(b+\lambda)(\lambda-a)}}\right)^2 = e^{2\sqrt{(b+\lambda)(\lambda-a)}l/\gamma}.$$
(79)

This equation can also be written

$$\frac{b-a+2\lambda-2\sqrt{(b+\lambda)(\lambda-a)}}{b-a+2\lambda+2\sqrt{(b+\lambda)(\lambda-a)}} = e^{2\sqrt{(b+\lambda)(\lambda-a)}t/\gamma},$$
(80)

or, showing the analyticity,

$$-\frac{2(b-a+2\lambda)}{(b+a)^2} = \frac{\sinh(2\sqrt{(b+\lambda)(\lambda-a)}l/\gamma)}{2\sqrt{(b+\lambda)(\lambda-a)}l/\gamma}\frac{l}{\gamma}.$$
(81)

Consider Eq. (47) and (49a). Then $b = 2\mu$. From (80) one finds that the critical length l of the interval and the parameter a = f'(0) are connected by the equation

$$\tan\frac{\sqrt{2\mu al}}{\gamma} = -\frac{2\sqrt{2\mu a}}{2\mu - a}.$$
(82)

For a qualitative discussion of Eq. (82) we keep μ fixed. The quotient l/γ is a decreasing function of the parameter a. For $a \to 2\mu$ the right hand side goes to infinity, thus the argument of the tangent is $\pi/2$, and $a = 2\mu$ corresponds to $l/\gamma = \pi/(4\mu)$. For $a \to \infty$ the right hand side goes to zero like $2\sqrt{2\mu}/\sqrt{a}$. Since $\tan x \approx x$ near x = 0, we find

$$\frac{l}{\gamma} \sim \frac{2}{a} \quad \text{for} \quad a \to \infty.$$
 (83)

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For $a \rightarrow 0$ the argument of the tangent goes to π , hence

$$\frac{l}{\gamma} \sim \frac{\pi}{\sqrt{2\mu a}}$$
 for $a \to 0.$ (84)

In the parabolic case we have, using Eq. (36) for a comparison,

$$\frac{l}{\gamma} = \frac{\pi}{\sqrt{2\mu a}}.$$
(85)

Thus the behavior for small l is markedly different.

The linear system (6) and (58) preserves positivity and the spectral bound (the eigenvalue with maximal real part) is real. The spectral bound can be obtained from the characteristic equation with a = 0. We put $\lambda = \mu\nu$ and we write the characteristic equation in the form

$$\frac{1+\nu-\sqrt{(2+\nu)\nu}}{1+\nu+\sqrt{(2+\nu)\nu}} - e^{2\sqrt{(2+\nu)\nu}(\mu l/\gamma)} = 0.$$
(86)

Let λ_0 be the spectral bound. Then λ_0/μ depends only on the parameter $\mu l/\gamma$. Notice that this number is different from the parameter $\mu l/\gamma^2$ that appears in the parabolic case. λ_0 is always negative. With some effort one can show [65] that the quotient λ_0/μ is an increasing function of $\mu l/\gamma$ and assumes the following special values,

$$\begin{array}{cccc} \mu l/\gamma \to 0 & \Longleftrightarrow & \lambda_0/\mu \to -\infty, & \mu l/\gamma = 1 & \Longleftrightarrow & \lambda_0/\mu = -2, \\ \mu l/\gamma = \pi/2 & \Longleftrightarrow & \lambda_0/\mu = -1, & \mu l/\gamma \to -\infty & \Longleftrightarrow & \lambda_0/\mu \to 0. \end{array}$$

The Neumann problem is somewhat simpler. The eigenvalues are $\lambda_0 = a$, with eigenvector (1,0), and

$$\lambda_k^{\pm} = \frac{1}{2} [a - b \pm \{(a + b)^2 - 4k^2 \gamma^2 / l^2\}^{1/2}, \quad k = 1, 2, \dots$$
(87)

Now we return to the case of several space dimensions. With f(0) = 0, f'(0) = a > 0, the linearized system to (54) is

$$u_t + \operatorname{div} v = au,$$

$$v_t + D \operatorname{grad} u + v = 0,$$
(88)

with boundary condition (65) or (68), respectively. The corresponding telegraph equation is

$$\tau u_{tt} + (1 - \tau a)u_t = D\Delta u + au. \tag{89}$$

The eigenvalue problem to Eq. (88) is

$$\lambda u + \operatorname{div} v = au,$$

$$\tau \lambda v + D \operatorname{grad} u + v = 0,$$
(90)

with boundary condition (65) or (68), respectively. In Eq. (90) one can eliminate v and find

$$\Delta u = \Lambda u \tag{91}$$

with

$$(\lambda - a)(1 + \tau \lambda) = D\Lambda \tag{92}$$

and boundary conditions

$$(1+\tau\lambda)u(x) = -\sqrt{\tau D}\,\frac{\partial u}{\partial\nu}(x), \quad x \in \partial\Omega, \tag{93}$$

ог

$$\frac{\partial u}{\partial \nu}(x) = 0, \quad x \in \partial\Omega, \tag{94}$$

respectively. Eqs. (91), (92) and (94) could also be obtained from Eqs. (89) and (69).

Let Λ_k , U_k , k = 0, 1, 2, ... be the sequence of eigenvalues and eigenvectors of Eqs. (91) and (94), normalized in $L_2(\Omega)$, with $\Lambda_0 = 0$. Then the eigenvalues of problem (90) and (94) are $\lambda_0 = a$ and

$$\lambda_k^{\pm} = -\frac{1-\tau a}{2\tau} \pm \frac{1}{2\tau} \sqrt{(1+\tau a)^2 + 4\tau D\Lambda_k}, \quad k = 1, 2, \dots$$
(95)

The eigenvalues λ with large absolute values are complex and their asymptotic behavior is $\Re \lambda = -(1 - a\tau)/(2\tau)$, $\Im \lambda \sim \sqrt{D|\Lambda|/\tau}$. Thus, for small τ , the eigenvalues approach a line parallel to the imaginary axis at about $\Re \lambda \approx -1/(2\tau)$.

As in the one-dimensional case [67], [6] one can find solutions to the linear initial boundary value problem (88) and (69) by separation of variables. The ansatz

$$u(t,x) = \sum_{k} T_k(t) U_k(x) \tag{96}$$

for (89) leads to the ordinary differential equation

$$\tau T_k + (1 - \tau a)T_k = (D\Lambda + a)T_k. \tag{97}$$

The characteristic exponents are λ_k^{\pm} as given by Eq. (95). If $u(0,x) = \sum_k c_k U_k(x)$, $u_t(0,x) = \sum_k c'_k U_k(x)$, then $T_k(0) = c_k$, $\dot{T}_k(0) = c'_k$. Hence we find the representation

$$u(t,x) = c_0 e^{at} U_0(x) + \sum_{k=1}^{\infty} \frac{1}{\lambda_k^+ - \lambda_k^-} \left[(e^{\lambda_k^+ t} - e^{\lambda_k^- t}) c_k' + (e^{\lambda_k^- t} \lambda_k^+ - e^{\lambda_k^+ t} \lambda_k^-) c_k \right] U_k(x).$$
(98)

As in the reaction diffusion case the ultimate goal is the description of the qualitative behavior of the solutions of the semilinear equations with appropriate boundary conditions. A useful tool are invariants and Lyapunov functions which have been found by Brayton and Miranker [4] for n = 1 and can be generalized to several space dimensions and also to some vector-valued problems (see also [40]). Let

$$V(u,v) = \frac{1}{2} \int_{\Omega} (u_t^2 + \frac{\tau}{D} v_t^2) dx - M \int_{\Omega} (\frac{1}{2D} v^2 + F(u) - u \nabla v) dx.$$
(99)

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Then along trajectories

$$\frac{d}{dt}V(u,v) = -\int_{\Omega} [(M - f'(u))u_t^2 + \frac{1}{D}(1 - M\tau)v_t^2]dx - \int_{\partial\Omega} (u_t + Mu)\nu^T v_t dS.$$
(100)

If the damping condition $\sup_u f'(u) < 1/\tau$ is satisfied then one can find M such that $\sup_u f'(u) < M < 1/\tau$. Then the term containing the space integral becomes nonpositive. The boundary integral vanishes in the case of the Neumann condition.

Several authors have shown that specific damped wave equations have compact attractors (Webb [71], Lopes [50], Fereisl [16], Hale [36]).

The arguments for the scalar case can be easily carried over to the case of several dependent variables. Then one arrives at hyperbolic systems that mimics reaction diffusion systems. For one space dimension, let $u = (u_1, \ldots, u_m)$ be a vector of species, $M = (\mu_i \delta_{ij})$, $\Gamma = (\gamma_i \delta_{ij})$ and let $f : \mathbb{R}^m \to \mathbb{R}^m$ be the vector field that describes the interaction of species. Then the generalization of (44) is

$$u_t^+ + \Gamma u_x^+ = M(u^- - u^+) + \frac{1}{2}f(u),$$

$$u_t^- - \Gamma u_x^- = M(u^+ - u^-) + \frac{1}{2}f(u).$$
(101)

This system is equivalent to

$$u_t + \Gamma v_x = f(u),$$

$$v_t + \Gamma u_x = -2Mv,$$
(102)

and the function u is a solution to the vector telegraph equation

$$u_{tt} + (I - 2Mf'(u))u_t = \Gamma^2 u_{xx} + 2Mf(u).$$
(103)

5 Branching processes, random walks and travelling fronts

In the standard interpretation of the reaction diffusion equation (2), with f(u) = u(1-u), say, either the function $u(t, \cdot)$ represents a particle density at time t or the number u(t,x) is a probability describing an event at time t at the point x. McKean [51] has given a totally different interpretation of the same equation in terms of branching processes. He designs a stochastic process of the following form. At any time $t \ge 0$ there are $\nu(t)$ particles. These have positions on the real axis $X_1(t), \ldots, X_{\nu(t)}(t)$. Thus there are $\nu(t) + 1$ random variables. The process is constructed in such a way that these are independent. Each of the particles performs a Brownian motion independent of all the other particles. At the same time the particles are subject to a branching process. Any existing particle has exponential holding time. When it splits it gives rise to finitely many daughters (two in the special case). The daughters start their motion at the position of the mother. Brownian motion and branching act independently of each other.

Thus the process is characterized by the following parameters: The diffusion rate D, the Poisson parameter b and the distribution of the number of daughters given by its generating function

$$g(z) = \sum_{k=2}^{\infty} g_k z^k, \quad g_k \ge 0, \quad k = 2, 3, \dots; \quad \sum_{k=2}^{\infty} g_k = 1.$$

In the simplest case, branching into two daughters, we have $g(z) = z^2$.

McKean defines a function u(t, x) as a probability for the position of the most advanced particle,

$$u(t,x) = Prob\{X_i(t) < x, i = 1, \dots, \nu(t)\}.$$
(104)

Clearly, u(t, x) is a nondecreasing function of x with $u(t, x) \to 0$ for $x \to -\infty$, and $u(t, x) \to 1$ for $x \to +\infty$. He proves that the function u satisfies a reaction diffusion equation

$$u_t = \frac{1}{2}u_{xx} + f(u), \quad f(u) = b(g(u) - u).$$
(105)

Consider the process that starts with a single particle at x = 0. Then the initial datum is

$$u(0,x) = \begin{cases} 0, & x < 0, \\ 1, & x \ge 1. \end{cases}$$
(106)

Then the solution to the initial value problem will develop into a travelling front solution. Thus we have the same situation as in Fisher's model.

McKean's idea of connecting a branching process to a process for spatial spread has been carried over to correlated random walks by Dunbar and Othmer [14], [15]. They consider a stochastic process with the following properties. At time t there are $\nu(t)$ particles at positions $X_1(t), \ldots, X_{\nu(t)}(t)$. These particles multiply according to a branching process and move according to a correlated random walk. It is assumed that the branching of particles and the motion of particles act independently. Again they consider the function (104) and they show that it satisfies a reaction telegraph equation

$$u_{tt} + (2\mu + 2f'(u))u_t = \gamma^2 u_{xx} - (2\mu + b)f(u)$$
(107)

Here μ and γ are the parameters of the correlated random walk, and b defines the holding time of the branching process. For $\mu \to \infty$, $\gamma \to \infty$, $\gamma^2/\mu \to 1$, Eq. (107) becomes Eq. (105).

As indicated in the introduction, reaction diffusion equations started with a travelling front problem. In the parabolic case consider the scalar equation (2) with $f \in C^1[0,1], f(0) = f(1) = 0, f'(0) > 0, f'(1) < 0, f(u) > 0$ for 0 < u < 1. A travelling front is a solution $u(t,x) = \phi(x - ct)$ where the shape function ϕ satisfies $0 < \phi(x) < 1$ and $\lim_{x\to-\infty} = 1$ and the speed c is positive. There is a minimal speed c_P (depending on f) and for every $c \ge c_P$ there is, up to translation, exactly one travelling front (see [48], [2], [35], the literature in [31], and [21] for more recent developments in a stochastic setting). For the hyperbolic problem (44), with the same hypothesis on f, a travelling front is a solution $u^+(x - ct)$, $u^-(x - ct)$ with $u^+(x) > 0$, $u^-(x) > 0$, $u^+(x) + u^-(x) < 1$, $u^s(-\infty) = 1/2$, $u^s(+\infty) = 0$ for $s = \pm$. Under suitable conditions on f and μ there is a positive minimal speed $c_H \in (0, \gamma)$, and for every $c \in [c_H, \gamma)$ there is, up to translation, a unique travelling front. A sufficient condition for this statement is the inequality $f'(u) < 2\mu$ for all $u \in [0, 1]$. For the proof and extensions see [30], [31].

Travelling front solutions can be found in other reaction random walk systems, where such solutions exist in the corresponding reaction diffusion equations. As an example one can consider a set of equations that describe epidemic spread by migrating infectives

$$u_{t} = -\beta u(v^{+} + v^{-}),$$

$$v_{t}^{+} + \gamma v_{x}^{+} = \mu(v^{-} - v^{+}) - \alpha v^{+} + \beta u(\tau v^{+} + (1 - \tau)v^{-}),$$

$$v_{t}^{-} - \gamma v_{x}^{-} = \mu(v^{+} - v^{-}) - \alpha v^{-} + \beta u((1 - \tau)v^{+} + \tau v^{-}).$$

(108)

Here one can ask for travelling front solutions that connect two stationary points of the underlying reaction system [32].

6 Pattern formation and other problems from biology

From the view point of Biology one of the main applications of reaction diffusion equations are models for pattern formation. Although there are several schools which have developed such models (mostly with rather specific nonlinearities, not so much supported by experimental evidence but rather by tradition, to name some of the earliest, [22], [24]), the underlying idea is that of Turing [70]: A stable spatially constant equilibrium of the underlying reaction scheme can be destabilized by diffusion, if different species have rather distinct diffusion rates. The simplest case occurs for two variables. Consider

$$u_t = Du_{xx} + Au \tag{109}$$

with

1

$$u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \quad D = \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix}, \quad A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}.$$
 (110)

Assume that the zero solution is stable with respect to the reaction, $a_{11} + a_{22} < 0$, $a_{11}a_{22} - a_{12}a_{21} > 0$, and that u_1 acts as an "activator", u_2 as an "inhibitor", i.e. $a_{11} > 0$, $a_{22} < 0$, $a_{12} < 0$, $a_{21} > 0$. Let [0, l] be a bounded interval. Consider the system (109) with homogeneous Neumann conditions. If d_1 is small and d_2 is large (a short range activator with a long range inhibitor) then there are modes k and lengths l such that these modes grow exponentially. Hillen [39] has studied systems of the form (109) that show the same behavior and he has determined the exact stability conditions.

Several authors, e.g. Hadeler [30], Sánchez-Garduño and Maini [69] have considered density-dependent diffusion, i.e. diffusion equations where the diffusion coefficient itself depends on density,

$$u_t = (D(u)u_x)_x + f(u).$$
(111)

Systems of this form have been extensively studied ("cross diffusion") by Mimura, e.g. in [54]. In the case where D is uniformly positive, many results carry over from the case $D \equiv const$. Particular attention has been paid to the porous medium version [69]. A similar dependence on density can be incorporated in Eq. (44),

$$u_t^+ + (\gamma(u)u^+)_x = \mu(u)(u^- - u^+) + \frac{1}{2}f(u),$$

$$u_t^- - (\gamma(u)u^-)_x = \mu(u)(u^+ - u^-) + \frac{1}{2}f(u).$$
(112)

or Eq. (46)

$$u_t + (\gamma(u)v)_x = f(u),$$

$$v_t + (\gamma(u)u)_x = -2\mu v.$$
(113)

The boundary conditions remain (58-63). The travelling front problem can be solved if γ'/γ is not too large [33].

Greenberg [27] has studied the classical Stefan problem for a generalized heat equation. As we have observed earlier, the boundary value problem for the random walk system does not approximate to that of the diffusion equation if the appropriate limit in the coefficients is taken. Using an energy balance argument, Greenberg specifies a nonlinear Stefan condition for the hyperbolic problem that in the limit yields the Stefan boundary. Here we propose to stay in the class of linear problems (i.e. the only nonlinearity is the dependence on the boundary itself). Thus we consider the standard problem (44) in a domain

$$\Omega = \{(t, x) : 0 \le t \le T, 0 \le x \le s(t)\}.$$

The boundary condition at x = 0 is of Dirichlet type $u^+(t, 0) = \varphi(t)$. The boundary condition at x = s(t) is of Stefan type. We assume that a proportion $\kappa \in (0, 1)$ of particles is reflected, $u^-(t, s(t)) = \kappa(u^+(t, s(t)) \text{ and the boundary is pushed forward}$ by the unreflected particles, $\dot{s}(t) = \tau(u^+(t, s(t)) - u^-(t, s(t)))$. Equivalently, we can assume $\dot{s}(t) = \tau(1 - \kappa)u^+(t, s(t))$. Initial conditions are $u^+(0, x) = u_0(x)$, $u^-(0, x) = u_0^-(x)$ for 0 < x < s(0).

Reaction diffusion equations play a prominent role in neurobiology (see [49],[11). The Hodgkin-Huxley model and its simplified version, the Fitzhugh-Nagumo model, are actually three models each. The basic model is an ordinary differential equations system that describes the excitation of a (short) piece of nerve membrane (the so-called space clamp situation). The same equations with an additional parameter modeling the dendritic input describe, via a Hopf bifurcation, the onset of oscillatory

behavior at the axon hillock ([34], [29]). Finally, one can model the axon as a one dimensional domain, the ordinary differential equation is acting at each space point, and the transmission between adjacent areas is modeled by the cable equation (which corresponds to nearest neighbor coupling in a discrete setting). Then a (degenerate) reaction diffusion system results. There is a vast literature on these problems [11]. The first proof of existence for a travelling pulse solution was given by Carpenter [7]. Fitzgibbon and Parrot [19] reconsidered the original papers and found, that originally the system was designed as a hyperbolic system and later has been "simplified" to a parabolic system by putting a presumably small parameter equal to zero. Already Lieberstein [49] pointed out that this parameter (self-induction) should not be neglected. In the Fitzhugh-Nagumo case the hyperbolic system has the form

$$\epsilon u_{tt} + (1 + \epsilon g(u))u_t = u_{xx} + f(u) - \delta v,$$

$$v_t = u - \nu v$$
(114)

with $f(u) = u(1-u)(u-\alpha)$, $\alpha \in (0,1)$. One of the most interesting features of these equations is the existence of travelling pulses and travelling wave trains. A travelling wave ansatz u(x - ct), v(x - ct) leads to

$$\begin{aligned} \epsilon c^2 \hat{u} - c(1 + \epsilon g(u)) \hat{u} &= \ddot{u} + f(u) - \delta v, \\ \dot{v} &= (\nu v - u)/c. \end{aligned} \tag{115}$$

We put w = u to obtain a three-dimensional first order system,

$$(1 - \epsilon c^2)\dot{w} = -c(1 + \epsilon g(u))w - f(u) + \delta v,$$

$$\dot{v} = (\nu v - u)/c,$$

$$\dot{u} = w.$$
(116)

For this system, for small ϵ , one can again use the arguments of [7].

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Random differential equations and applications

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Abstract

We introduce some basic methods and results in the field of random differential equations. These methods and results center on the concepts of exponential dichotomy, Lyapounov type number, and rotation number. They are applied to two problems in random bifurcation theory.

1 Introduction

The purpose of this paper is to discuss some basic methods and results in the field of "random differential equations" and to delineate in some detail an application of those methods to bifurcation theory. Despite the use of the word "random", and despite a certain formal similarity to the theory of stochastic differential equations, the techniques we introduce are only partly probabilistic in nature, and in fact we will not consider stochastic differential equations. This being the case, it seems natural to begin the paper by delimiting in broad outline the problems one *does* discuss in the field of random differential equations and the basic techniques used to deal with them. We will indicate several areas in which the methods of this field have found application. Then we will turn to the particular case of bifurcation theory and consider a bifurcation scenario intermediate between those considered in the well-developed fields of smooth quasi-periodic and stochastic bifurcation theory.

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As promised, we begin by discussing what we mean by the term "random differential equation". These are non-autonomous linear or non-linear differential equations, viewed from a direction which permits the use of ideas of topological dynamics and ergodic theory in their study. As we will see, our point of view encompasses a very wide variety of time-dependent equations. The time dependence may be periodic, or "deterministically" chaotic, or "indeterministically" chaotic so long as it is bounded. Though we do not consider stochastic differential equations as these are usually defined, the methods we discuss apply to all non-autonomous equations satisfying a boundedness condition with respect to the time variable.

Our starting point is, then, the non-autonomous differential equation

$$x' = f(t, x) \qquad x \in \mathbb{R}^n, \ t \in \mathbb{R}$$
(1.1)

where the t-dependence is defined by a flow $\{T_t \mid t \in \mathbb{R}\}$ on a compact metric space Y. That is, $\{T_t\}$ is a one-parameter group of homeomorphisms of Y [52]. This amounts to viewing (1.1) as just one of a family of equations

$$x' = f(T_t(y), x) \qquad y \in Y, \ x \in \mathbb{R}^n \tag{1.1}_y$$

where now $f: Y \times \mathbb{R}^n \to \mathbb{R}^n$ is a jointly continuous function which is at least Lipschitz continuous in x, so that standard theorems about existence, uniqueness, and continuity of solutions with respect to y are valid. Frequently (but not always), Y will support a probability measure μ which is *ergodic* with respect to the flow $\{T_t \mid t \in \mathbb{R}\}$. That is to say

- (i) μ is invariant: $\mu(T_t(B)) = \mu(B)$ for each $t \in \mathbb{R}$ and each Borel set $B \subset Y$;
- (ii) μ is indecomposable: if $B \subset Y$ is a Borel set such that $T_t(B) = B$ for all $t \in \mathbb{R}$, then $\mu(B) = 0$ or 1.

The presence of a topological structure on Y tends to distinguish our approach to "random" differential equations from that of the Bremen school (see, e.g. [1] for a review). Here the emphasis is on the measurable structure corresponding to an ergodic measure μ . Stochastic differential equations can be studied in this framework and indeed these have been considered in detail by L. Arnold, F. Colonius, H. Crauel, W. Kliemann, and co-workers. In this article we will make considerable use of the compact metric structure on Y. It is this structure that will allow us to apply tools of topological dynamics.

It is easiest to give examples of random ordinary differential equations when f is linear in x, and this is what we now do

Example 1 Let

$$x' = a(t)x \qquad x \in \mathbb{R}^n \tag{1.2}$$

be a linear differential equation with bounded measurable coefficient matrix $a(\cdot)$. We "randomize" equation (1.2) in the following way. Let $L^{\infty}(\mathbb{R}, M_n)$ be the set of bounded measurable functions in the algebra M_n of $n \times n$ real matrices. We introduce the weak-* topology in this space: $\hat{a}_n \to \hat{a}$ if and only if

$$\int_{-\infty}^{\infty} \widehat{a}_n(t)\varphi(t)\,dt \ \longrightarrow \ \int_{-\infty}^{\infty} \widehat{a}(t)\varphi(t)\,dt$$

for every function $\varphi \in L^1(\mathbb{R})$. Then closed norm-bounded subsets of $L^{\infty}(\mathbb{R}, M_n)$ are compact. We define a flow in $L^{\infty}(\mathbb{R}, M_n)$ by translation:

$$(T_t \widehat{a})(s) = \widehat{a}(t+s) \qquad \widehat{a} \in L^{\infty}(\mathbb{R}, M_n).$$

This is the so-called *Bebutov* flow [38]; see also [36]. Returning to equation (1.2), define

 $Y = \operatorname{cls} \{T_t(a) \mid t \in \mathbb{R}\} \subset L^{\infty}(\mathbb{R}, M_n).$

Then Y is compact, the set $\{T_t \mid t \in \mathbb{R}\}$ defines a flow on Y, and equation (1.2) is one of the family of equations

$$x' = y(t)x \qquad y \in Y. \tag{1.2}_y$$

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We have randomized equation (1.2). When convenient, we can fix an ergodic measure μ on Y and discuss properties of equations $(1.2)_y$ which are valid for μ a.a. y (but not necessarily for the original equation (1.2)). This not infrequently leads to important insights which are not at all obvious if attention is restricted to equation (1.2). A basic example is the Oseledec theory [39] which will be discussed later. On the other hand the existence of an ergodic measure on Y (there is always at least one; see [38]) is quite irrelevant for the discussion of some questions which are posed naturally in terms of random differential equations. For example, stability and smoothness problems arising in the theory of exponential dichotomy are often solved without use of ergodic theory.

When convenient, one can write equation $(1.2)_{y}$ in the form

$$x' = A(T_t(y))x \qquad x \in \mathbb{R}^n \tag{1.2}'_y$$

where $A: Y \to M_n$ is a bounded Borel function. For example, define

$$A(y) = \lim_{n \to \infty} n \int_0^{1/n} y(s) \, ds \quad (y \in Y);$$

then for each $y \in Y$, $A(T_t(y))$ is defined and equals y(t) Lebesgue-a.e. Sometimes it is useful to have a continuous function $A: Y \to M_n$ in $(1.2)'_y$; this is possible if (and only if) the original function $a(\cdot)$ is uniformly continuous on \mathbb{R} .

As a special case, suppose a is periodic with period 1: a(t + 1) = a(t). Then the above construction produces a circle $Y \subset L^{\infty}(\mathbb{R}, M_n)$. The flow $\{T_t \mid t \in \mathbb{R}\}$ is equivalent to translation on the standard unit circle: $T_t(e^{2\pi i\theta}) = e^{2\pi i(\theta+t)}$ $(0 \le \theta < 1)$. There is exactly one ergodic measure on Y, which corresponds to normalized Lebesgue measure on the circle $\{0 \le \theta < 1\}$.

Example 2 Suppose $a : \mathbb{R} \to M_n$ is quasi-periodic with k frequencies $\gamma_1, \ldots, \gamma_k$. That is, a(t) is a uniform limit of trigonometric polynomials

$$\sum c_{n_1\dots n_k} e^{2\pi i (n_1\gamma_1 t + \dots + n_k\gamma_k t)}.$$

In this case the construction of Example 1 produces a k- torus Y (assuming the frequencies $\gamma_1, \ldots, \gamma_k$ are rationally independent), and the translation flow on Y is equivalent to a Kronecker twist flow:

$$T_t(\theta_1,\ldots,\theta_k) = (\theta_1 + \gamma_1 t,\ldots,\theta_k + \gamma_k t) \mod \mathbb{Z}^k.$$

There is a unique invariant measure μ on Y, which corresponds to the normalized Lebesgue measure $d\theta_1 \wedge \ldots \wedge d\theta_k$ on T^k .

Example 3 We refer to the book of Doob [15] for the definitions of the terms from probability theory used below. Let (Ω, ν) be a probability space, and let $\{Z_t \mid t \in \mathbb{R}\}$ be a stationary ergodic, stochastically continuous family of differential equations

$$x' = Z_t(\omega)x \quad (\omega \in \Omega).$$
 (1.3) _{ω}

Let X be the uncountable product $X = \prod_{t \in \mathbb{R}} \Omega$, and let ν_{∞} be the probability mea-

sure defined on the σ -algebra \mathcal{B} generated by finite products $A = \{(\omega_t)_{t \in \mathbb{R}} \mid \omega_{t_1} \in B_{t_1}, \ldots, \omega_{t_k} \in B_{t_k}\} \subset X$ (where $B_{t_1}, \ldots, B_{t_k} \subset \Omega$ are ν -measurable) by the formula $\nu_{\infty}(A) = \nu(B_{t_1}) \cdots \nu(B_{t_k})$. Define

$$i: X \longrightarrow L^{\infty}(\mathbb{R}, M_n); \qquad i((\omega_t)) = Z_t(\omega_0)$$

where ω_0 means the zero-th "coordinate" of $(\omega_t) \in X$. Let $Y = \operatorname{cls} i(X)$ in the weak-* topology. Then it can be shown that *i* is a Borel map and that the image measure $i(\nu_{\infty}) = \mu$ is an ergodic measure on Y.

We take the point of view that the family of differential equation $(1.3)_{\omega}$ is equivalent to the random differential equation

$$x' = y(t)x \qquad (y \in Y)$$

with $Y = \operatorname{cls} i(X)$. Thus all methods we develop for random differential equations can be applied to equations $(1.3)_{\omega}$.

At this point it is instructive to observe that there is natural progression in the collection of all random ODEs as regards the "degree of randomness" of the triple $(Y, \{T_t\}, \mu)$. A periodic differential equation exhibits no randomness. It is rather surprising that, even though a quasi-periodic flow (Example 2) exhibits very strong recurrence properties, solutions of a random ODE with quasi-periodic flow $(Y, \{T_t\})$ can exhibit quite irregular behavior. This is evidenced by results concerning the Lyapounov exponents of such equations; see especially the examples of Millionščikov [37] and Vinograd [51]. More recently, it has been shown that the quasi-periodic Schrödinger operator can exhibit a "substantial amount" of point spectrum; see [18].

In any case, one can imagine that the ergodic flow on Y may satisfy mixing conditions, have positive entropy, etc. In particular the entire range of possibilities of "deterministic chaos" may be present in the flow on Y. It is to be expected that the randomness of the flow on Y will make itself felt in the behaviour of the solutions of equations $(1.1)_y$.

At this point one may object that the concept of random differential equation is too general. One of the lessons of the last twenty-five years is that potent tools are available for the study of all such equations, the application of which leads not infrequently to useful insights. These tools are (1) the concept of exponential dichotomy; (2) Lyapounov type numbers adapted to the random frameworks; (3) rotation number. We will illustrate all three of these concepts in our treatment of random bifurcation.

Some fields in which one or more of these concepts have been fruitfully applied in recent years are the following.

(1) The random Schrödinger operator. Textbooks are now available on this subject [9, 16]. It is interesting to compare their contents with the discussion in the carly "reviews" ([26, 50]). It is clear that many interesting problems in this field need further study, for example the Cantor spectrum problem for quasi-periodic operators and the Schrödinger inverse problem together with its relation to the Korteweg-de Vries equation.

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- (2) The study of transversal homoclinic orbits and the numerical study of chaotic systems. These fields have benefited from the use of exponential dichotomy as a tool. Palmer [40, 41] first related exponential dichotomy to the existence of transversal homoclinic orbits. For further developments see, e.g., [2, 3, 42]. The Contemporary Mathematics volume [33] is devoted to chaotic numerics and contains several papers which use Palmer's exponential dichotomy approach to orbit shadowing.
- (3) Control theory of non-autonomous systems. The present author and M. Nerurkar have discussed the relation between local and global controllability for linear systems using Lyapounov exponents [31]. Exponential dichotomy is very useful in studying the random linear stabilization problem [29]. We also wish to mention the papers of Bougerol [4, 5] who discusses the random Kalman filter using Lyapounov exponents.
- (4) Random orthogonal polynomials have been studied systematically by J. Geronimo and his co-authors [20, 21]. In particular, an inverse problem for such polynomials has been formulated and solved by extending a basic result of Kotani from the theory of the random Schrödinger operator [34] and using ideas of algebraic curve theory [22].
- (5) Random bifurcation theory. In Section 3 below we will discuss the random saddle node bifurcation (see also [1, 12]). In Section 4 a bifurcation scenario worked out by the author and Y.F. Yi [32] will be discussed.

2 Basic concepts

In this section we consider some basic definitions and facts having to do with exponential dichotomies, Lyapounov exponents, and rotation numbers.

Let

$$x' = A(T_t(y))x \qquad x \in \mathbb{R}^n \tag{2.1}_y$$

be a random family of linear equations where $\{T_t \mid t \in \mathbb{R}\}$ is a flow on a compact metric space Y. We will assume for convenience that $A: Y \to M_n$ is continuous though, as discussed in § 1, it would suffice to assume that Y is a weak-* compact, translation invariant subset of $L^{\infty}(\mathbb{R}, M_n)$ (or more generally of $L^p_{loc}(\mathbb{R}, M_n)$ for $p \ge 1$).

Definition 2.2 Equations $(2.1)_y$ are said to have an *exponential dichotomy* (ED) if there are constants C > 0, $\gamma > 0$ and a continuous family $\{P_y \mid y \in Y\}$ of projections $P_y : \mathbb{R}^n \to \mathbb{R}^n$ such that

$$\begin{aligned} \|\Phi_{y}(t)P_{y}\Phi_{y}(s)^{-1}\| &\leq Ke^{-\gamma(t-s)} & (t \geq s) \\ \|\Phi_{y}(t)(I-P_{y})\Phi_{y}(s)^{-1}\| &\leq Ke^{+\gamma(t-s)} & (t \leq s). \end{aligned}$$

Here $\Phi_y(t)$ is the fundamental matrix solution of $(2.1)_y$ (i.e. it is an $n \times n$ matrix function which satisfies the differential equation and the initial condition $\Phi_y(0) = I$).

A basic fact concerning the existence of an exponential dichotomy is due to Sacker-Sell [45, 46] and Selgrade [48]. First recall that the flow on Y is called *chain recurrent* if given $y \in Y, T > 0$, and $\epsilon > 0$, there is a finite sequence $y = y_1, y_2, \ldots, y_N = y$ of points in Y and a corresponding sequence $t_1 > T, \ldots, t_{N-1} > T$ such that

distance $(y_{i+1}, T_{t_i}(y_i)) < \epsilon$ $1 \le i < N$.

Theorem 2.3 Suppose that the flow on Y is chain recurrent. Then equations $(2.1)_y$ have an ED if and only if, for each $y \in Y$ the only solution x(t) of $(2.1)_y$ which is bounded on all of \mathbb{R} is the zero solution.

The ED property is extremely useful because of the remarkable stability properties and smoothness properties of the projections P_y . Basic stability results are due to Coppel [14] and Sacker-Sell [46], while Palmer [40], Yi [53] and others have proved smoothness results.

We next give a brief discussion of Lyapounov exponents. Fix $y \in Y$; the Lyapounov exponent of a non-zero solution x(t) of equation (2.1)_y is

$$\beta(x) = \lim_{t \to \infty} \frac{1}{t} \ln ||x(t)||.$$
 (2.4)

(If the limit does not exists, one replaces lim by lim sup in (2.4)). Also the maximal Lyapounov exponent of equation $(2.1)_y$ is

$$\beta_y = \lim_{t \to \infty} \frac{1}{t} \ln \|\Phi_y(t)\|.$$
 (2.5)

The limits in (2.4) and (2.5) need not exist; however in the random context one has the fundamental theorem of Oseledec [39] which has been reproved several times (e.g. [1]) and which has a non-linear version developed by Ruelle [43]. To state the linear version, we introduce the *skew-product* flow defined by equations $(2.1)_y$. This is the flow $\{\hat{T}_t \mid t \in \mathbb{R}\}$ defined on the product space $Y \times \mathbb{R}^n$ in the following way:

$$\overline{T}_t(y,x) = (T_t(y), \Phi_y(t)x).$$

The reason for the term "skew-product" is that the y-part of the flow does not depend on x.

Theorem 2.6 Let μ be an ergodic measure on Y. There is a set $Y_0 \subset Y$ of full μ -measure such that, if $y \in Y_0$, then there are $k \leq n$ Lyapounov exponents β_1, \ldots, β_k of equation $(2.1)_y$. That is, for each non-zero solution $x(\cdot)$ of equation $(2.1)_y$, the limit in (2.4) exists and is among $\{\beta_1, \ldots, \beta_k\}$. The set $\{\beta_1, \ldots, \beta_k\}$ is independent of

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 $y \in Y_0$. Furthermore, there are measurable subbundles $W_1, \ldots, W_k \subset Y_0 \times \mathbb{R}^n$ which are invariant with respect to the flow $\{\widehat{T}_t \mid t \in \mathbb{R}\}$ and which satisfy

$$Y_0 \times \mathbb{R}^n = W_1 \oplus \cdots \oplus W_k;$$

the bundle W_i has the following description:

$$W_i = \{(y, x) \in Y_0 \times \mathbb{R}^n \mid \lim_{t \to \pm \infty} \frac{1}{t} \ln \|\Phi_y(t)x\| = \beta_i\}.$$

Finally, $\beta_y = \max \{\beta_1, \ldots, \beta_k\}$ for μ -a.a. $y \in Y$.

This theorem states that there is a "measurable decomposition" of $Y \times \mathbb{R}^n$ into invariant measurable subbundles, where the subbundles are defined by the μ -Lyapounov exponents of the random differential equation $(2.1)_y$. Of course the measurable decomposition can be viewed as a random analogue of the decomposition of \mathbb{R}^n into the generalized eigenspaces of a constant matrix A, because the generalized eigenspaces of A are invariant under the action of the fundamental matrix solution $\Phi(t) = e^{At}$ of the constant-coefficient system x' = Ax.

Next, we discuss the relation between the Sacker-Sell theory of exponential dichotomy and the Oseledec theory. Define the dynamical spectrum Σ of the random differential equation $(2.1)_y$ as follows: $\Sigma = \{\lambda \in \mathbb{R} \mid \text{the translated equations} x' = [-\lambda I + A(T_t(y))]x$ do not admit an exponential dichotomy}. Then it is proved in [46] that Σ is a union of finitely many closed intervals $[a_1, b_1] \cup \ldots \cup [a_r, b_r]$ where $a_1 \leq b_1 < a_2 \leq b_2 \leq \ldots < a_r \leq b_r$ and $r \leq k$. There are continuous subbundles $\widehat{W}_1, \ldots, \widehat{W}_r \subset Y \times \mathbb{R}^n$ such that

(i)
$$W_1 \oplus \cdots \oplus W_r = Y \times \mathbb{R}^n$$
;

(ii) if
$$(y, x) \in \widehat{W}_i$$
, then $\lim_{t \to \pm \infty} \lim_{t \to \pm \infty} \frac{1}{t} \ln \|\Phi_y(t)x\| \in [a_i, b_i]$.

Furthermore, each continuous bundle \widehat{W}_i is a direct (measurable) sum of Oseledec bundles: $\widehat{W}_i = W_{j_1} \oplus \cdots \oplus W_{j_i}$. The endpoints $e \in \{a_1, b_1, \ldots, a_r, b_r\}$ of the spectral intervals are distinguished in the sense that, for each such number e, there is an ergodic measure $\mu = \mu_e$ on Y with respect to which e is an almost everywhere Lyapounov exponent in the sense of the Oseledec theory.

Suppose now that the linear random differential equation $(2.1)_y$ is 2-dimensional, i.e., $x \in \mathbb{R}^2$. Let x(t) be a non-zero solution of $(2.1)_y$, and let $\theta(t)$ be the polar angle of x(t) in the $x = (x_1, x_2)$ -plane. Of course we suppose that $\theta(t)$ is determined in a continuous way. We define the rotation number

$$\alpha = \lim_{t \to \infty} \frac{\theta(t)}{t}.$$
 (2.6)

The right hand side of (2.6) is clearly independent of the initial value $\theta(0)$. The limit need not exist for every $y \in Y$ (though it does if $(Y, \{T_t\})$ admits exactly one ergodic measure). As in the case of the Lyapounov exponent, if μ is an ergodic

measure on Y, then the limit in (2.6) exists for μ -a.a. y and is constant, independent of y and of the initial value $\theta(0)$. Proofs of these statements are mostly in [28], though the results stated there are given for the almost periodic Schrödinger operator. The proofs in [28] are generalized to the case we are considering in [23].

The rotation number is of fundamental importance in the theory of the onedimensional random Schrödinger operator, and the paper [28] marks the foundation of the systematic development of that theory in the 1980s. The utility of the rotation number derives from its strong continuity properties with respect to parameters. This feature will be illustrated in our discussion of bifurcation theory. There is a higherdimensional version of the rotation number, defined for example if the function $A(\cdot)$ takes values in the Lie algebra $sp(n, \mathbb{R})$ of infinitesimally symplectic matrices, or more generally in u(p,q). This quantity is discussed in [27, 30] and an application to the random feedback stabilization problem of control theory is given in [29]. We will not discuss the higher-dimensional rotation number here because its definition would take us too far afield and because we will not use it in the sequel.

3 Random bifurcation theory: the random saddle node

We consider one of the simplest random bifurcation problems which, however, still has instructive features. See [6, 12]. The random saddle node is modelled by the random differential equation

$$x' + x^{2} = -\lambda + q(T_{t}(y))$$
(3.1)_y

where $(Y, \{T_t\})$ is a compact metric flow and $q: Y \to \mathbb{R}$ is a continuous function. If q = 0, then one checks directly that $x^{\pm} = \pm \sqrt{-\lambda}$ determines, for each $\lambda < 0$, a pair of fixed points, one of which is attracting and one of which is repelling. On the other hand, if $\lambda > 0$, then all solutions x(t) of $x' + x^2 = -\lambda$ tend to $-\infty$ in finite time.

If q is non-zero, the situation is similar but there are some interesting possibilities that merit mention. Let us begin by changing variables, writing $\varphi = \frac{x'}{x}$. Then the equation for φ is simply the random one-dimensional Schrödinger equation where λ plays the role of an eigenvalue parameter:

$$-\varphi'' + q(T_t(y))\varphi = \lambda\varphi. \tag{3.2}_y$$

Since q is bounded, the operator $L_y = -\frac{d^2}{dt^2} + q(T_t(y))$ is self-adjoint and bounded from below in $L^2(\mathbb{R})$ for each $y \in Y$.

We now make use of some of the most basic facts from the theory of the random Schrödinger operator (see [28, 50, 9, 16]). Fix an ergodic measure μ on Y and suppose for convenience that the "topological support" of μ is all of Y (that is, $\mu(V) > 0$ for every open subset $V \subset Y$). Then the spectrum $\Sigma \subset \mathbb{R}$ of the operator L_y is constant (as a closed subset of \mathbb{R}) for μ -a.a $y \in Y$. Let λ_0 be the left endpoint of Σ . Then, for Random differential equations and applications

 $\lambda < \lambda_0$, the associated differential equation

$$\begin{pmatrix} \varphi \\ \varphi' \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -\lambda + q(T_t(y)) & 0 \end{pmatrix} \begin{pmatrix} \varphi \\ \varphi' \end{pmatrix}$$
(3.3)_y

has an exponential dichotomy. Using the fact that the coefficient matrix in $(3.3)_y$ has trace zero, this implies that, in the $\varphi - \varphi'$ space, there is an expanding direction and a contracting direction, and these directions vary continuously with y. More precisely, one has

$$Y \times \mathbb{R}^2 = W^+ \oplus W^-$$

where W^{\pm} are the continuous invariant subbundles discussed in § 2: each is onedimensional.

Define now

$$x_y^+ = \frac{\varphi'_+(0)}{\varphi_+(0)}, \qquad x_y^- = \frac{\varphi'_-(0)}{\varphi_-(0)}$$

where $\varphi_{\pm}(t)$ ($\varphi_{\pm}(t)$) is a solution of $(3.3)_y$ in the expanding (contracting) direction. It can be shown that x_y^{\pm} are finite for all $y \in Y$, or equivalently that $\varphi_{\pm}(t) \neq 0$ for all $t \in \mathbb{R}$, for each $y \in Y$.

A moment's reflection shows that the sections $\{(y, x_y^{\pm}) \mid y \in Y\} \subset Y \times \mathbb{R}$ are analogues of the attracting-repelling fixed points arising for $\lambda < 0$ when q = 0. These sections support ergodic measures μ^{\pm} (the natural lifts of μ under the projection $\pi : Y \times \mathbb{R} \to Y$). Thus one can also speak of attracting and repelling invariant measures in $Y \times \mathbb{R}$.

On the other hand, if $\lambda > \lambda_0$, then the rotation number $\alpha = \alpha(\lambda)$ of equations $(3.3)_y$ is strictly positive ([28, 23]). This implies (see § 2) that, for μ -a.a y, all non-zero solutions $\begin{pmatrix} \varphi(t) \\ \varphi'(t) \end{pmatrix}$ of $(3.3)_y$ rotate around the origin in $\varphi - \varphi'$ space infinitely often as $t \to \infty$. This means that all solutions of the x-equation $(3.1)_y$ blow up in finite time for μ -a.a. y.

These features have of course direct analogues when q = 0. When $\lambda = \lambda_0$, however, an interesting possibility arises which has no analogue in the case q = 0 (nor in the case when q is periodic). Namely, at $\lambda = \lambda_0$, the two ergodic measures μ^+ and μ^- need not collapse together to form one measure (this is what does happen if q = 0 or if q is periodic), but rather they may remain distinct. It so happens that they remain distinct if and only if the maximal Lyapounov exponent $\beta(\lambda_0)$ with respect to μ of equations (3.3)_y when $\lambda = \lambda_0$ is strictly positive. This phenomenon in turn is common when the flow $(Y, \{T_t\})$ admits non-trivial recurrence properties. Its discovery for almost periodic flows is due to Millionščikov ([37]; see also Vinograd [51]). For "highly random" flows it is due to Furstenberg and Kesten [19].

In any case, consider now the linearization of $(3.1)_y$ around a given solution x(t): one obtains

$$(\delta x)' + 2x(t)\delta x = 0. \tag{3.4}_y$$

We may linearize equations $(3.1)_y$ "around μ^+ ", where μ^+ is the limit as λ increases to λ_0 of the measures $\mu^+(\lambda)$. It is easy to make sense of this idea; intuitively speaking

one substitutes in $(3.4)_y$ solutions x(t) of $(3.1)_y$ which are in the support of μ^+ . Since $x = \frac{\varphi'}{\varphi}$, we see that the Lyapounov exponent of equations $(3.4)_y$ which corresponds to the measure μ^+ is $-2\beta(\lambda_0)$.

The moral of these remarks is that the stability of an invariant measure (in the sense that the corresponding Lyapounov exponent of equations $(3.4)_y$ is strictly negative) does not guarantee the continuability of the invariant measure. Indeed $Y \times \mathbb{R}$ carries no measures invariant for equations $(3.1)_y$ (which project to μ) if $\lambda > \lambda_0$. If the continuability is given, however, then negativity of the Lyapounov exponent does indeed guarantee the stability of the continued invariant measure for nearby parameter values [6].

4 Random bifurcation theory II: a two-dimensional problem

We begin by formulating a quite general one-parameter bifurcation problem with two degrees of freedom. Let Y be a compact metric space with flow $\{T_t \mid t \in \mathbb{R}\}$, and let $I \subset \mathbb{R}$ be an open interval containing the origin $\lambda = 0$. Consider the random differential equations

$$x' = l_{\lambda}(T_t(y))x + n_{\lambda}(T_t(y), x) \qquad x \in \mathbb{R}^2$$

$$(4.1)_y$$

where $n_{\lambda}(y, x)$ is jointly continuous in (λ, y, x) , is C^2 -smooth in x, and satisfies $n_{\lambda}(y, x) = O(||x||^2)$ as $x \to 0$. The flow $\{T_t\}$ is allowed to vary with λ ; we assume that $T_t = T_t^{\lambda}$ is jointly continuous.

Suppose now that x = 0 is an asymptotically stable solution of $(4.1)_y$ for each $\lambda < 0$, but that asymptotic stability is lost as λ passes through zero. A natural and important question arises: is there a new asymptotically stable invariant set (attractor) if $\lambda > 0$? If so, what does it look like?

In a moment we will consider two situations in which variants of this general problem arise. First let us rephrase the problem slightly. Note that, for fixed λ , the solutions of $(4.1)_y$ define a skew-product flow $\{\widehat{T}_t\}$ on $Y \times \mathbb{R}^2$ in the following way:

$$T_t(y, x_0) = (T_t(y), x(t))$$

where x(t) is the solution of $(4.1)_y$ satisfying $x(0) = x_0$. It is easy to see that $\{\hat{T}_t\}$ defines a flow on $Y \times \mathbb{R}^2$, at least if solutions of $(4.1)_y$ exist on $-\infty < t < \infty$. But this latter condition can be assured by multiplying $n_\lambda(y, \cdot)$ by a suitable bump function of x centered at x = 0.

Note now that the set $Y \times \{0\} \subset Y \times \mathbb{R}^2$ is compact and invariant with respect to the flow $\{\widehat{T}_t = \widehat{T}_t^{\lambda}\}$ for each $\lambda \in I$. By hypothesis this set is asymptotically stable for $\lambda < 0$ but ceases to be so at $\lambda = 0$. We will search for compact, invariant, asymptotically stable subsets Z of $Y \times \mathbb{R}^2$ which are near $Y \times \{0\}$ when $\lambda > 0$.

Let us now consider two problems which motivate the study of $(4.1)_y$. The first is that of the breakdown of stability of an invariant two-torus in a non-linear dynamical

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system. Consider a one-parameter family of equations

$$z' = f_{\lambda}(z) \qquad z \in \mathbb{R}^N \tag{4.2}_{\lambda}$$

where as before λ lies in an open interval $I \subset \mathbb{R}$ containing zero. Suppose that $\{Y_{\lambda} \mid \lambda \in I\}$ is a continuous family of invariant 2-tori, which is stable for $\lambda < 0$ but loses stability at $\lambda = 0$. One asks if $(4.7)_y$ admits an invariant attractor for $\lambda > 0$.

There is a well-known way, indicated by Ruelle and Takens [44], by which a family of invariant 2-tori can arise in parametrized family of nonlinear dynamical systems. Thus this problem is of significant interest. Two approaches to studying the problem were developed in the late 1970s by Sell and Flockerzi ([49, 17]) and by Chenciner-Iooss ([10, 11]). In both approaches, strong smoothness conditions together with a diophantine assumption on the flow on the 2-torus at the critical value $\lambda = 0$ are of crucial importance.

It should be emphasized that Chenciner and Iooss wrote down a (strong) condition guaranteeing the *existence* of a smooth family of invariant 2-tori for $\lambda > 0$, i.e., after the breakdown of asymptotic stability. Our theory presupposes the persistence of the family of 2-tori for $\lambda > 0$. In situations where this persistence does not hold, our theory is not applicable.

If persistence does hold, however, then $(4.2)_{\lambda}$ can be reduced to $(4.1)_y$ by the device of linearizing $(4.2)_{\lambda}$ around the compact invariant set Y_{λ} and making appropriate assumptions concerning the existence of a center manifold. See [32] for details.

A second type of problem, to which our methods apply directly, is illustrated by the noisy Duffing van der Pol oscillator

$$v'' = (\alpha + y(t))v + \beta v' - v^2 v' - v^3.$$
(4.3)

Here $y(\cdot) \in Y$, and Y is a weak-* compact, translation invariant subset of $L^{\infty}(\mathbb{R}, M_n)$. Thus one has a "parameter-disturbed" bifurcation problem. Note that v = v' = 0 is a solution of (4.3); one studies the stability of this solution as α and β vary. The problem (4.3) was studied by Holmes and Rand [24] when y = 0. They divided the α - β parameter space into eight regions, with various bifurcation scenarios as one crosses the boundary between one region and another.

When $y(t) = \xi(t)$ = white noise, this problem has been studied numerically by K.R. Schenk of Bremen [47]. Motivated by the work of Holmes-Rand, he also divides the α - β parameter space into eight regions. He describes the "attracting invariant measures" in $Y \times \mathbb{R}^2$ in each region (here Y is the path space of white noise). He observes that the attracting invariant measure has a "two-peak" structure in certain regions, and a "crater" structure in others. The two-peak structure is produced by what he calls a stochastic pitchfork bifurcation, and the crater structure by a stochastic Hopf bifurcation.

Schenk does not give an analytical discussion of these very interesting bifurcation patterns. The bifurcation scenario we now discuss resembles in a general way Schenk's stochastic pitchfork bifurcation (and not the stochastic Hopf bifurcation, despite the title of [32]). It must be quickly noted that the randomness $y(\cdot)$ which we study is defined by a flow on a 2-torus, very far indeed (one might think) from white noise. Yet

we have the impression that our scenario has more in common with that described by Schenk than with those discussed in quasi-periodic bifurcation theories ([10, 11, 49, 17] and more recently [25, 35, 7, 8]).

Let us now return to equations $(4.1)_y$. Recall that the parameter λ takes values in an open interval I containing $\lambda = 0$. We suppose that $y \in Y$, a fixed 2-torus, and write

$$y = (y_1, y_2)$$

where $y_1, y_2 \in [0, 1) \simeq \mathbb{R}/\mathbb{Z}$ are angular coordinates on Y. The flow $\{T_t^{\lambda} \mid t \in \mathbb{R}\}$ is assumed to be generated by a vector field V_{λ} on Y. We take for granted that standard existence and uniqueness results are satisfied by the solutions of the equations $y' = V_{\lambda}(y)$. We shall assume throughout that the vector fields V_{λ} ($\lambda \in I$) are jointly continuous in (λ, y) and that they are all transversal to a fixed simple closed curve $K \subset Y$ which is not homotopic to a point. Changing coordinates on Y, we can and will assume that K is given by $\{(y_1, y_2) \mid y_1 = 0\}$.

As an example of the flows on Y which we have in mind, consider

$$T_t^{\lambda}(y_1, y_2) = (y_1 + t, y_2 + \rho(\lambda)t)$$

(the quasi-periodic case). The frequencies are 1 and $\rho(\lambda)$. The quantity $\rho(\lambda)$ is obviously the classical rotation number [13] of the first return map $m_{\lambda} : K \to K : y_2 \to y_2 + \rho(\lambda)$, which in this case coincides with the time-one map.

In general we will write $\rho(\lambda)$ for the classical rotation number of the first return map $m_{\lambda} : K \to K$ ($\lambda \in I$), which need not coincide with any time- t_0 map of $\{T_t^{\lambda}\}$. Since m_{λ} is a homeomorphism of the circle K to itself, $\rho(\lambda)$ has all the usual properties, which we will use below with limited further comment.

We next introduce a useful decomposition. Write

$$l_\lambda(y) = \left(egin{array}{cc} a_\lambda(T_t(y)) & 0 \ 0 & a_\lambda(T_t(y)) \end{array}
ight) + b_\lambda(y) \quad ext{where } ext{tr} \, b_\lambda(\cdot) \equiv 0,$$

and let $\beta_b(\lambda)$ be the maximal Lyapounov exponent of the "traceless" equation

$$x' = b_{\lambda}(T_t(y)) x.$$

Then the maximal Lyapounov exponent $\beta(\lambda)$ of the linearization of $(4.1)_y$:

$$x' = l_{\lambda}(T_t(y)) x \tag{4.4}_y$$

is the sum:

$$\beta(\lambda) = \beta_a(\lambda) + \beta_b(\lambda). \tag{4.5}$$

It is necessary to add a caveat to this discussion. If the rotation number $\rho(\lambda)$ is irrational, then there is exactly one measure on Y which is ergodic with respect to the flow $\{T_t^{\lambda}\}$. In this case β_a , β_b and β are all well-defined and (4.5) is true. On the other hand, if $\rho(\lambda)$ is rational, then there may be several ergodic measures on Y. One must make a choice of ergodic measure in order to define the maximal

Lyapounov exponents. This will not always be convenient, so in what follows we will tacitly assume that $\rho(\lambda)$ is irrational whenever we apply the formula (4.5).

We now suppose that $\beta(\lambda) < 0$ for $\lambda < 0$ but that $\beta(\lambda) > 0$ for at least some λ in every interval $(0, \lambda_1)$ with $\lambda_1 > 0$. We pose the question: do equations $(4.1)_y$ possess an attractor in $Y \times \mathbb{R}^2$ for at least some $\lambda > 0$? We shall see that, subject to some more or less reasonable assumptions, the answer is yes. In the scenario we study, there will be an attractor for *some* but not all λ in each interval $(0, \lambda_1)$ with $\lambda_1 > 0$. In fact there will be an attractor for a "large" set of positive λ , but these attractors definitely do not form a continuous family on $(0, \lambda_1)$.

It is convenient to divide the possible relations between β_b and β into three cases:

- (R1) $\beta_b(\lambda) \gg \beta(\lambda)$ for $\lambda > 0$, λ near zero;
- (R2) $\beta_b(\lambda) \simeq \beta(\lambda)$ for $\lambda > 0$, λ near zero;
- (R3) $\beta_b(\lambda) \ll \beta(\lambda)$ for $\lambda > 0$, λ near zero.

In what follows we will assume that the first relation holds. It holds in particular if $\beta_b(0) > 0$ and if β_b is continuous at $\lambda = 0$. There are grounds for believing that these conditions are verified rather often for the random linear equations $(4.4)_y$. However satisfactory rigorous results are not yet available which would bolster this belief, so we omit further discussion of the matter. Moreover, for technical reasons we shall have to assume that $\beta_b(0) = 0$ in order to prove our main result. We feel, however, that our main theorem is true if $\beta_b(0) > 0$, and that proving our results under this hypothesis would contribute substantially to understanding the breakdown of stability of the zero solution of equations $(4.1)_y$.

An important hypothesis of our main theorem will be that $l_{\lambda}(\cdot)$ is not too smooth as a function of y. In fact we will require that l_{λ} be no more than $C^{1-\delta}$ -smooth for some $\delta > 0$. This is because the conclusion of our Theorem 4.6 is almost certainly false if l_{λ} is C^{r} -smooth for r > 1. Thus our bifurcation scenario should be viewed as complementary to theories in which a high degree of smoothness is required.

Before turning to a discussion of our results, we remark that condition (R3) is satisfied in theories where a stable 3-torus bifurcates cleanly from the family of 2-tori at $\lambda = 0$ ([10, 11, 49, 17]). Roughly speaking, the "hyperbolic" part of the linearized system (4.4)_y is dominated by the "elliptic" part. The relation (R2) seems rather unpleasant from a theoretical point of view. An example which displays transversal homoclinic behaviour in (4.1)_y when (R2) holds is given in [32].

We now begin the analysis of equations $(4.1)_y$ when x = 0 loses asymptotic stability at $\lambda = 0$ and when condition (R1) above holds. We will impose further assumptions of a "generic" nature, meant to hold for as large a class of problems as possible. We begin with the family of vector fields $\{V_{\lambda}\}$. If the rotation number $\rho(\lambda)$ of the first-return map $m_{\lambda} : K \to K$ is rational, then (generically) the circle K supports qattractor-repeller pairs, i.e., there is frequency locking. While it is certainly reasonable that frequency locking should occur for an open dense set of $\lambda \in I$, we assume that it does *not* occur at $\lambda = 0$. If it did, then our loss-of-stability problem would reduce to a (non-smooth!) version of the bifurcation problem studied in [44]. Further investigation of this matter would be interesting. Here, however, we will assume that, at $\lambda = 0$, the rotation number $\rho(0)$ is irrational. In fact the important set of λ -values will be those for which $\rho(\lambda)$ is irrational. With this in mind, we define

$$\Lambda_{\bullet} = \operatorname{cls} \left\{ \lambda \in I \mid \rho(\lambda) \notin \mathbb{Q} \right\},\$$

and note that $0 \in \Lambda_*$.

Next we consider the linear equations

$$x' = l_{\lambda}(T_t(y))x. \tag{4.4}_y$$

The solutions of this equation exhibit a rich range of behaviour; its theory is far from completely developed. On the other hand one has sufficient knowledge to permit our analysis of equations $(4.1)_y$. The basic result which we will need states that, roughly speaking, a generic one-parameter family $x' = b_\lambda(T_t(y))x$ of trace-zero linear systems has an exponential dichotomy for an open dense set of parameter values in Λ_* .

To state this result more precisely, let $sl(2, \mathbb{R})$ be the Lie algebra of 2×2 real matrices with trace zero. Let B be the set of all $C^{1-\delta}$ -mappings from the 2-torus Y into $sl(2, \mathbb{R})$ where $0 < \delta \leq 1$. Further let s be any non-negative number $(s = \infty \text{ is allowed})$. Define $C^s(I, B)$ to be the collection of all C^s -mappings from the interval I to the Banach space B. The number s is not important in our theory, but the number δ is. The result we now enunciate is very likely false if $1-\delta$ is replaced by r for r > 1.

Theorem 4.6 Let $\{V_{\lambda} \mid \lambda \in I\}$ be a family of vector fields on Y satisfying the conditions enunciated earlier. There is a residual subset $E \subset C^{s}(I, B)$ with the following property: if $b = b_{\lambda}(\cdot) \in E$, then the equations

$$x' = b_{\lambda}(T_t(y))x \tag{4.7}_y$$

have an exponential dichotomy for all λ in an open dense subset of Λ_* .

The idea in what follows is quite simple. Since ED is an extremely robust property, it is natural to study the non-linear equations $(4.1)_y$ for parameter values $\lambda \in \Lambda_*$ for which an exponential dichotomy is present in equations $(4.7)_y$. One expects that the presence of ED in the linear equations will make itself felt in the behavior of solutions of the nonlinear equations.

We return to equations $(4.1)_y$. The fact is that these are too general for us to handle, even with the relation (R1) and Theorem 4.6 at our disposal. However, we can deal with the problem

$$x' = \lambda[l_{\lambda}(T_t(y))x + n_{\lambda}(T_t(y), x)]$$

$$(4.8)_y$$

by using a generalization of the method of averaging, as described in [32].

To analyze equations $(4.8)_{y}$, we write

$$l_{\lambda} = a_{\lambda} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \gamma_{\lambda} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} + \delta_{\lambda} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \epsilon_{\lambda} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Random differential equations and applications

Let (r, θ) be polar coordinates in the x-plane. Then equations $(4.8)_y$ take the form

$$r' = \lambda \{ [a_{\lambda} + U_{\lambda}]r + d_{\lambda}r^{2} + \widehat{f}_{\lambda} \}$$

$$\theta' = \lambda \{ L_{\lambda} + G_{\lambda}r + \widehat{g}_{\lambda} \}$$

where a_{λ} is a function of $T_t(y)$; $U_{\lambda}, d_{\lambda}, L_{\lambda}$ and G_{λ} are functions of $(T_t(y), r(t), \theta(t))$. One has explicitly:

$$U_{\lambda}(y,\theta) = \delta_{\lambda}(y)\cos 2\theta + \epsilon_{\lambda}(y)\sin 2\theta$$
$$L_{\lambda}(y,\theta) = \gamma_{\lambda}(y) + \epsilon_{\lambda}(y)\cos 2\theta - \delta_{\lambda}(y)\sin 2\theta.$$

The function $d_{\lambda}(y,\theta)$ depends on the nonlinearity n_{λ} . In addition $\hat{f}_{\lambda} = O(r^3)$ and $\hat{g}_{\lambda} = O(r^2)$ as $r \to 0$, uniformly in (y,θ) .

Define another function

$$p_{\lambda}(y,\theta) = rac{\partial U_{\lambda}}{\partial heta} = 2\epsilon_{\lambda}(y)\cos 2\theta - 2\delta_{\lambda}(y)\sin 2\theta.$$

Introduce the following hypotheses.

- (H1) $\beta_b(\lambda) \gg \beta(\lambda)$ for small positive λ , and $\beta_b(0) = 0$.
- (H2) When $\lambda = 0$, there is a unique measure on the "projective bundle" $Y \times \mathbb{P}^1(\mathbb{R})$ which is invariant under the natural flow-of lines on $Y \times \mathbb{P}^1(\mathbb{R})$ defined by $x' = l_0(T_t(y))x$. See [32]. This hypothesis can be viewed as a very weak version of the diophantine condition in the smooth quasi-periodic theory. It allows our averaging procedure to work.
- (H3) The average $\overline{d}_0 = \lim_{T \to \infty} \frac{1}{T} \int_o^T d_0(T_s(y), \theta(s)) \, ds$ is less than zero. The average is well-defined by (H2). This is a generalized weak-attractor condition.
- (H4) The mean values $\overline{p}_{\lambda} = \lim_{T \to \infty} \frac{1}{T} \int_{0}^{T} p_{\lambda}(T_{s}(y), \theta(s)) ds$ satisfy $\overline{p}_{0} = 0$ and $\overline{p}_{\lambda} \leq c\beta_{b}(\lambda)$ for a certain constant c. This may be viewed as a weak normal form condition; it is satisfied if, at $\lambda = 0$, $l_{0} = \begin{pmatrix} 0 & -\gamma_{0} \\ \gamma_{0} & 0 \end{pmatrix}$.
- (H5) Four quantities which we do not write explicitly do not deviate too much from their mean values.

We can now state our main theorem.

Theorem 4.9 Let Λ_b be the set of points $0 < \lambda \in \Lambda_*$ such that $x' = b_{\lambda}(T_t(y))x$ has an ED. Assume that hypotheses (H1)-(H5) hold.

(a) If $\lambda \in \Lambda \cap (0, \lambda_1)$ for sufficiently small λ_1 , then equations (4.1)_y admit an attractor-repeller pair $Z^-(\lambda), Z^+(\lambda)$ in $Y \times \mathbb{R}^2$. These sets tend to $Y \times \{0\} \subset Y \times \mathbb{R}^2$ as $\lambda \to 0$.

(b) The sets Z⁻(λ) vary discontinuously as λ → 0 in a precise sense as λ → 0⁺; so do the sets Z⁺(λ).

We finish this paper with a brief discussion of point (b) of Theorem 4.9. It is here that the rotation number $\alpha(\lambda)$ of equation (4.7)_y plays a role. Here we speak of the rotation number defined in § 2 and not of the classical quantity $\rho(\lambda)$.

The main point is that there is a "time-changed" version $\hat{\alpha}(\lambda)$ of the rotation number such that, if equations $(4.7)_y$ have an ED at λ , then

$$\widehat{\alpha}(\lambda) = n_{\lambda} + m_{\lambda}\rho(\lambda)$$

where n_{λ}, m_{λ} are integers. Now, by removing a set of first category from the set E of Theorem 4.6, one can assume that $\hat{\alpha}(0)$ is not of the form $n + m\rho(0)$ for integers n, m. Since $\hat{\alpha}(\cdot)$ is continuous, the integers n_{λ}, m_{λ} must vary wildly as $\lambda \to 0$.

Now, the integers n_{λ}, m_{λ} are winding numbers, and it turns out that they reflect the way in which $Z^{-}(\lambda)$ is embedded in $Y \times \mathbb{R}^{2}$. It is in this sense that the sets $Z^{-}(\lambda)$ vary discontinuously as $\lambda \to 0$.

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Adaptive dynamics, a geometrical study of the consequences of nearly faithful reproduction

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Abstract

We set out to explore a class of stochastic processes, called "adaptive dynamics", which supposedly capture some of the essentials of long term biological evolution. These processes have a strong deterministic component. This allows a classification of their qualitative features which in many aspects is similar to classifications from the theory of deterministic dynamical systems. But they also display a good number of clear-cut novel dynamical phenomena.

The sample functions of an adaptive dynamics are piecewise constant functions from \mathbb{R}_+ to the finite subsets of some "trait" space $\mathbb{X} \subset \mathbb{R}^k$. Those subsets we call "adaptive conditions". Both the range and the jumps of a sample function are governed by a function s, called "fitness", mapping the present adaptive condition and the trait value of a potential "mutant" to \mathbb{R} . Sign(s) tells which subsets of \mathbb{X} qualify as adaptive conditions, which mutants can potentially "invade", leading to a jump in the sample function, and which adaptive condition(s) can result from such an invasion.

Fitnesses supposedly satisfy certain constraints derived from their population/community dynamical origin, such as the fact that all mutants which are equal to some "resident", i.e., element of the present adaptive condition, have zero fitness. Apart from that we suppose that s is as smooth as can possibly be condoned by its community dynamical origin. Moreover we assume that a mutant can differ but little from its resident "progenitor".

In sections 1 and 2 we describe the biological background of our mathematical framework. In section 1 we deal with the position of our framework relative to present and past evolutionary research. In section 2 we discuss the community dynamical origins of s, and the reasons for making a number of specific simplifications relative to the full complexity seen in nature.

In sections 3 and 4 we consider some general, mathematical as well as biological, conclusions that can be drawn from our framework in its simplest guise, that is, when we assume that X is 1-dimensional, and that the cardinality of the adaptive conditions stays low. The main result is a classification of the adaptively singular points. These points comprise both the adaptive point attractors, as well as the points where the adaptive trajectory can branch, thus attaining its characteristic treelike shape.

In section 5 we discuss how adaptive dynamics relate through a limiting argument to stochastic models in which individual organisms are represented as separate entities. It is only through such a limiting procedure that any class of population or evolutionary models can eventually be justified. Our basic assumptions are (i) clonal reproduction, i.e., the resident individuals reproduce faithfully without any of the complications of sex or Mendelian genetics, except for the occasional occurrence of a mutant, (ii) a large system size and an even rarer occurrence of mutations per birth event, (iii) uniqueness and global attractiveness of any interior attractor of the community dynamics in the limit of infinite system size.

In section 6 we try to delineate, by a tentative listing of "axioms", the largest possible class of processes that can result from the kind of limiting considerations spelled out in section 5. And in section 7 we heuristically derive some very general predictions about macro-evolutionary patterns, based on those weak assumptions only.

In the final section 8 we discuss (i) how the results from the preceding sections may fit into a more encompassing view of biological evolution, and (ii) some directions for further research.

1 The larger context

1.1 Evolutionary basics

The most conspicuous, if not the defining, properties of life are that living objects (1) reproduce almost faithfully, and (2) die. It is a mathematical necessity that the independent reproduction of particles leads to exponential population growth (or to rapid extinction, but such populations habitually escape our attention) (Jagers, 1975, 1991, 1995). Therefore in any finite world organisms will (3) interact, both directly through jostling or fighting, and indirectly through the consumption of resources and the sharing of predators. The consequence of (1) to (3) is that life evolves: Those types that do a better job in contributing to future generations will inherit the earth. Until a copying error during the reproductive act creates a still "better adapted" type. Evolution will grind to a halt only when it has reached a combination of types which cannot be bettered under the current condition of the environment.

Simple though it may seem, this scenario becomes interestingly complicated due to the fact that those same types are (co-)instrumental in creating the current environmental condition.

Remark: That there is no sign yet that evolution on this earth is going to freeze has two causes. The easy one is that the physical configuration of the world keeps changing. But it usually does so relatively slowly. Much to the biologist's luck, since it allows him/her (sometimes) to predict organismal properties from evolutionary considerations. The second cause is more involved: (a) There is no need that ecology drives evolution to a point attractor, even in models which only consider simple external (phenotypic) representations of organisms. But if we assume that too extreme phenotypes are weak survivors, as is generally the case in the real world, we may expect at least convergence to some nice attractor. However, there is a snag. (b) Since the internal (genotypic) representation of organisms is almost infinitely complicated, the map from genotype to any simple phenotypic representation is very many to one. Dolphins, Ichthyosaurs, tuna, and sharks may look similar, but underneath they are very different creatures. Consequently the mutational supply (due to copying errors of the genetic material) of new phenotypic variation shows considerable history dependence. (a) and (b) together make that when the evolutionary process is looked at in somewhat greater detail, it appears that non-point attractors with some recurrency property just don't exist. Evolution either halts, or progresses indefinitely, though not necessarily progressively. Luckily, here again, proper modes of abstraction as well as time scale differences come to the rescue of those who nevertheless want to make predictions.

1.2 History: the changes in attention paid to ecological and genetic complexity

The mechanistic theory of evolution started public life with the publication of Charles Darwin's "On the Origin of Species" in 1859. The one flaw in the reasoning of the early Darwinists was their, lukewarm, adherence to the concept of blending inheritance (the blending of the properties of the parents in their offspring), since by mathematical necessity evolution can only occur among particles which reproduce sufficiently faithfully. But they clearly saw evolution as driven by the interaction between individuals, as is proved by Darwin's statement that he owed his idea of the "struggle for existence" to the writings of Thomas Malthus.

At the turn of the century the inheritance problem was solved by the rediscovery of a piece of contract research by a Moravian monk with physicist leanings, Gregor Mendel. It aren't the organisms which reproduce almost faithfully, but their genes. This considerably complexifies the logic, since the genes inhabiting one organism affect each other's reproductive potential. In the twenties a reconciliation of the Mendelian and Darwinian paradigms was effected by the three great mathematical population geneticists, Sir Ronald Fisher, J.B.S Haldane, and Sewall Wright. The handwaving linking up in the forties and fifties of the resulting circle of ideas with those of the paleontologists and taxonomists of the day is now referred to as the Modern Synthesis. The strength of that link is still among the biologists' articles of faith.

Ironically the mathematical framework underlying the Modern Synthesis dealt almost exclusively with the genetics of populations of non-interacting individuals. For this was one of the main simplifications made by the early theoretical population geneticists in order to cope with the complexities of realistic inheritance laws. It is even more ironical that this assumption of non-interaction makes it particularly hard on model populations to split into lines going their separate ways. The origin of species was, and is, still one of the less well understood problems of population genetics. The second point on which the population genetics of the time fell short as a cornerstone for the theory of adaptive evolution is that it almost exclusively concentrated on the changes in the relative frequencies of types from a fixed genetic repertoire. For this is the scale where contact could be made between theory and genetic observations on real populations. Yet, the overall features of long term adaptive evolution crucially depend on the existence of a continual trickle of new mutants. The stream of novel adaptive variation is that small and fickle, that it is essentially beyond direct observation. But its effects can be seen in overwhelming profusion. We are but one instance

Around 1970 both conceptual omissions were rectified by W.D. Hamilton (1967), G.R. Price and John Maynard Smith (Maynard Smith & Price, 1973; Maynard Smith, 1982), who put to the fore the concept of Evolutionarily Unbeatable Strategy. An EUS is a strategy which when played by everybody prevents all comparable strategies from increasing in numbers. Such strategies are the natural longer term evolutionary traps. (By now EUSes are more often called Evolutionarily Stable Strategies. Unfortunately this is a misnomer as EUSes need not be stable in the dynamic sense.) Of course there was a price. Only the statics of adaptive evolution was considered. Moreover, it became common usage to assume clonal reproduction (i.e., the almost faithful reproduction of individuals), in order to concentrate on behavioural interactions. Luckily later research has shown that a good number of the general results kept their ground for more realistic types of inheritance. But exceptions that are neither trivial nor contrived have been found as well.

1.3 About this paper

In this paper we set out to construct in a general manner the simplest possible dynamical counterpart to the EUS concept. Since we primarily want to cope with general types of ecological complexities we stick to the by now time-honoured assumption of clonal reproduction. Moreover we assume that the ecological and evolutionary time scales are clearly separated. Finally we shall assume that the types can be characterized by a finite number of numerical traits, that the ecology satisfies some continuity conditions (to be expounded below) and that mutation only produces small steps in trait space.

1.4 Relation to present day views of the evolutionary process

No doubt red-blooded biologists will find our assumptions artificial. To them we have the following three remarks to make in our defense. (i) It is always better to start hunting for patterns in some well chosen caricature of reality, and to leave it for a second stage to see to how those patterns modify when additional realism is added, than not to see any wood for the trees. (However, till we reach that second stage our conclusions about long term evolution should be taken with a pinch of salt.) (ii) The least we do is develop an internally consistent picture of a class of evolutionary processes, well worth of study in their own right. It is only by studying various classes of evolutionary processes that one may ever hope to bring out their essence. (iii) Our picture is the simplest one allowing the eventual development of a bifurcation theory of EUSes. Anyone who knows what bifurcation theory has done for differential equations will appreciate the usefulness of such a development.

For mathematicians we may add that there is a wholy new, and rather unusual, class of dynamical systems waiting to be explored.

As a final point we should make clear that we are by no means the first to venture on the present path. Some notable forerunners are Ilan Eshel (1983, 1991,1995; – & Feldman, 1982, 1984), Jonathan Roughgarden (1976, 1979, 1983), Freddy Bugge Christiansen (1984, 1988, 1991; – & Loeschcke, 1980, 1987, Loeschcke & -, 1984a,b), Peter Taylor (1989), Karl Sigmund (Hofbauer & -, 1990; Nowak & -, 1990), Simon Levin (Cohen & -, 1987; Ludwig & -, 1992), Peter Hammerstein (1995, - & Selten, 1994), and Carlo Matessi (- & Di Pascuale, 1995). The main difference of our effort from theirs is that we strive to construct a clear mathematical framework that should abstractly encompass a greater deal of ecological complexity (but at the cost of highly oversimplifying the genetical end). Tom Vincent and co-workers (1990; -& Brown, 1984, 1987, 1988, 1989; Brown & -, 1987a,b, 1992; - & Fisher, 1988; - et al., 1993) followed a line of thought that superficially is rather similar to ours. Our approach differs from theirs both in its greater formal abstraction and in that we try to stick to formalisms that consistently allow an interpretation in individual-based terms concordant with the basic philosophy with which we started this discourse (see also Metz & De Roos, 1992).

2 Reconciling the population dynamical and taxonomical viewpoints

2.1 Fitness

The catch phrase of the theory of evolution by natural selection is "fitness". Definitions abound, most of them rather special or not very clear. Here we shall stick to the definition expounded in Metz et al. (1992), as this is the only one coping with a range of ecological scenario's which is sufficient for our purpose: Fitness is the asymptotic average rate of exponential growth ρ which results from a thought experiment in which we let a clone of the type under consideration grow in an ergodic environment. This definition immediately makes clear that the fitness of a type, say X, also depends on the environment in which it lives, E. We shall bring this out in our notation by writing $\rho_E(X)$.

Remark: The underlying mathematical idea is:

(i) The dynamics of a sufficiently large (spatially and/or physiologically structured) population can, for a given time dependence of the environmental conditions, be described by a positivity-preserving linear evolutionary (in the mathematical sense) system. For ergodic environmental conditions, and subject to some biologically innocent regularity conditions, there exists a unique number ρ such that

$$\frac{\log |N(t)|}{t} \rightarrow \rho, \quad \text{a.s.},$$

|N(t)| the total population mass. (This has not been proven yet in as much generallity as we would wish. But the special model classes that so far have yielded to analysis all show the same pattern; see Tuljapurkar 1990; Inaba 1989; Ferrière & Gatto, 1995). In mathematics ρ is better known as the dominant Lyapunov exponent.

(ii) What results there are for special classes of branching processes (Jagers, 1975, 1991, 1995; Athreya & Karlin, 1971a,b) all tell that (a) a branching process starting with a single individual either goes extinct, or starts growing exponentially with a growth rate ρ equal to that of its mean process, (b) the probability of non-extinction is zero when $\rho \leq 0$, and positive when $\rho > 0$.

In a non-virgin world the current environment is necessarily (co-)determined by

those types that are already in residence. Let those types be denoted by X_1, \ldots, X_n (we confine the discussion to situations where that number of types is finite), let $C := (X_1, \ldots, X_n)$ denote the combination of those types, and let a unique environment E(C) be created by the resulting interactions. If we interpret "being resident" as "staying bounded away from zero population size (on the population dynamical time scale!)" we expect E(C) to be ergodic with $\rho_{E(C)}(X_i) = 0$, $i = 1, \ldots, n$. For (i) by assumption the masses of none of the types goes to zero, (ii) in a finite world none of those masses can go to infinity either.

Remark: We always think of the world as intrinsically noisy. This not only does away with some considerable mathematical complications (see e.g. Ruelle 1989 and Rand et al., 1994), but it also has the advantage of being realistic.

Let Y generically denote a mutant type. In our discussion of the determination of the environmental condition by the resident population we implicitly assumed that population to be numerically large. (Populations which stay numerically small quickly go extinct by chance fluctuations.) Mutants arrive as single individuals. Therefore the effect of the mutant population on the environment is that diluted that its initial growth is the same as that of a Y population in the ergodic environment E(C).

We shall denote the fitness of Y in a C population dynamical background as

$$s_C(Y) := \rho_{E(C)}(Y).$$
 (2.1)

We assume that (i) mutants for which $s_C(Y) < 0$ are unable to invade a C community, (ii) mutants with $s_C(Y) > 0$ can invade (but will not necessarily always do so as a result of random fluctuations due to the small initial size of the mutant population; see sections 4 and 5.4).

Mutants that do indeed invade are traditionally referred to as successful.

2.2 Traits

We shall assume that the types come parameterized by some compact and simply connected subset X of \mathbb{R}^k . Moreover we shall assume that a mutant Y differs but slightly from the type X_i from which it derives. The components of X_i , Y stand for the values of some numerical traits, like leg length, metabolic rate, duration of juvenile period, etc..

Communities with only one evolving type are called monomorphic, with two evolving types dimorphic, etc.. (To keep the arguments simple we assume that the remaining species of the community don't evolve. We surmize that the theory can be extended to multi-species co-evolution by making appropriate notational changes; see also Dieckmann & Law, 1995.)

The trait values determine the population dynamical characteristics of a type. Simple trait evolution in an n-morphic community, in which every successful mutant just oust its progenitor, can therefore be visualized as a movement through the parameter space of a community dynamical model. It also can occur that the new mutant and all the old resident types can coexist, or that replacement of one of the former resident types by a mutant drives some other resident type(s) to extinction. In the first case evolution leads to an enriched, (n+1)-morphic, community, in the second case to an impoverished, (n-m)-morphic, $1 \le m < n$, community. See also figure 8.

2.3 The "taxonomic" perspective

Many traits are easy observables, even on fossils (think of leg length). This in direct opposition to the population dynamical characteristics which they engender (think of the issue of determining in the field the probability of outrunning a predator). Therefore much biological research focusses on trait evolution per se, with little attention for the population dynamical gears of the evolutionary machinery. One of our goals is to accommodate this viewpoint to the greatest possible extent. This was the overriding reason for the assumptions that (i) there is a separation between the population dynamical and the evolutionary time scales, (ii) any combination of residents C engenders a unique E. For these two assumptions justify the introduction of the function

$$s: (C, Y) \mapsto s_C(Y),$$

thereby making it possible to talk about the relation of trait values and fitness per se.

The theoretical framework that we shall develop below is based on the Ansatz that such a function s (i) exists, (ii) provides an evolutionarily sufficient summary of the underlying community dynamics, and (iii) satisfies some appropriate smoothness properties.

The whole of section 6, setting out a tentative axiom system for a theory of Adaptive Dynamics, is devoted to staking out the land concealed behind (ii) and (iii) of the Ansatz. In sections 3 and 4 we explore some of its more immediate landmarks.

2.4 More about the community dynamical justification

The recent spate of attention for the non-linear phenomena occurring already in simple population dynamical models may have given the impression that multiple attractors are almost the rule in community dynamics. We believe that this impression is wrong, at least when it comes to evolutionary considerations. Deterministic community models are idealisations made with a purpose, the charting of particular types of community phenomena. More realistic models incorporating environmental noise usually have unique attractors, here to be interpreted as stationary probability measures on the set of functions mapping time to environmental conditions.

The following example may illustrate our point. A famous model for the outbreaks of the Canadian spruce budworm (Ludwig, Jones & Holling, 1978) gives rise to two stable equilibria. Yet the very reason that the model was built, was to explain the observed occurrences of shifts between two rather extreme defoliation regimes. On a slightly longer time scale we also have to account for the factors bringing about these shifts. The introduction of noise also tends to smoothen the deterministic bifurcation of an attractor into a more gradual change of the probability measure on the set of functions mapping time to environmental conditions.

2.5 Aside: a helpful special class of community dynamical models

If one wants to develop a general theory it helps to have some simple examples to guide one's way. Unfortunately it is rarely possible to calculate s for a specific community dynamical model other than by doing a direct simulation to determine E(C). To compound our misfortune those cases where we can find an explicit expression for s almost invariably give rise to relatively trivial types of adaptive dynamics. However, there is an outstanding exception, which goes by the name of generalized Lotka-Volterra models (Hofbauer et al., 1987; Rand et al., 1994). These are models with community equations which can be written as either

$$\frac{dn_i(t)}{dt}(t) = \left[r(X_i, E_0(t)) - \sum_{j=1}^m a(X_i, X_j)g(X_j, n_j(t), E_0(t))\right]n_i(t)$$
(2.2)

or

$$n_i(t+1) = \exp\left[r\left(X_i, E_0(t)\right) - \sum_{j=1}^m a(X_i, X_j)g\left(X_j, n_j(t), E_0(t)\right)\right]n_i(t)$$
(2.3)

where n_i is the population density of the individuals of type X_i , and E_0 some ergodic driver (think of the weather). For such a model let $C = (X_1, \ldots, X_m)$ be a trait combination such that all *m* types can coexist, i.e., for any initial condition with all $n_j(0) > 0$, lim inf $n_i(t) > \epsilon_i > 0$, $i = 1, \ldots, m$, then

$$s_C(Y) = \left[\rho(Y) - \sum_{j=1}^m a(Y, X_j) \gamma_j(X_1, \dots, X_m)\right]$$
(2.4)

with $\rho(Y)$ the time average of $r(Y, E_0(t))$, and $\gamma_j(X_1, \ldots, X_m)$ the time average of $g(X_j, n_j(t), E_0(t))$. The latter can be calculated from the equations

$$\sum_{j=1}^{m} a(X_i, X_j) \gamma_j(X_1, \dots, X_k) = \rho(X_i)$$
(2.5)

derived by setting $s_C(X_i) = 0$.

Note that for the Lotka-Volterra models $s_C(Y)$ is well defined even when the dynamics of the C community has multiple attractors.

2.6 About this paper

Below you find the prolegomena to a formal theory of Adaptive Dynamics. In section 3 we treat the only well established part: evolution close to monomorphism for one

Adaptive dynamics

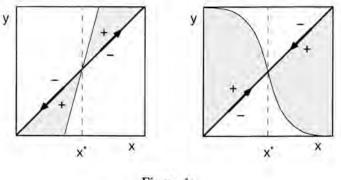


Figure 1:

dimensional trait spaces. This is the one area where the barest possible of assumptions already give strong results. In section 4 we discuss, with the help of an example, the natural extension of the theory from section 3 to higher degrees of polymorphism. Near the end of that section it is found that a number of imminently relevant points have to remain undecided unless further assumptions are introduced. Luckily population dynamical considerations of a very general kind can guide us when we pick these assumptions. However, the maximal set of assumptions that can be derived in this manner is just a little less than is needed to get into some really interesting arguments. Therefore we in one place also introduce an assumption pertaining to the production of mutations by individual organisms, which, though fair, is less firmly supported by basic biological laws.

In section 5 we consider, with the help of the same example as in section 4, the relation of our taxonomically abstracted schemes to the fully individual-based point of view. This section should provide a background for judging the tentative "axiom system" for Adaptive Dynamics that we present in section 6. There we aim at listing a set of assumptions that are mathematically sufficiently weak to have a certain minimum amount of biological firmness and yet are mathematically sufficiently strong, and sufficiently many, to erect an interesting theory on, leading to novel biological insights. In section 7 we list some provisional conclusions from that theory. In the final section we discuss some pro's and con's of our approach in a wider biological perspective, and indicate some directions for future research.

3 Adaptive Dynamics in one dimension: I evolution close to monomorphism

3.1 Graphical constructions

In this section we shall heuristically treat Adaptive Dynamics for one dimensional trait spaces. To keep things simple we shall moreover assume that the trait space X coincides with the set $\mathbb{P}_1 := \{x \in X \mid s(x) > 0\}$, where s(x) denotes the fitness of x in a (relatively) virgin world.

3.1.1 Monomorphic populations

We begin with a consideration of the monomorphic situation. Figure 1 shows two potential sign structures for $s_x(y)$. (Notice that $s_x(x) = 0$, so that generically s changes sign on the diagonal of the (x, y)-plane.) We start with discussing two situations where successful mutants oust their progenitors without arguing as yet why they may be supposed to do this.

We first consider figure 1a. For any x to the left of x^* only smaller mutants can invade, for any x to the right of x^* only larger mutants can do so. Therefore each subsequent successful mutation moves x further away from x^* . The situation is analogous to the cobwebbing (or rather staircasing!) construction used to analyse recurrence relations in one variable. Only this time the steps come at random times and have stochastic sizes.

In figure 1b the opposite happens. For all x to the left of x^* only larger, and for all x to the right of x^* only smaller mutants can invade. If the mutational step size is bounded by ϵ , and if the process does not run out of successful mutations, evolution will eventually bring x within an ϵ -distance of x^* . And here the analogy with recurrence relations ends.

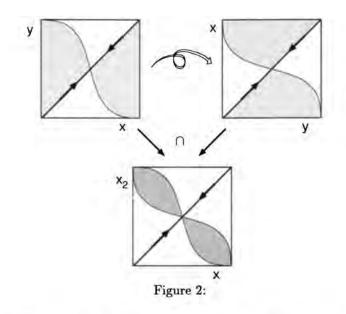
3.1.2 Dimorphisms

As a next step we consider the conditions which make a mutant oust or not oust its progenitor. To find these conditions we return to the underlying community dynamical scenario. When a mutant ousts its progenitor the community necessarily passes through a phase during which the progenitor is present only in very low densities. Therefore that progenitor no longer contributes to the setting of the environmental stage. This is done by the mutant in its stead; population dynamically yestertime's resident and mutant have switched roles. We conclude that for a successful mutant y to oust its progenitor x, it is necessary that $s_y(x) \leq 0$. We shall assume that this condition is also sufficient, as this accords best with our earlier assumption that the community dynamics always has a global attractor.

To construct the subset of \mathbb{X}^2 for which both $s_{x_1}(x_2) > 0$ and $s_{x_2}(x_1) > 0$, we flip copies of the diagrams of figure 1 over the diagonal and superimpose them on the originals. See figure 2. The intersection of the regions marked "+" we call \mathbb{P}_2 . \mathbb{P}_2 parametrizes the so-called "protected" dimorphisms.

Remark: Our choice not to include in \mathbb{P}_2 the points $C = (X_1, X_2)$ characterized by $s_{X_1}(X_2) = 0$ or $s_{X_2}(X_1) = 0$, is based on the usual pattern of soft bifurcation of community dynamical equilibria: If a parameter change moves a globally stable interior equilibrium of some decent community dynamics smoothly onto the boundary of the positive cone, then at the bifurcation point the community dynamics has a boundary equilibrium attracting the whole interior of the positive cone.

To have both the monomorphisms and the dimorphisms represented in one picture we embed X, and with it \mathbb{P}_1 , as the diagonal in \mathbb{X}^2 . After all, a combination of two identical types is ecologically indistinguishable from a single type. The potential adaptive conditions of the population, up to and including dimorphisms, correspond



to the union of \mathbb{P}_1 and \mathbb{P}_2 . Its representation as a subset of \mathbb{X}^2 we shall refer to as \mathbb{A}_2 . The example in figure 3 indicates how such a representation can help us portray patterns of evolutionary movement.

The invasion of a y mutant into a dimorphic population consisting of the type combination (x_1, x_2) is determined by the sign of $s_{x_1,x_2}(y)$. If y is successful, and if, say, $(x_1, y) \in \mathbb{P}_2$, $(y, x_2) \notin \mathbb{P}_2$, $s_{x_1,y}(x_2) < 0$, then a step is made to (x_1, y) . When the mutational steps are only small the most usual pattern is that a mutant ousts its progenitor. This is the situation hinted at in figure 3. If ousting the progenitor results in a jump over the boundary of \mathbb{P}_2 only the mutant remains. The cases in which mutant and progenitor will coexist will be discussed in section 4.

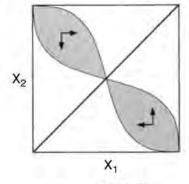


Figure 3:

3.1.3 More about the space of adaptive conditions

A neater way of looking at our embedding trick is by noticing that the real objects of evolutionary interests are sets, not ordered lists, of trait values. This observation produces a natural equivalence between the diagonal of X^2 and X. By the same token the labelling as 1 and 2 of the two types making up a point in X^2 is arbitrary. Therefore \mathbb{P}_2 should be invariant under a permutation of the indices of the x_i . In figure 3 this symmetry is seen as a mirror symmetry around the diagonal.

Terminological remark: We call the elements of A_2 adaptive "conditions", instead of adaptive "states" since we customarily tie the notion of state to being Markovian, and we don't want to assume yet that the distribution of the mutational steps is determined in full by the adaptive condition.

3.2 The classification of evolutionarily singular points

3.2.1 Evolutionarily Singular Strategies

The consideration of figures 1 to 3 makes clear that a very special role is played by points x^* where a(n other) 0-level set of the function $s_x(y)$ crosses the diagonal. We shall refer to such points as Evolutionarily Singular Strategies, or just as singular points. Such points correspond to the rest points of the movement in \mathbb{P}_1 . Moreover \mathbb{P}_2 and \mathbb{P}_1 connect only in singular points $x^* (\equiv (x^*, x^*) \in \partial \mathbb{P}_2)$ of \mathbb{P}_1 : It is only near such points x^* that evolution can step up from \mathbb{P}_1 to \mathbb{P}_2 . (Downstepping from \mathbb{P}_2 to \mathbb{P}_1 is possible from all points near $\partial \mathbb{P}_2$ for which mutants in the direction of the nearby part of $\partial \mathbb{P}_2$ are potentially successful.)

Singular points can be characterized by

$$\frac{\partial s_x(y)}{\partial y}\Big|_{x=y=x^*} = 0. \tag{3.1}$$

Remark: Please notice that, contrary to the usual situation in dynamical systems, evolutionarily singular strategies, as defined by us, aren't the rest points of the adaptive dynamics. The rest points are the (globally) Evolutionarily Unbeatable Strategies, i.e., the strategies X^* such that $s_{X^*}(Y) < 0$ for all $Y \neq X^*$. The local variant of EUSes are characterized by

$$\frac{\partial s_X(Y)}{\partial Y}\big|_{X=Y=X^*} = 0 \quad \text{and} \quad \frac{\partial^2 s_X(Y)}{\partial Y^2}\big|_{X=Y=X^*} \text{ negative definite},$$

i.e., in addition to (3.1) a second order condition should be satisfied. All rest points of an adaptive dynamics are local EUSes. And any local EUS can be made into a rest point by sufficiently restraining the size of the mutational steps.

3.2.2 The expansion of $s_x(y)$

To classify the different types of singular points we linearize. To this end we define

$$u := x - x^*, \quad v := y - x^*.$$
 (3.2)

We shall with a slight abuse of notation use the same symbol s for the local coordinate version of the fitness function. Our assumption that s is sufficiently smooth allows us to write

$$s_u(v) = a + b_1 u + b_2 v + c_{11} u^2 + 2c_{12} uv + c_{22} v^2 + \text{ h.o.t.}.$$
(3.3)

The fact that any mutation indistinguishable from the resident should be selectively neutral, i.e., have zero fitness, translates into

$$s_u(u) = 0 \quad \text{for all } u, \tag{3.4}$$

allowing us to conclude that

$$a = 0, \quad b_1 + b_2 = 0, \quad c_{11} + 2c_{12} + c_{22} = 0.$$
 (3.5)

Finally (3.1) tells us that

$$b_2 = 0.$$
 (3.6)

Therefore

$$s_u(v) = c_{11}u^2 - (c_{11} + c_{22})uv + c_{22}v^2 + \text{ h.o.t.}.$$
(3.7)

Apparently we need only two parameters, c_{11} and c_{22} , at this stage of the classification (and only the ratio of c_{11} and c_{22} really matters, since all the pictures locally are invariant under scaling).

Figure 4 shows the dependence of the local sign structures of s on c_{11} and c_{22} . The local direction of evolutionary movement in \mathbb{P}_1 and the local configuration of \mathbb{P}_2 , both deduced from the local sign structure of s in figure 4, are depicted in figure 5.

3.3 The expansion of $s_{x_1x_2}(y)$

To complete the picture we need the pattern of movement in \mathbb{P}_2 . From now on we confine attention to the cases $c_{22} > -c_{11}$ to ensure that \mathbb{P}_2 is not locally empty (see fig. 5). We define

$$u_1 := x_1 - x^*, \quad u_2 := x_2 - x^*, \quad v := y - x^*, \quad (3.8)$$

and write

$$s_{u_1u_2}(v) = \alpha + \beta_1 u_1 + \beta_2 u_2 + \beta_3 v + \gamma_{11} u_1^2 + 2\gamma_{12} u_1 u_2 + \gamma_{22} u_{22} + 2\gamma_{13} u_1 v + 2\gamma_{23} u_2 v + \gamma_{33} v^2 + \text{h.o.t.},$$
(3.9)

The numbering of the resident types is arbitrary. Therefore s should be invariant under a permutation of those numbers:

$$s_{u_1u_2}(v) = s_{u_2u_1}(v). \tag{3.10}$$

Another invocation of the principle of selective neutrality of the resident types gives

$$s_{u_1 u_2}(u_1) = s_{u_1 u_2}(u_2) = 0. \tag{3.11}$$

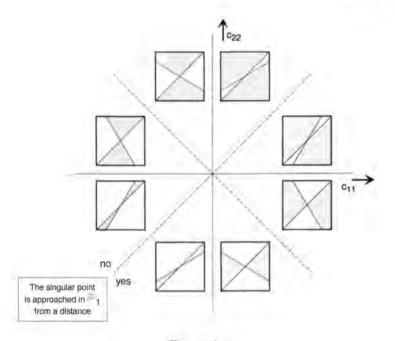


Figure 4:

As a final step we use that there is a single point, $u_1 = u_2 = 0$, where \mathbb{P}_2 toucnes the diagonal of \mathbb{X}^2 . In that point u_1 and u_2 are equal, so that we are back in the monomorphic case. Therefore

$$s_{00}(v) = s_0(v). \tag{3.12}$$

Combining all this information leads to

$$s_{u_1u_2}(v) = (v - u_1)(v - u_2)[c_{22} + \text{h.o.t.}].$$
 (3.13)

Apparently the whole classification can be done in terms of the two parameters c_{11} and c_{22} only!

Remark: The above derivation was based on the, in afterthought somewhat unwarranted, assumption that the smoothness of s on \mathbb{P}_2 extends to the point $(x^*, x^*) \in \partial \mathbb{P}_2$. In section 6 we shall argue that in general the behaviour of community dynamical equilibria under parameter changes only condones assuming (i) that s is smooth on the closure of \mathbb{P}_2 with the exception of the points of $\partial \mathbb{P}_2$ where \mathbb{P}_2 touches the diagonal of \mathbb{X}^2 , and (ii) that s.(y) has continuous first and second (and higher) directional derivatives in the directions pointing to the interior of \mathbb{P}_2 . In the points where \mathbb{P}_2 touches the diagonal of \mathbb{X}^2 full higher order derivatives fail to exist generally. However, for the case considered above it so happens that the condition that the resident types should be evolutionarily neutral together with (ii), implies that s is twice differentiable for (x_1, x_2, y) on (closure $\mathbb{P}_2 > \mathbb{X}$, the points (x^*, x^*, y) not excepted.

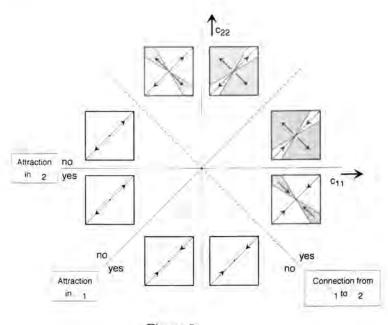


Figure 5:

3.3.1 Local evolution

From figure 4 we immediately see that locally the monomorphic substitutions bring the adaptive condition of the population closer to x^* when $c_{22} < c_{11}$, and move the adaptive condition away from x^* when $c_{22} > c_{11}$. Figure 5 shows that \mathbb{P}_2 is locally non-empty when $c_{22} > -c_{11}$ and empty when $c_{22} > -c_{11}$. From a consideration of both figures together we conclude that locally around x^* transitions from the monomorphic condition to a dimorphic condition occur almost surely when and only when $-c_{11} < c_{22} < c_{11}$, and never when $c_{22} > c_{11}$, or $c_{22} < -c_{11}$. (Assuming, of course, that the process never runs out of mutational variation.)

To see how evolution proceeds from points in \mathbb{P}_2 we observe that, according to (3.13) $s_{u_1u_2}(v)$ for given values of u_1 and u_2 is a parabola in v which crosses the v-axis in the points $v = u_1$ and $v = u_2$.

We first consider the case $-c_{11} < c_{22} < 0$. In that case only mutants v between u_1 and u_2 can invade. A consideration of the local geometry of \mathbb{P}_2 tells that v will oust at least that u_i for which sign $(u_i) = \text{sign}(v)$. The other resident may or may not be ousted. A more detailed calculation shows that, if there is a continuous supply of mutations, (i) \mathbb{P}_2 will almost surely be left for \mathbb{P}_1 , (ii) the distance to 0 decreases by at least a factor $\theta < 1$ for every excursion that is made from \mathbb{P}_1 into \mathbb{P}_2 and back. Every step from \mathbb{P}_1 into \mathbb{P}_1 also leads to a decrease of the distance to 0. Therefore the linearized adaptive dynamics almost surely converges to 0.

When $c_{22} > 0$ only mutants v outside the interval (u_1, u_2) can invade. A consideration of the local geometry of \mathbb{P}_2 tells that v will always oust the nearest resident.

When in addition $c_{11} > 0$ the linearized adaptive dynamics (i) stays in \mathbb{P}_2 and (ii) keeps increasing the distance between u_1 and u_2 . When $c_{11} < 0$ the linearized adaptive dynamics can also jump over the boundary of \mathbb{P}_2 , to \mathbb{P}_1 ; once in \mathbb{P}_1 it moves away from x^* (and from \mathbb{P}_1 it never enters \mathbb{P}_2 again).

In figure 5 the arrows in \mathbb{P}_2 symbolically summarize the results about the evolutionary movement in \mathbb{P}_2 locally near (x^*, x^*) which we have just described.

3.3.2 Types of singular points

The main classification resulting from a combined consideration of the movement in $\mathbb{P}_1 \cup \mathbb{P}_2$ is threefold:

evolutionary repellers characterized by c₂₂ > c₁₁,

(ii) evolutionary attractors characterized by $c_{22} < c_{11}$ and $c_{22} < 0$,

(iii) branching points characterized by $0 < c_{22} < c_{11}$.

A look forward to figure 7 will explain our choice of the latter name.

Of course we may everywhere replace c_{11} and c_{22} by

$$\frac{\partial^2 s_x(y)}{\partial x^2}\Big|_{x=y=x^*} = 2c_{11}, \qquad \frac{\partial^2 s_x(y)}{\partial y^2}\Big|_{x=y=x^*} = 2c_{22}. \tag{3.14}$$

The classification shown in figure 5 underscores our remark in subsection 1.2 that Evolutionarily Unbeatable Strategies are not necessarily evolutionarily attracting, a point first made by Ilan Eshel in 1983 (see also Eshel, 1995). Intriguingly the condition which locally characterizes an EUS, a singular strategy with $c_{22} < 0$, in retrospect turns out to be also the condition for attractivity in \mathbb{P}_2 . For an EUS to be a locally asymptotically stable fixed point of the adaptive dynamics it has to be locally attractive in \mathbb{P}_1 as well, i.e., it is also needed that $c_{22} < c_{11}$. In the litterature such fully attractive EUSes are called Continuously Stable Strategies (Eshel, 1983; as opposed to the "Evolutionarily Stable Strategies" which correspond to what we here call EUSes).

The general classification of singular points for one dimensional trait spaces was first derived by Peter Taylor (1989), though in a rather different disguise, and from a very different perspective. Another derivation, somewhat closer in spirit to ours, was give by Ludwig & Levin (1992).

4 Adaptive Dynamics in one dimension: II polymorphic evolution

4.1 An example

The following community equations should exemplify the results from the previous section.

$$\frac{dn(x_i)}{dt} = \left[1 - \frac{\sum_j a(x_i, x_j) n(x_j)}{k(x_i)} n(x_i)\right],$$
(4.1a)

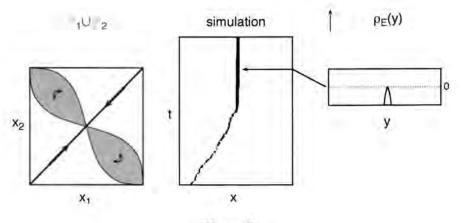


Figure 6:

with

$$a(x_i, x_j) = e^{\alpha (x_i - x_j)^2}, \qquad k(x) = 1 - x^2, \qquad -1 < x < 1,$$
 (4.1b)

and the summation extending over all values of the trait x supporting a non-zero population mass. In subsection 2.5 it was indicated how (4.1) translates into a fitness function s. (This example is a slight adaptation of a time honoured model for competition along a resource axis, first introduced by Robert MacArthur and Richard Levins (1964; see also MacArthur, 1970, 1972) and extensively studied by i.a. Freddy Bugge Christiansen and Volker Loeschcke (1980, 1987; see also Christiansen, 1984, 1988; Loeschcke, 1984; Loeschcke & Christiansen, 1984).)

The left panes of figure 6 to 8 show $\mathbb{P}_1 \cup \mathbb{P}_2$ together with the directions of adaptive movement. The middle panes show the result of numerically solving the differential equation (4.1), with the following modifications: (i) The trait axis was discretized. (ii) Any trait bin with zero population mass adjacent to one with positive mass, had a fixed probability per unit of time to receive a small population mass of size ν_1 . (iii) Any population mass which dropped below $\nu_0 < \nu_1$ was instantaneously set to zero. The panes show, in a style conventionally used by paleontologists, those populations which had masses either larger than ν_2 or than ν_3 , $\nu_3 > \nu_2 > \nu_1$. Finally the right hand panes show the instantaneous fitness, $1 - \sum_i a(y, x_i)n(x_i)$, of a potential mutant in the community indicated with an arrow in the middle pane. Figures 6 to 8 only differ in the value of α (respectively 1/3, 2, and 3). The most conspicuous feature of figures 7 and 8 is the occurrence of branching events, one in figure 7 and several in figure 8. All these branching events are dichotomies, in accordance with the graphical results from subsection 3.2.

Remark: Instantaneous fitness is a useful concept for non-structured populations only. In a constant environment such populations immediately start growing, or declining, exponentially. The instantaneous fitness $r_{E(t)}(Y)$, at time t of a type Y in an environment E, is the relative growth rate of Y clone in an environment which is

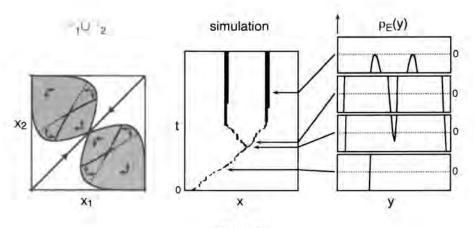


Figure 7:

forever kept in condition E(t). For non-structured populations, and generically only for them, the fitness $\rho_E(Y)$ can be calculated from these instantaneous fitnesses as

$$\rho_E(Y) = \lim_{t \to \infty} \frac{1}{t} \int_0^t r_{E(\tau)}(Y) \, d\tau.$$

Remark: Preliminary explorations of an extension of the theory to higher dimensional trait spaces indicate that there polytomies should be possible, at least in principle. The maximum number of branches that can sprout from a single very small (a term in need of explanation, see section 7.1 for some ideas on this topic) region in trait space, after a line of descent has entered that region, is one plus the dimension of the trait space.

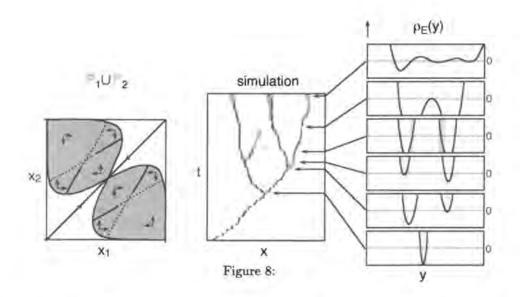
4.2 Stagnation sets

In the left panes of figures 7 and 8 we also have drawn the lines defined by

$$\frac{\partial s_{x_1,x_2}(y)}{\partial y}\Big|_{y=x_i} = 0, \qquad i = 1, 2.$$
(4.2)

From these lines the adaptive condition either cannot make local jumps in the x_i -direction, or can equally jump in positive or negative x_i -directions. This can be deduced from the following thought experiment: When we forbid x_j , j = 2, 1, to mutate, we are back in a monomorphic adaptive dynamics, with only x_i , i = 1, 2, evolving. (4.2) corresponds to the equation for the singular points of that monomorphic x_i -dynamics, parametrized by x_j .

For one dimensional trait spaces the stagnation sets are somewhat comparable to the isoclines of a differential equation. More in particular, if we let the jump size



go to zero, and the mutation rate to infinity in such a manner that [mean mutation distance]×[mutation rate] goes everywhere to the same constant we end up with a set of differential equations for the x_i , which have the stagnation sets for their isoclines (Dieckmann & Law, 1995). Moreover, the intersection of the x_1 - and x_2 -stagnation sets in \mathbb{P}_2 corresponds to the rest points of the dimorphic adaptive dynamics. This is well illustrated in figure 7, where that rest point is also stable towards higher degrees of polymorphism.

Termological remark: When we speak of the dimorphic dynamics in situations where trimorphisms aren't naturally excluded, we refer to the adaptive dynamics conditioned on the sample path staying dimorphic.

4.3 Colour-coding the stagnation sets

It is of course tempting to try to extend the classification of singular points from subsection 3.2 to the points $(_ix_{1,i}x_2)$ of an x_i -stagnation set. But we should be a little careful. Those parts of the classification that referred to attractivity or repulsivity in \mathbb{P}_1 are not particularly meaningful in a \mathbb{P}_2 context, due to the potential for movements of the remaining coordinate.

Let

$${}_{i}c_{11} = \frac{1}{2} \frac{\partial^{2} s_{x_{1},x_{2}}(y)}{\partial x_{i}^{2}} \Big|_{\substack{y=z_{i}\\z_{1}=(z_{1},z_{2}=z_{2})}}, \qquad {}_{i}c_{22} = \frac{1}{2} \frac{\partial^{2} s_{x_{1},x_{2}}(y)}{\partial y^{2}} \Big|_{\substack{y=z_{i}\\z_{1}=(z_{1},z_{2}=iz_{2})}}.$$
 (4.3)

We shall call points of an x_i -stagnation set black when $_ic_{22} < -_ic_{11}$, and coloured when $_ic_{22} > -_ic_{11}$. Coloured x_i -stagnation points with $_ic_{22} < 0$ we call green, and

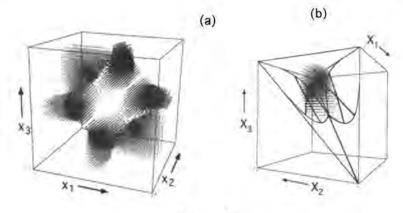


Figure 9:

coloured x_i -stagnation points with $ic_{22} > 0$ we call red. In figures 7 and 8 the red parts of the stagnation sets are drawn as interrupted lines.

The thought experiment in which we forbade one of the two types to mutate also tells us that the coloured parts of a stagnation set in \mathbb{P}_2 make contact with the set of protected trimorphisms \mathbb{P}_3 .

Remark: The term contact should be interpreted in terms of the threefold embedding of \mathbb{X}^2 in \mathbb{X}^3 , as the three diagonal planes $x_1 = x_2$, $x_1 = x_3$, $x_2 = x_3$, which follows from the natural equivalence relation $(x_1, \ldots, x_n) \sim (x_1, \ldots, x_m) :\Leftrightarrow \{x_1, \ldots, x_n\} =$ $\{x_1, \ldots, x_m\}$. By the same token \mathbb{P}_3 should be invariant under permutations of the indices of (x_1, x_2, x_3) , and the three diagonal planes should divide \mathbb{X}^3 up in six segments, each of which contains a canonical piece of \mathbb{P}_3 , see figure 9. Each diagonal plane consists of two equivalent parts, just as did \mathbb{X}^2 , plus the diagonal line $x_1 = x_2 = x_3$, separating them. These two parts each connect a different pair of segments of \mathbb{X}^3 .

For the green parts of the stagnation sets this contact is inconsequential, as can be seen from figure 7, but near to the red part of an x_1 -stagnation set there is the possibility that a transition $(_1x_1 + \epsilon_{1,1} x_2 + \delta) \rightarrow (_1x_1 + \epsilon_{1,1} x_1 + \epsilon_{2,1} x_2 + \delta)$ is followed by steps moving the adaptive condition further and further away from the diagonal plane, and the same holds true for the x_2 -stagnation sets. In other words, from, and only from, near to a red x_i -stagnation point there may occur a visible dichotomy in the line descending from x_i . This effect is illustrated in figure 8. Whether we really will see a fully developed dichotomy depends on the relative speeds of the movement in the directions parallel and orthogonal to the diagonal plane. In the example from figure 8 the branchings occur near a rest point of the dimorphic adaptive dynamics, so that the motion orthogonal to the diagonal plane dominates. Local domination of the component of adaptive motion parallel to the diagonal plane will lead in a few adaptive steps to a jump across $\partial \mathbb{P}_3$, back to \mathbb{P}_2 .

4.4 Extinctions and treeness

Reductions in the number of types are results of jumps over the boundary of \mathbb{P}_n . When a disappearing type differs appreciably (a term in need of explanation, see section 7.1 for some ideas on this topic) from any of the remaining types we shall speak of an extinction.

An example of an extinction can be seen in the middle pane of figure 8, where the sample path jumps $\partial \mathbb{P}_4$ to \mathbb{P}_3 .

The particular extinction event from figure 8 owes its occurrence to a geometrical peculiarity which directly relates to our earlier classification of the singular points. In the four-type stage the various members of the community are seen evolving in such a manner that the two middle branches are pushed towards each other. Geometrically this corresponds to a movement towards the diagonal plane $x_2 = x_3$ (assuming that we number the types from left to right). To see what happens geometrically we consider the slice through X^4 which results from keeping x_1 and x_4 constant. From the direction of movement of the middle two branches, we infer that the geometry of that slice is locally similar to the diagram depicted in figure 5 between three o'clock and four thirty. This conclusion is corroborated by the right hand pane of figure 8, second graph from above. Therefore we may imagine the trajectory in \mathbb{P}_4 as descending from some fixed height into a narrow furrow, with a codimension 1 bottom. Since the adaptive movement has a considerable stochastic slack there is essentially zero chance that the trajectory ever hits precisely that bottom.

To develop the last argument a little further we assume that the mutational steps have length less than ϵ , and that we consider a family of adaptive dynamics parametrized with ϵ , where ϵ acts as a scaling factor for the distribution of the mutational steps. Otherwise the distribution of the mutational steps is assumed to be fixed. Moreover we assume that mutations in the different types occur in independent Poisson processes with rates scaling as ϵ^{-1} , and otherwise only dependent on the composition of the community. Finally we assume that these rates are for fixed ϵ bounded away from both infinity and zero, the latter with the exception of points near to a boundary of the \mathbb{P}_n under consideration where that type is pushed to extinction. (These assumptions are the simplest ones compatible with our wish to accommodate general types of community dynamics; see subsection 6.4.1).

Our new assumptions imply that the crossing of a unit distance by our descending trajectory brings with it a sideways wobble scaling as $\epsilon^{1/2}$. Therefore we predict that it hits the side walls of the furrow at a distance from the bottom which scales as ϵ^{θ} , with $0 \leq \theta \leq 0.5$ depending on the particular assumptions that we make about its starting point.

The argument which we just developed applies to any situation in which evolution of the members of a community pushes two lines of descent towards each other. Except for a set of initial conditions with vanishing measure the chance that two lines of descent will ever come within an ϵ -distance from each other, once they have diverged further than that distance, should go to zero faster than ϵ .

The pleasant conclusion is that the trajectories of an adaptive dynamics in which the sizes of the mutational steps are bounded by ϵ , ϵ small, should, when observed at a resolution coarser than ϵ , look like good trees, without any merging branches.

4.5 About the speeds of adaptive movement, and, again, branching

In the polymorhic situation, as in more species co-evolution, the relative speeds of stepping in different directions starts to matter. (For higher dimensional trait spaces this is already the case for monomorphic evolution.) Biologically this speed is determined by two classes of processes: Intra-individual ones, determining (i) the probability that a birth event produces a mutated individual as well as (ii) the sizes of the mutational steps (and for higher dimensional trait spaces also the correlations between the various directions in which that step may be made). And ecological ones, determining (iii) the birth rate into a population and (iv) the probability that a mutant gets established.

We shall argue below that population dynamical considerations suggest that in nature the latter probability is roughly proportional to the fitness of the mutant, as long as that fitness is but small. Therefore we shall make an assumption to this effect in section 6 where we describe the directions in which we think that taxonomic level theory should be developed. For the time being we only point to one important effect of this assumption: It makes the initial development of a dichotomy a relatively slow process, and thereby usually precludes the development of fulblown dichotomies when a sample path gets in the neighbourhood of a red stagnation set, except near rest points of the n-type adaptive dynamics under consideration.

Remark: In the simulations from figures 6 to 8, the probability of a mutant with positive fitness getting established was set equal to a constant. For the combination of the particular initial condition chosen and the fitness function deriving from (4.1), this difference in assumptions effectively only affects the time scale of the middle panes.

5 The individual based justification

5.1 Two examples of the justification of deterministic population models at the level of the individuals comprising the population

The middle pane of figure 10 shows the results of a simulation of a stochastic population model, in which the individuals are counted in integers $N(x_i)$, that may be thought as underlying the model from subsection 4.1.

The individual-based models underlying the differential equation (4.1) have in common that, conditional on the present condition of their environment E(t), with

$$E = \{(x_j, n(x_j))\}, \quad n(x_j) := N(x_j)/\Omega, \quad \Omega \text{ the "system size"}, \quad (5.1)$$

(i) individuals are independent, (ii) die at random, with death rate $\mu(x_i, E(t))$, (iii)

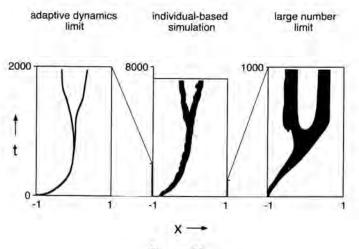


Figure 10:

a living individual gives birth in a Poisson process with rate $\lambda(x_i, E(t))$, and (iv)

$$\lambda(x_i, E(t)) - \mu(x_i, E(t)) = \left[1 - \frac{\sum_j a(x_i, x_j) n(x_j)}{k(x_i)}\right]$$
(5.2)

As a result the counts form a continuous time Markov process with transition rates

$$N(x_i) \stackrel{\mu(x_i, E(t))N_i}{\to} N(x_i) - 1, \qquad N(x_i) \stackrel{\lambda(x_i, E(t))N_i}{\to} N(x_i) + 1$$
(5.3)

(4.1) is interpreted as the large number limit of such processes, i.e., the limit in distribution of a sequence of processes $\{n(x_i) = N(x_i)/\Omega\}$, for $\Omega \to \infty$ (see e.g. van Kampen, 1981; Kurtz, 1981; Ethier & Kurtz, 1986).

To speed up the simulations we chose to set the birth rates uniformly equal to one and put all dependence on E in the death rates. Moreover we discretized the trait axis into 99 equal intervals, or bins, with x_i the midpoint of the i^{th} bin. Ω was set equal to 2500. Finally (5.2) was modified to the extent that at each birth event the newborn was put only with probability $1 - \theta$ in the bin of its parent, and with probability $\theta/2$ in either of the adjacent bins. The mutation probability θ was set equal to 0.003; the value of the "competition strength" is the same as that from figure 7, $\alpha = 2$.

The right most pane of figure 10 shows the results from approximating the full individual-based model by the large number limit

$$\frac{dn(x_i)}{dt} = \left[1 - \theta - \frac{\sum_j a(x_i, x_j) n(x_j)}{k(x_i)}\right] n(x_i) + \frac{1}{2} \theta \left[n(x_{i-1}) + n(x_{i+1})\right], \quad i = 1, \dots, 99.$$
(5.4)

(Note that (5.4) formally turns into (4.1) when we let $\theta \to 0$.) The dark area corresponds to $n(x_i, t) > 0.005$.

5.2 The Adaptive Dynamics formulation of the same population models

The left most pane of figure 10 shows the result of a simulation of the adaptive dynamics type. This figure is comparable to the middle pane of figure 7, except that we (i) assumed that the rate at which mutants were produced by type x_i was proportional to the system size times the equilibrium density $\tilde{n}(x_i)$ of that population, calculated from (4.1), (ii) we set the probability that a mutant got established equal to

$$\left[1-\mu(y,\widetilde{E})\right]_{+}, \qquad \widetilde{E} = \{(x_1,\widetilde{n}(x_1)),\ldots,(x_{99},\widetilde{n}(x_{99})). \tag{5.5}$$

These assumptions are based on the following arguments: (i) If mutants appear sufficiently rarely then the population dynamics has time to reach equilibrium before the appearance of the next mutant. (ii) Mutants appear as single individuals. As long as N(y) is small, and Ω large, (a) it still makes sense to count the mutants in integer numbers, (b) the mutants contribute only negligibly to E as perceived by the individuals (i.e., through the functions $\mu(x, E(t))$). Therefore the mutant population initially grows according to a linear birth and death process with per capita birth and death rates

$$\lambda = \lambda(y, \widetilde{E}) = 1, \qquad \mu = \mu(y, \widetilde{E}) = \frac{\sum_j a(y, x_j) \tilde{n}(x_j)}{k(y)}. \tag{5.6}$$

The sample path of such a process hits zero in finite time with probability $\min\{1, \mu/\lambda\}$, and with probability $(1 - \mu/\lambda)_+$ eventually grows exponentially at rate $\rho = \lambda - \mu$. Only mutants which get into the exponential growth regime eventually get established, with a time to establishment which scales as $\log(\Omega)/\rho$.

Remark: The stochastic process $\{n(x_i)\}$ cannot equilibrate in the strict sense since "everybody dead" is an absorbing state. However, (i) the average time to extinction scales exponentially in Ω , (ii) when $\theta = 0$ the functionals $n(x_i, t)$ converge in distribution to the solution of (4.1) for any bounded time, and (iii) an interior fixed point of (4.1) attracts the full interior of the positive cone. (i) to (iii) combine into the statement that for $\theta = 0$ (a) the convergence to quasi-equilibrium (i.e., convergence to equilibrium of the process that results from a conditioning on non-extinction) is much faster than extinction, (b) the distribution of $n(x_i)$ at quasi-equilibrium weakly converges to a point mass at $\tilde{n}(x_i)$ for $\Omega \to \infty$.

5.3 A comparison of the results from the three different formulations

All three simulations in figure 10 show the same branching pattern. The most obvious difference is in the overall speed of the three processes: The large number limit is about 15 times, and the adaptive dynamics approximation about 3 times as fast as the real thing. We believe that latter difference is largely due to the demographic noise resulting from the smallness of Ω (nessecitated by the limited computer speed at our disposal): The realized instantaneous fitnesses for the full model fluctuated

considerably over short time spans, and their moving time averages were much flatter functions of y than the $s_{C}(\cdot)$ calculated from the adaptive dynamics approximation. (The latter effect also resulted in a much decreased propensity for further branching in simulations at higher values of α .) The increased speed of the large number limit is due to the presence of all possible types immediately after t = 0, even when the differential equation is started up with all but one $n(x_i)$ equal to zero. These types may be present in extremely low densities, corresponding to a number much lower than 1 for any realistic value of Ω , but they can make up for this lack in numbers by their rapid reproduction. (In simulations for smaller values of α this even resulted in the growth of a secondary peak, seemingly out of the blue, opposite to the primary peak, followed by a movement of the two peaks towards each other ending in their merger into a single peak around the EUS.)

5.4 The justification of any general theory of Adaptive Dynamics

Generalizing from the previous example we argue that adaptive dynamics type models should be seen as limits, for the system size Ω going to infinity, of stochastic individualbased models in which (i) the influences of individuals on E scale as $1/\Omega$, (ii) the initial numbers of individuals are proportional to Ω , (iii) the mutation probabilities per birth event scale as θ , where $\Omega \theta \to 0$ when $\Omega \to \infty$, while (iv) we look on a time scale $T = \Omega \theta t$, t the old time scale, and (v) concentrate on following the trait values which are represented by numbers of individuals that are not $o(\Omega)$.

(i) and (ii) should guarantee that the population dynamical influences on E becomes free from demographic fluctuations on the t-scale, and (iii) should guarantee that that limiting population dynamics is not influenced by the occurrence of mutations. Finally (iv) guarantees that (a) the average number of mutations per unit of T-time remains bounded and bounded away from zero, provided the original process had mutation rates which were so bounded, (b) the E dynamics converges to its attractor infinitely quickly in T-time, provided that the limiting E dynamics in t-time has the right convergence properties, and (c) only time averaged properties in t-time E dynamics matter in T-time (but we should be careful to do our averaging right!).

It is in the light of this interpretation that we should judge the list of assumptions in the next section.

6 Prolegomena to a general theory of Adaptive Dynamics

6.1 Some notational conventions

Adaptive Dynamics are stochastic processes with piecewise constant sample functions mapping \mathbb{R}_+ to finite subsets of a compact and simply connected trait space $\mathbb{X} \subset \mathbb{R}^k$, with elements X, X_1, \ldots, X_n, Y , satisfying certain special assumptions which we shall outline below.

For notational purposes it is useful to introduce

3

$$\overline{\mathbf{X}} := \bigcup_{n=0}^{\infty} \mathbf{X}^n, \tag{6.1}$$

where

$$\mathcal{L}^{0} := \{\mathcal{V}\}, \quad \mathcal{V} \text{ the "virgin world".}$$
(6.2)

The elements of \overline{X} will generically be denoted as $C = (X_1, \ldots, X_n)$. The connection between \overline{X} and the finite subsets of \overline{X} is made through the map

$$\operatorname{Set}: C \mapsto \operatorname{Set}(C) := \{X_1, \dots, X_n\}, \quad \operatorname{Set}(\mathcal{V}) := \emptyset, \tag{6.3}$$

and the equivalence relation

$$(X_1,\ldots,X_n)\sim (X_1,\ldots,X_m):\Leftrightarrow \{X_1,\ldots,X_n\}=\{X_1,\ldots,X_m\}.$$
 (6.4)

The equivalence class of C can be written as $\operatorname{Set}^{-1}(\operatorname{Set}(C))$.

For later use we moreover define

$$C/\{i_1,\ldots,i_m\} := (X_1,\ldots,X_{i_1-1},X_{i_1+1},\ldots,X_{i_m-1},X_{i_m+1},\ldots,X_n\}.$$
(6.5)

6.2 Fitness and protected polymorphisms

6.2.1 Preliminaries about the fitness s

Each process is "governed" by a function

$$s: \overline{\mathbb{P}} \times \mathbb{X} \to \mathbb{R}: (P, Y) \mapsto s_P(Y), \tag{6.6}$$

where

 $\overline{\mathbb{P}} \subset \overline{\mathbb{X}}$ is the set of "protected polymorphisms". (6.7)

The elements of $\overline{\mathbb{P}}$ will generically be denoted as P. A recursive definition of \mathbb{P} , itself involving s, will be given in the next subsection. For the time being we only note that $(\overline{\mathbb{P}}, s)$ and \sim should be compatible, in the sense that

P0: Set⁻¹(Set($\overline{\mathbb{P}}$) = $\overline{\mathbb{P}}$,

S0: $s_{P'}(Y) = s_P(Y)$ whenever $P' \sim P$.

Moreover s satisfies the selective neutrality of residents condition:

S1: $s_P(X_i) = 0$ for all $X_i \in Set(P)$.

6.2.2 Delineating the protected polymorphisms, first go

A taxonomically oriented theory of adaptive dynamics requires that we can decide whether $C \in \overline{\mathbb{P}}$ by a consideration of all expressions $s_{C'}(X)$, with $\operatorname{Set}(C') \subset \operatorname{Set}(C)$, and $X \in \operatorname{Set}(C) \setminus \operatorname{Set}(C')$. A rather straightforward generalization of the constructions from sections 3 and 4 leads to the tentative definition Adaptive dynamics

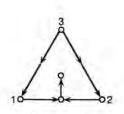


Figure 11:

 $\mathbb{P}_0 := \{\mathcal{V}\},\$

$$\mathbb{P}_n := \{ C \in \mathbb{X}^n \mid \text{ for all } P \text{ such that } (1) \text{ Set}(P) \subset \text{Set}(C), \text{ and}$$

$$(2) P \in \mathbb{P}_{n-k} \text{ for some } k > 0,$$

there is at least one $X \in Set(C) \setminus Set(P)$

for which $s_P(X) > 0$,

and

P1b:
$$\mathbb{P}_{< n} := \bigcup_{j=0}^{n-1} \mathbb{P}_j,$$

 $\mathbb{D}_n := \{C \in \mathbb{X}^n \mid \operatorname{Set}(C) \in \operatorname{Set}(\mathbb{P}_{< n})\},$
 $\mathbb{A}_n := \mathbb{P}_n \cup \mathbb{D}_n,$
 $\overline{\mathbb{P}} := \bigcup_{n=0}^{\infty} \mathbb{A}_n.$

Figure 11 exemplifies the meaning of P1a: The three numbered corners of the triangle symbolize three trait values X_1, X_2 , and X_3 . Vertices midway between two corners, say i and j, symbolize combinations of two trait values, $C = (X_i, X_j)$. The vertex at the center represents the combination of all three trait values, $C = (X_1, X_2, X_3)$. Vertices corresponding to trait combinations $P \in \overline{\mathbb{P}}$ have been encircled. An outgoing arrow from such an encircled vertex pointing to the ith corner signifies that $s_P(X_i) > 0$, and an ingoing arrow that $s_P(X_i) < 0$. The arrows attached to the three corner vertices tell us that (X_1, X_2) is the only protected dimorphism (up to equivalence) that can be made out of $\{X_1, X_2, X_3\}$. We consider (X_1, X_2, X_3) a protected polymorphism since all four encircled non-center vertices have at least one outgoing arrow attached to them.

P1a is a direct adaptation to the clonal case of a definition appearing in various places in the population genetical litterature (see e.g. Eshel, 1995). But this definition is not without problems, as we shall see in the next subsection. However, before we deal with these problems we first go a little further into the population dynamical intuition underlying P1a, or rather figure 11.

At the community dynamical level the vertices in figure 11 should be interpreted as representing a community with one, two or three types present out of $\{X_1, X_2, X_3\}$.

Explanatory remark: The state space of a single X_i population necessarily is a positive cone. Negative population densities don't exist. The state space of a

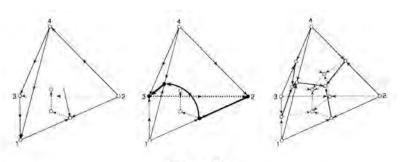


Figure 12:

community comprising a combination $C = (X_1, \ldots, X_n)$ of n types necessarily is a product of n of these positive cones times the state space of the remainder of the community. When the state of the X_i population is zero we say that X_i has been deleted from the community. The faces of the community state space defined by the deletion one or more of the X_1, \ldots, X_n , are community dynamically invariant. We call an attractor of a community global when it attracts for almost all initial conditions for which the states of all its ingredient populations are essentially nonzero (meaning that there is a positive mass of individuals which are still able to reproduce effectively). An internal global attractor of a k-type sub-community (a) globally attracts inside the face of the community state space which results from deleting the remaining n - k types, (b) puts no community mass on the faces of the state space of the sub-community.

The fact that the three corner vertices are encircled tells us that the faces of the community state space corresponding to the three single-type sub-communities are supposed to have internal global attractors. The arrows attached to these vertices tell us that each of these internal attractors is externally unstable in the (X_1, X_2, X_3) community. The same arrows also tell us that only one of the three possible two type communities can ever have an internal global attractor. For believers in a bounded noisy world the arrow pattern also strongly suggest that it indeed has such an attractor. (But few general theorems to this effect have been proved as yet; see e.g. Ellner (1984) and Chesson and Ellner (1989).) The total arrow pattern does not point to any structure in the combined faces of the community state space with the potential to attract all community mass from the interior. By a leap of faith we take this as an indication that the three type community should have an internal attractor.

6.2.3 Some flies in the ointment, and two optional axioms

Figure 12 shows, in a notation comparable to that of figure 11, three possible sign configurations of s on subsets of $\{X_1, \ldots, X_4\}$ which according to **P1a** should make (X_1, \ldots, X_4) into an element of \mathbb{P}_4 . The left and right configurations are unproblem-

Adaptive dynamics

atical, but the middle configuration contains a "heteroclinic loop". Any community dynamical model underlying this sign configuration necessarily sports a heteroclinic loop in the standard sense of the word.

It is possible to construct community dynamical models with heteroclinic loops, or, more generally, heteroclinc networks, which attract with respect to the interior of the positive cone. **P1a** fails to exclude that an underlying population dynamics possesses an attracting heteroclinic network. Therefore "space of protected polymorphisms" is somewhat of a misnomer for a $\overline{\mathbb{P}}$ which just satisfies **P1**. (NB: There is no inherent contradiction in the existence of a combination ($\overline{\mathbb{P}}$, s) satisfying **P1**, and of a corresponding formal adaptive dynamics, which makes no community dynamical sense.)

There are three ways in which we can proceed:

- (i) We just ignore the complication. Although it is impossible to interpret the resulting mathematical theory fully in terms of individual-based processes, there is no immediate reason that it contains internal inconsistencies. Of course we should be somewhat careful how we interpret any ensuing theorems. But none of our results so far seems to be particularly vulnerable to interpretational problems caused by the ensuing semantic gap.
- (ii) We modify P1a by including some additional conditions which should exclude from (include in) \mathbb{P}_n any (X_1, \ldots, X_n) supporting attracting (repelling) heteroclinic networks of an underlying community dynamics. This strategy will only fit in our taxonomically oriented approach when it is generally possible to distinguish unequivocably between attracting and non-attracting heteroclinic networks solely in terms of our function s. Since all results so far known about the (non-)attractivity of heteroclinic networks in (differential equation models for) community dynamics are phrased in terms of that s (Brannath, 1994; Hofbauer, 1994) there is some hope that such an approach may become feasible in the future.
- (iii) We just exclude any s which happens to produce heteroclinic loops from our consideration by adding an axiom to that account:

P2: No $P \in \overline{\mathbb{P}}$ supports a heteroclinic loop.

Unfortunately we don't have easy ways for checking P2 for a given function s. Moreover, so far we never made explicit use of P2 in deriving results. Therefore strategies (i) and (iii) essentially amount to the same.

P2 is but one way of singling out a special subclass of adaptive dynamics. A still smaller subclass is determined by

P3: $P \in \overline{\mathbb{P}}$ implies that $P/\{i\} \in \overline{\mathbb{P}}$ for all $i = 1, ..., \sharp Set(P)$.

The rightmost diagram of figure 12 provides an illustration. **P3** trivially implies **P2**. Moreover it excludes all adaptive dynamics with sign configurations of s for which the existence of a good internal attractor of any underlying community dynamics may be

contentious. (But we wish to point out here that we have devised community models not satisfying P3 that behaved perfectly well adaptive-dynamically.)

The following proposition, given without proof, provides a somewhat more easily checkable sufficient condition for **P3**: s satisfies **P3** if (i) for every P there is at least one i such that $P/\{i\} \in \overline{\mathbb{P}}$, and (ii) $s_P(Y) > 0 \Rightarrow S_{P/\{i_1,\dots,i_k\}}(Y) > 0$ for all pairs $P, P/\{i_1, \dots, i_k\} \in \overline{\mathbb{P}}$.

6.3 Smoothness of s

The two main reasons to develop any high level theory, i.e., a theory which is not immediately tied to a particular class of models, are that (i) such a theory may point at results which risk to go unnoticed under the clutter of detail inherent in the analysis of special models, (ii) it is only through those means that we can bring out the robust properties of larger classes of models. Both (i) and (ii) hold water only if the ensuing results are sufficiently unexpected. Adaptive dynamics starts to get interesting when we may assume that s is sufficiently smooth. But there is a snag: It is rather hard to find what kind of smoothness conditions are condoned by our requirement that the theory can be tied to at least some classes of community dynamical models. Below we give our present insights in this matter, but this clearly is a topic in need of greater scrutiny.

6.3.1 Smoothness of s away from the diagonal planes of X^n

Away from the diagonal planes of X^n it is relatively harmless to assume fairly unrestricted smoothness of s. This smoothness may be flouted for some specific community dynamical models, but the models that remain form a sufficiently large class. Moreover, when smoothness is flouted we often can produce the complete picture by gluing together the results for a number of regions inside which smoothness holds fine. An example of a useful smoothness assumption is

S2a: s can be continuously extended to $(\operatorname{closure} \mathbb{P}_n) \times \mathbb{X}$, n = 1, 2, ..., and for all $P \in (\operatorname{closure} \mathbb{P}_n) \setminus \mathbb{E}_{\delta}$, \mathbb{E}_{δ} the δ -neighbourhood of the diagonal planes of \mathbb{X}^n , this extension satisfies, for both $Q \in \mathbb{R}^{nk}$ and $V \in \mathbb{R}^k$ small,

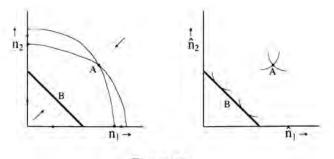
$$s_{P+Q}(Y+V) = s_P(Y) + Ds_P(Y)(Q,V) + \frac{1}{2}(Q,V)^T D^2 s_P(Y)(Q,V) + R(P,Y;Q,V),$$

with the remainder term

$$R(P,Y;Q,V) = O(|(Q,V|^3))$$

uniformly in (P, Y) on $(closure \mathbb{P}_n) \setminus \mathbb{E}_{\delta}$,

where D^i denotes the i^{th} derivative of s with respect to (P, Y). The reason for removing \mathbb{E}_{δ} is disclosed in the next subsection.





6.3.2 Smoothness of s on closure \mathbb{P}_n

Figure 13 illustrates the problems that we run into when we try to extend S2 to the intersection of closure \mathbb{P}_n and the diagonal planes of \mathbb{X}^n . The left hand diagram shows the isocline pattern for two members of a family of hypothetical unstructured two-type communities. In community A the two types differ, and there is a single, stable, internal equilibrium; community B consists of two exactly equal types, so that the two isoclines become a straight line connecting the two equivalent single species equilibria. The right hand diagram once more shows the position of these equilibria, but now accompanied by two pairs of paths traced by the equilibrium when we move along smooth curves in closure \mathbb{P}_2 . The two curves passing through the parameter vector of community A map into two paths which intersect at the position of the single A equilibrium. However, there is no reason at all why the paths corresponding to the curves passing through the parameter vector of community B, should intersect.

Remark: We drew the latter paths as staying on one side of the line of B equilibria, instead of crossing that line, since this happens to be the generic pattern for Lotka-Volterra models. (Remember that the places where $closure\mathbb{P}_2$ intersects the diagonal of \mathbb{X}^2 are strongly constrained; it is this constraint which is at the heart of an otherwise maybe rather unexpected result.) We haven't yet tried to prove that this pattern extends to general ODE community models though. The same Lotka-Volterra models also provide immediate counterexamples against the existence of a derivative of s on (closure \mathbb{P}_n) $\times \mathbb{X}$.

The upshot is that community dynamical considerations may condone assuming that s has smooth directional derivatives in closure \mathbb{P}_n , but not that it has smooth derivatives. Since these considerations only apply to the *P*-component of (P, Y) we conjecture that any overall smoothness assumptions on s should take the following format

S2b: s can be continuously extended to $(\operatorname{closure} \mathbb{P}_n) \times \mathbb{X}$, $n = 1, 2, \ldots$, and this

extension satisfies, for $V \in \mathbb{R}^k$ small,

$$s_P(Y+V) = s_P(Y) + B(P,Y)V + V^T C(P,Y)V + O(|V|3)$$

with B and C continuous in (P, Y), and, for $Q \in \mathbb{C}(P)$ (see below), |Q| = 1,

$$\begin{aligned} s_{P+\epsilon Q}(Y) &= s_P(Y) + \epsilon a_1(P, Y; Q) + \epsilon^2 a_2(P, Y; Q) + O(\epsilon^3), \\ B(P+\epsilon Q, Y) &= B(P, Y) + \epsilon B_1(P, Y; Q) + O(\epsilon^2), \\ C(P+\epsilon Q, Y) &= C(P, Y) + O(\epsilon), \end{aligned}$$

with $a_1(P,Y;Q)$, $a_2(P,Y;Q)$, $B_1(P,Y;Q)$, homogeneous in Q, and continuous in P, Y, and Q, and the various order estimates uniform on \mathbb{P}_n , where

$$\mathbb{C}(P) := \text{closure} \{ Q \in \mathbb{R}^{nk} \mid P + \epsilon Q \in \mathbb{P}_n \text{ for all sufficiently small } \epsilon \}.$$
(6.8)

Remark: S2b almost implies S2a. (The proof follows the lines of the proof of theorem 12.11 in Apostol (1974).) The exceptions are the corners of \mathbb{P}_n (the set of points of non-smoothness of $\partial \mathbb{P}_n$), not only the corners where \mathbb{P}_n touches a diagonal plane of \mathbb{X}^n .

6.3.3 Extending S0, and some consequences

Below we shall no longer distinguish between s and its extension to closure \mathbb{P} . However, before we can do this we first have to assume explicitly that our old

S0: $s_{P'}(Y) = s_P(Y)$ whenever $P' \sim P$,

also holds good for that extension.

By applying S1 to S2b we find that, for small $Q = (U_1, \ldots, U_n)$ and V,

$$s_{P+Q}(X_i+V) = {}_iB(P)(V-U_i) + {}_iB_1(P,Q)(V-U_i) -U_i^T {}_iC_{22}(P)U_i + V^T {}_iC_{22}(P)V + O(|(Q,V)|^3),$$
(6.9)

with

$${}_{i}B(P) := B(P, X_{i}), \quad {}_{i}B_{1}(P, Q) := B_{1}(P, X_{i}; Q), \quad {}_{i}C_{22}(P) := C(P, X_{i}).$$
 (6.10)

S1 and **S2a** tell us that away from the diagonal planes of X^n (6.9) may be replaced by the stronger

$$s_{P+Q}(X_{i}+V) = iB(P)(V-U_{i}) + \sum_{j=1}^{n} U_{j}^{T} iB_{1,j}(P)(V-U_{i}) -U_{i}^{T} iC_{22}(P)U_{i} + V^{T} iC_{22}(P)V + O(|(Q,V)|^{3}), = iB(P)(V-U_{i}) + \sum_{j=1,j\neq i}^{n} U_{j}^{T} iB_{1,j}(P)(V-U_{i}) +U_{i}^{T} iC_{11}(P)U_{i} + 2U_{i}^{T} iC_{12}(P)V + V^{T} iC_{22}(P)V +O(|(Q,V)|^{3}),$$
(6.11)

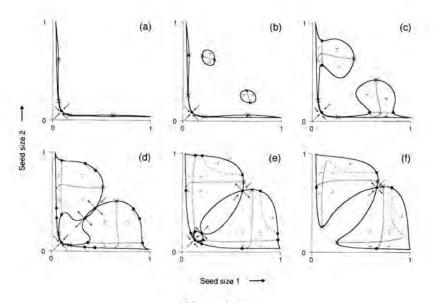


Figure 14:

with

$${}_{i}C_{11}(P) := -\frac{1}{2} \left({}_{i}B_{1i}(P) + {}_{i}B_{1i}^{T}(P) \right) - {}_{i}C_{22}(P), \qquad {}_{i}C_{12}(P) := \frac{1}{2} {}_{i}B_{1i}(P), \quad (6.12)$$

so that

 $_{i}C_{11}(P) + _{i}C_{12}(P) + _{i}C_{12}^{T}(P) + _{i}C_{22}(P) = 0.$ (6.13)

Formulas (6.9), (6.11), and (6.13) are the real workhorses.

S2 may also be used together with S0 and S1 to justify the assumption made in section 3 for 1-dimensional X, that $s|_{P_2\times X}$ unrestrictedly allows a second order Taylor formula. S2a already tells that this is the case away from the diagonal. For $P = (x^*, x^*)$ we use an elegant argument due to Christiansen & Loeschcke (1987). The first formula of S2b says that $s_{P+Q}(x_i+v)$ consists of a quadratic in v plus a third order correction term, with the leading term of the quadratic equal to $_ic_{22}(P)v^2$, and the other coefficients also depending on $Q = (u_1, u_2)$. The equality of the components of P in combination with S0 tell us that $_{1}c_{22}(P) = _{2}c_{22}(P)$, so that we can drop the *i*. The equality of the components of P combines with S1 to tell us that this quadratic should be zero when either $v = u_1$ or $v = u_2$. But for a single variable, and only for a single variable, this implies that the quadratic equals $c_{22}(P)(v-u_1)(v-u_2)$.

6.3.4 Consistency conditions connecting s on different \mathbb{P}_n

Figure 14 shows the \mathbb{A}_2 's, with the stagnation sets drawn in, for a sequence of parameter values measuring the steepness of competition between differently sized seedlings, of a family of models for the competition among plants differing evolutionarily only in the sizes of the seeds which they produce. On the part of the boundary of where x_2 goes extinct the (x_1, x_2) -community reduces to a pure x_1 community. Therefore the x_1 -stagnation set should intersect this boundary exactly at the values of x_1 where the monomorphic x_1 -dynamics has a singular point. Moreover the local colour of the stagnation set should match the type of that singular point. A slightly more involved graphical argument shows that the x_2 -stagnation sets should intersect the x_1 -extinction boundary at the local extrema of that boundary in the x_1 -direction. Local convexity of \mathbb{P}_2 around such an an extremum, call it (x_1°, x_2°) , implies that $_{2}c_{22}(x_1^\circ, x_2^\circ) > 0$, local concavity that $_{2}c_{22}(x_1^\circ, x_2^\circ) < 0$. Figure 14 also shows that these rules considerably constrain how \mathbb{P}_2 can transform when we change process parameters.

The previous observations form the motivation for the introduction of two assumptions, of increasing strength, which tell how $s|_{\mathbf{P}_n\times\mathbf{X}}$ connects to some of the $s|_{\mathbf{P}_m\times\mathbf{X}}$, m < n. But before we can state these assumptions we first need to introduce some additional notation: Let $J \subset \{1, \ldots, n\}, 0 \leq \sharp J \leq n-1$ and let $i \in \{1, \ldots, n\}, i \notin J$. With this convention we define the smooth boundary components

 $\partial_{i;J} \mathbb{P}_n := \{ C \in \mathbb{X}_n \mid (1) \ (a) \ C/\{i\} \cup J \in P_{n-\sharp(\{i\} \cup J)} \\ (b) \ s_{C/\{i\} \cup J}(X_i) = 0 \\ (c) \ s_{C/\{i\} \cup J}(X_j) < 0 \text{ for all } j \in J, \\ (2) \text{ for any } P \text{ such that} \\ (a) \ \operatorname{Set}(P) \subset \operatorname{Set}(C) \\ (b) \ \operatorname{Set}(P) \neq \operatorname{Set}(C) \\ (c) \ \operatorname{Set}(P) \neq \operatorname{Set}(C) \\ (c) \ \operatorname{Set}(P) \neq \operatorname{Set}(C/\{i\} \cup J), \text{ and} \\ (d) \ P \in \mathbb{P}_{n-h} \text{ for some } h > 0, \\ \operatorname{there is at least one } X \in \operatorname{Set}(C) \setminus \operatorname{Set}(P) \\ \operatorname{for which} s_P(X) > 0 \}, \qquad (6.14)$

together with the corners

$$\partial_{i_1,\dots,i_k;J_1,\dots,J_k} \mathbb{P}_n := (\text{closure } \partial_{i_1;J_1} \mathbb{P}_n) \cap \dots \cap (\text{closure } \partial_{i_k;J_k} \mathbb{P}_n), \tag{6.15}$$

with the convention that when $\sharp J = 0$ we just write $\partial_i \mathbb{P}_n$ instead of $\partial_{i;J} \mathbb{P}_n$. (Of course many of these boundary components may be empty!)

For completeness we moreover introduce the boundary components, for $J \subset \{1, \ldots, n\}, 1 \leq \sharp \leq n$,

$$\Delta_{J} = \{ C \in \mathbb{X}_{n} \mid (1) \ (a) \ C/J \in \partial \mathbb{P}_{n-\sharp J}$$

$$(b) \ s_{C/J}(X_{j}) = 0 \text{ for all } j \in J$$

$$(2) \text{ for any } P \text{ such that}$$

$$(a) \ \operatorname{Set}(P) \subset \operatorname{Set}(C)$$

$$(b) \ \operatorname{Set}(P) \neq \operatorname{Set}(C)$$

$$(c) \ \operatorname{Set}(P) \neq \operatorname{Set}(C/J), \text{ and}$$

$$(d) \ P \in \mathbb{P}_{n-h} \text{ for some } h > 0,$$

$$\operatorname{there is at least one } X \in \operatorname{Set}(C) \setminus \operatorname{Set}(P)$$

$$(6.16)$$

and

$$\delta_i \mathbb{P}_n := \{ P = (X_1, \dots, X_n) \in \mathbb{P}_n \mid X_i \in \partial \mathbb{X} \}.$$
(6.17)

To simplify the discussion we shall below sometimes invoke the transversality condition

 $\mathbf{T}_{\leq n}$: the graph of $s|_{\mathbb{P}_{\leq n} \times \mathbf{X}}$ is transversal to the graph of the nul-function on $\mathbb{P}_{\leq n} \times \mathbf{X}$. From the definition of \mathbb{P}_n and the continuity of s it immediately follows that, whenever $\mathbf{T}_{\leq n}$,

$$\partial \mathbb{P}_{n} = \bigcup_{\substack{1 \leq i \leq n, J \subset \{1, \dots, n\}, 0 \leq \sharp J \leq n-1 \\ \bigcup_{J \subset \{1, \dots, n\}, 0 \leq \sharp J \leq n}} \operatorname{closure} \Delta_{J} \mathbb{P}_{n} \cup \bigcup_{0 \leq i \leq n} \delta_{i} \mathbb{P}_{n}.$$
(6.18)

We start with an assumption about the behaviour of s near the smooth boundary components:

S3:
$$s_P(Y) = s_{P/\{i\}\cup J}(Y)$$
 for all $P \in \partial_{\{i\}, J} \mathbb{P}_n$.

S3 may be thought of as expressing the community level assumption that the attractors of the community dynamics depend smoothly on the parameters differentiating the constituting species.

S3 nicely does away with the $\Delta_J \mathbb{P}_n$ in the sense that, whenever $\mathbf{T}_{< n}$,

$$\partial \mathbb{P}_n = \bigcup_{1 \le i \le n, J \subset \{1, \dots, n\}, 0 \le \sharp J \le n-1} \text{closure } \partial_{i;J} \mathbb{P}_n \cup \bigcup_{0 \le i \le n} \delta_i \mathbb{P}_n.$$
(6.19)

(The proof goes by induction on n.)

Next we observe that the combination of S2 and S3 implies that

$$s_P(Y) = s_{P/\{i_1\}\cup J_1}(Y) = \dots = s_{P/\{i_k\}\cup J_k}(Y) \text{ whenever } P \in \partial_{i_1,\dots,i_k;J_1,\dots,J_k} \mathbb{P}_n,$$
(6.20)

i.e., in the corners the full functions $s_{P/\{i_j\}\cup J_j}(\cdot)$, $j = 1, \ldots, k$, should coincide. This would be rather a coincidence, except when it so happens that we are basically dealing with an invasion rate into one and the same P', such that $\operatorname{Set}(P') \subset \bigcap_j \operatorname{Set}(P/\{i_j\} \cup J_j)$. (The points $P/\{i_j\} \cup J_j$, $P \in \partial_{i_1,\ldots,i_k;J_1,\ldots,J_k} \mathbb{P}_n$, then should be also boundary points of $\mathbb{P}_{n-\sharp}(\{i_j\}\cup J_j)$.) This observation suggests that we may without great loss of community dynamical generality assume:

S4: $s_P(Y) = s_{P/\{i_1,\dots,i_k\}\cup J_1\cup\dots\cup J_k}(Y)$ for all $P \in \partial_{i_1,\dots,i_k;J_1,\dots,J_k}\mathbb{P}_n$.

S4 trivially implies S3, but not vice versa.

S4 has two immediate consequences. The first is, not unexpectedly,

$$\left(\partial_{i_1,\dots,i_k;J_1,\dots,J_k}\mathbb{P}_n\right)/\{i_1,\dots,i_{j-1},i_{j+1},\dots,i_k\} \cup \bigcup_{j=1}^k J_j \subset \partial \mathbb{P}_{n-\sharp(\{i_1,\dots,i_k\}\cup\cup_{j=1}^k J_j)+1}.$$
(6.21)

The second one is slightly more involved. Therefore we will only give an example: For figures 6, 7, 8 and 14, S4 together with S1 implies that near to the outer corners of \mathbb{P}_2 the adaptive movement is away from the corner.

6.4 The trait substitution process

An adaptive dynamics is governed by its s not only through its sample functions being maps from \mathbb{R}_+ to $\operatorname{Set}(\overline{\mathbb{P}})$; s also governs the mechanics of the trait substitution process.

A trait substitution, i.e., a jump in the sample function, is generated by the composition of three processes:

- (1) The production of a mutant $Y = X_i + V$ from an $X_i \in \text{Set}(P)$. Mutations result from rare copying errors of the genetic material during individual reproduction events. A mutation gets expressed as a step in the trait vector of the mutant relative to that of its parent only through the action of the developmental process on the individual mutated genotype.
- (2) The establishment of that mutant. When $s_P(Y) \leq 0$ the mutant will fail to establish and the sample function continues smoothly, when $s_P(Y) > 0$ there is a chance that the mutant gets established.
- (3) The production of a new value of the sample function. The establishment of a mutant leads to a shake-up of the community in which one or more of the X_i ∈ Set(P) may be lost.

Only the end result of these three processes is visible at the level of the sample function, as the positions and types of jumps.

6.4.1 The production of mutants

Since the production of mutants contains a large intra-individual component we have but few a priori considerations to base our assumptions on. The list of assumptions below tries to strike a compromise between being biologically as weak as possible and yet being mathematically sufficiently useful. It is only at the intra-individual level that we strived for weakness. Where we could strengthen the assumptions by bringing in a community dynamical argument we have done so.

From the present jump moment till the next one, mutations in X_i may be assumed to occur in a Poisson process with rate λ_i .

Basic biological considerations tell us that λ_i (a) may depend on the history of the line of descent leading to X_i , and (b) depends on P. (a) is due to the fact that the map from genotype to any simple phenotypic representation necessarily is very many to one, so that there is no good reason to expect that on the phenotypic level the mutation process is Markovian, (b) to the fact that at the community dynamical level P determines the average birth rate into the X_i -population. We shall make only the weak assumption that the mutation probabilities per birth event are bounded away from both 0 and ∞ . If we make the same sort of continuity assumptions on the attractors of the community dynamics as before, we end up with the overall assumption:

M1: $0 < -\lambda_i(P) \leq \lambda_i \leq +\lambda_i(P)$, with

- (i) $\pm \lambda_i$ continuous in all points $P \in \text{closure } \mathbb{P}_n$, with the exception of P for which $X_j = X_i$ for some $j \neq i$,
- (ii) for $P = (X_1, \ldots, X_n) \rightarrow C = (X'_1, \ldots, X'_n) \in \partial_{i;J} \mathbb{P}_n, \ \sharp Set(C) = n,$

$${}_{\pm}\lambda_i(P) = O(|X_h - X'_h|) \quad \text{for } h \in \{i\} \cup J, \\ {}_{\pm}\lambda_i(P) \to {}_{\pm}\lambda_i(C/\{i\} \cup J) \quad \text{for } h \notin \{i\} \cup J,$$

(iii) for $P = (X_1, \dots, X_n) \to C = (X'_1, \dots, X'_n)$ with $X'_j = X'_i, j > i$, $\pm \lambda_i(P) + \pm \lambda_j(P) \to \pm \lambda_i(C/\{j\}).$

Of course, special adaptive dynamics may satisfy stronger assumptions, e.g. the Markovian dependence of λ_i on P. Biology also tells that the distribution of the mutational steps $V = Y - X_i$ may well depend on the history of the line of descent leading to X_i . Therefore we only make an overall non-degeneracy assumption:

M2a: The mutational steps are continuously distributed, with the possible exception of a concentration of mass on

$$\mathbb{B}(X_i) := \{ V \mid Y = V + X_i \in \partial \mathbb{X} \};\$$

the latter mass is continuously distributed on $\mathbb{B}(X_i)$.

M2b: Let f temporarily denote the density of Y in $\{V \mid Y = V + X_i \in X\}$, and g the density of Y in $\mathbb{B}(X_i)$. Both f and g are uniformly continuous on the closures of their domains and there exists a single constant c > 0 such that f(0) > c, and, when $X_i \in \partial X$, g(0) > c.

M2b guarantees that mutations effectively occur in all directions.

To make the smoothness assumptions on s pay, other than by providing some constraints on the possible shapes of $\overline{\mathbb{P}}$, we have to assume that the mutational steps are uniformly small:

M3: There exists an ϵ such that

 $\mathcal{P}\{|V| > \epsilon\} = 0.$

6.4.2 The establishment of a mutant

To get established, the mutant population has to grow from a single individual to a number of individuals which is of the order of the system size Ω (compare the discussion in section 5). The initial phase of this growth process is dominated by stochastic demographic fluctuations. In the limit of infinite Ω the probability of establishment should equal that of the stochastic branching process where Y type individuals reproduce in the environment E(P).

The estimates for the establishment probability of particular branching processes with low growth rates (Haldane 1927; Kendall, 1948, 1949; Eshel, 1981, 1984; Hoppe 1992a, b; Athreya 1992, 1993; Pollak 1992; Haccou & Iwasa, in prep) all have an initial term which is linear in the growth rate. Therefore it seems safe to assume that

B: The probability $\pi_P(Y)$ that a Y mutant successfully invades a P community is zero when $s_P(Y) < 0$, and when $s_P(Y) \ge 0$ we can bound $\pi_P(Y)$ by

$$\alpha s_P(Y) + o(s_P(Y)) \le \pi_P(Y) \le \beta s_P(Y),$$

with $\alpha, \beta > 0$, and the order term uniform on $\overline{\mathbb{P}}$.

Remark: We slightly oversimplified the argument above. On the community dynamical time scale both the birth rate of Y mutants and the probability that a mutant gets established are time dependent, except in the special cases that the community attractor is a deterministic equilibrium. Therefore the two processes, production of mutants by X_i and the establishment of a mutant, cannot be treated separately. The correct argument runs as follows: Let $\lambda'_i(t)$ denote the production rate of mutants from X_i , and $\pi'_P(Y)(t)$ the probability that a Y mutant gets established. Then

$$\lambda_i = \lim_{t \to \infty} t^{-1} \int_0^t \lambda_i'(\tau) \, d\tau, \qquad \pi_P(Y) = \lambda_i^{-1} \lim_{t \to \infty} t^{-1} \int_0^t \lambda_i'(\tau) \pi_P'(Y)(\tau) \, d\tau.$$

When moreover

$$a(t)s_P(Y) + o(s_P(Y)) \le \pi'_P(Y)(t) \le b(t)s_P(Y),$$

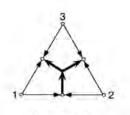


Figure 15:

with the order term uniformly in t, then **B** holds good with α and β the corresponding time averages of a(t) and b(t). With these definitions the only visible effect on the evolutionary time scale of a complicated community dynamics is a dependence of $\pi_P(Y)$ on the parent of Y, which we didn't make explicit in our notation. When **M3** is in operation this dependence is necessarily slight, and it should be possible to make the estimate **B** independent of the parent of Y.

6.4.3 The production of the post-jump value of the sample function

The establishment of a mutant leads to a shake-up of the community in which one or more of the $X_i \in \text{Set}(P)$ may be lost. The following assumption about the types that are kept around is directly in line with the arguments underlying **P1**.

- K: The new value of the sample function is chosen at random, with probabilities which depend only on P and Y, from among all P' such that
 - (i) $P' \in \overline{\mathbb{P}}$

(ii)
$$\operatorname{Set}(P') \subset \operatorname{Set}(P) \cup \{Y\}$$

(iii) for all $X \in (\operatorname{Set}(P) \cup \{Y\}) \setminus \operatorname{Set}(P')$

 $s_{P'}(X) \leq 0.$

Figure 15 provides an illustration.

Remark: On the community dynamical level **K** only holds water as long as any heteroclinic loops are repelling. When the theory gets modified to cope in an acceptable manner with such loops, as we hope that will be possible in the future, the natural assumption is that P' also may be any trait combination that occurs in a vertex of an attracting heteroclinic loop.

7 One research strategy and some conclusions

The assumptions made in the previous section aren't the only possible ones. We listed them to make explicit our own preconceptions and to get a discussion started about possible useful and/or justifiable alternatives. Moreover, it is possible to explore their consequences in a number of different directions. One useful direction is the development of a bifurcation theory for EUSes. In this section we discuss, without proofs, a number of heuristically derived macro-evolutionary results, as an example of one other direction that could be taken.

We emphasize that it is as yet unclear how robust the results below are with respect to relaxing our basic time scale argument.

7.1 The research strategy

The results below were derived by adhering to the following research strategy

- 1. Let the scale of the mutational steps, as measured by their maximum seize ϵ , go to zero, and simultaneously rescale time so that the process doesn't freeze (which choice of scale is appropriate depends on the phenomenon that is considered).
- Forget about features of the sample path that can only be seen at a resolution of O(ε^{1/2}).
- 2 b. Forget about events that only occur, in interestingly long stretches of the sample path, with probability o(1).
- 2 c. Concentrate on phenomena that are stable under slight changes of s.

Remark: 2a also provides an exegesis of some of the verbiage in sections 3 and 4: "Small" should be interpreted as " $O(\epsilon^{1/2})$ but not $o(\epsilon^{1/2})$ ", "very small" as " $o(\epsilon^{1/2})$ ", and "visible" as "not very small".

7.2 Overall environment constant on the evolutionary time scale

We start our discussion on the assumption that on the evolutionary time scale(s) the environment can be considered constant, i.e., the environmental fluctuations are fully restricted to the community dynamical time scale. In that case we should distinguish two time scales, each relevant to a particular type of evolutionary phenomena:

- 1. Both the number of steps needed to cover a fixed distance in any \mathbb{P}_n , $n = 1, 2, \ldots$, and the time needed for one step, scale as ϵ^{-1} (remember axiom **B**). Therefore starting from some point $P \in \mathbb{P}_n$, the time needed for convergence to an attractor in \mathbb{P}_m , $m \leq n$, and time pattern of the movement on a non-point attractor in \mathbb{P}_m , scales as ϵ^{-2} . We shall label the corresponding evolutionary time scale fast.
- 2. Branching, however, takes a time which scales as e^{-3} , since s is locally quadratic in $Y X_i$ near a branching point of X_i . We shall label the corresponding evolutionary time scale slow.

Adaptive dynamics

If the mutation process is Markovian the movement on the fast evolutionary time scale can, but for the jumps to a lower degree of polymorphism, be approximated by an ODE (Dieckmann & Law, 1995).

Branching only occurs on the slow time scale after the fast process has come to rest at a point attractor of the adaptive dynamics in \mathbb{P}_m which allows for the branching of, say, $h, 1 < h \leq m$, lines of descent. Even for $\epsilon \to 0$ the number of lines that branch may stay stochastic: Simulation results suggest that, due to the peculiar geometry of $\overline{\mathbb{P}}$, the fast evolution of those branches that happen to have taken a relatively larger lead, inhibits the branching of the remaining lines of descent.

The previous considerations may be translated into the following predictions about macro-evolutionary patterns that derive from our model assumptions: If there are no long term environmental changes due to external perturbations, the natural overall behaviour of an adaptive dynamics will often show a number of alternations between short periods of fast change in the species in the community, and long periods of stasis of the community as a whole. The time scale of these phases is set by the production rate of mutational variation. "Speciation" is initiated only during static phases, and the eventual divergence of the nascent species starts the next fast phase. This alternation goes on till the process gets trapped in a non-equilibrium attractor of the adaptive dynamics, or in a fully attractive evolutionarily unbeatable combination of strategies.

As a final point we mention once more that in higher dimensional trait spaces polytomies (in which one line of descent gives rise to more than two branches during a single slow phase) shouldn't be unusual, the higher the dimension of the trait space the higher the degree of polytomy.

7.3 Changing physical environments

As a final topic we consider the consequences of overall environmental fluctuations on the evolutionary time scale, say due to climate change.

Again we have to consider two time scales, but now of the environmental fluctuations. If the overall environment fluctuates on the fast evolutionary time scale the fluctuations will inhibit branching, by the same geometric mechanism by which progressive evolution of other lines of descent inhibited branching. (This may be seen as a, tongue in cheek, explanation for the low species diversity in the North, where the ice ages provided precisely this type of fluctuations.)

The second possibility is that the overall environment only fluctuates on the time scale of the static phases or even slower (the usual time scale of the geological record!). The typical patterns seen on that scale derive from the stable bifurcations of attractors of the adaptive dynamics. As this subject has hardly been broached, our conclusions all derive from a few immediate graphical arguments. Two stably occurring types of hard bifurcations are (i) saddle node type bifurcations and (ii) bifurcations in which an evolutionary point attractor located in, say, \mathbb{P}_n transforms into a branching point. Intriguingly the latter type of bifurcation need not be of the pitchfork type in \mathbb{P}_{n+1} : The constraints on the places where the stagnation sets touch the boundary of \mathbb{P}_{n+1} make that it is possible that an evolutionary point attractor located in \mathbb{P}_n

stably transforms into a branching point without making contact with evolutionarily singular points in \mathbb{P}_{n+1} . The result of such a bifurcation on the longest time scale is seen as the occurrence out of the blue, of an abrupt branching event, followed by fast progressive evolution of the novel "species".

In the parlance of paleontologists the patterns resulting from hard bifurcations of point attractors are called punctuated equilibria, (i) within a line of descent or (ii) with speciation.

One punctuation event may lead to more in its wake, as the fast evolution of one line of descent reverberates through the species assemblage, potentially resulting in extinctions and/or further branching events. We therefore may expect that the overall effect of a continually changing environment has the look of quasi-stasis interspersed with clusters of fast events, consisting of both extinctions and speciations.

8 Concluding remarks

In this section we place our main results in a larger biological context; in the final subsection we indicate some potentially fruitful further lines of research.

8.1 Branching

The prediction and characterization of branching events may well be considered the most interesting result from our attempt at classifying the various possible evolutionarily singular points. However, as was clearly put forward by Christiansen (1991), it is also the result which is the least robust against the introduction of a realistic diploid genetics (no obligate self-fertilisation or absolute assortative mating). To keep our other results obtained so far intact under realistic diploid genetics we have to assume that heterozygotes have phenotypes lying in between those of the two corresponding homozygotes. But this same assumption forces us to deal with the potential of a continual stream of intermediate types where the sample path of a clonal model would start branching. Branching can only be rescued by assuming some newly developing or pre-existing mechanism which impedes the mating between two individuals from the diverging strains. Interestingly the few working ecological models for speciation through the development of some mating barrier, indeed seem to be organized around an evolutionarily singular point of the branching type (e.g. Seger, 1985). Moreover, there recently has been a spate of publications (e.g. Henry, 1994) about so-called cryptic speciation, i.e., the development of mating barriers (based on special mate recognition systems, compare Paterson, 1993) which are not yet reflected in the divergence of some readily observable traits. Our hunch is that the crypsis will be lifted when, and more often than not only when, the community dynamically relevant trait values of those species come to lie in the neighbourhood of a branching point.

Remark: Only populations which are sufficiently strongly coupled by migration allow a representation by a single fitness function s. The existence of such a representation formed the basis for all our considerations. Therefore allopatric speciation, in which two populations become migratorily uncoupled before the onset of divergence, falls

outside the range of our formalism. Only the so-called sympatric and parapatric speciation modes fall squarely within its range (compare Meszéna, in prep). However, past opinion was that the latter modes of speciation were at best rare, compared to the allopatric one. However, recently more and more field evidence is coming available for the frequent occurrence of rapid speciation in populations which are not divided up by any clear physical barriers to migratory exchange (e.g. Meyer, 1993). And, better still, such events in a number of instances even have occurred in a repeatable manner following the immigration of a founder species into separate lakes or islands

8.2 On the non-commutativity of limits

(Schluter & Nagel, 1995; Losos, 1995).

The results from the previous section were based on three subsequent limiting arguments, (i) the approximation of an individual-based stochastic community model by a deterministic one, combined with (ii) the assumption of rarity of mutations, together allowing the transition from the framework of community dynamics to that of adaptive dynamics, and (iii) the assumption of uniform smallness of the mutational steps, allowing the deduction of the macro-evolutionary conclusions in section 7. Both intuition and figure 10 suggest that we cannot be too sure that these three arguments are all the way compatible.

The community dynamical time needed for a substitution of one type by another, say X_i by Y, scales as $\log(\Omega)/[s_P(Y) - s_{(P,Y)/\{i\}}(X_i)]$, Ω the system size. The denominator of this expression goes to zero when the size of the mutational steps, ϵ , goes to zero. Therefore the limits $\epsilon \to 0$, and $\Omega \to \infty$ together with $\Omega\theta \to 0$, θ the mutation probability per birth event, don't commute. Depending on the route we follow in $(\Omega, \theta, \epsilon)$ -space to $(\infty, 0, 0)$ we get a different limit process. To get the results described in the previous section for the fast phase we should have that $\Omega\theta \log(\Omega)/\epsilon \to 0$. The results for the slow phases may be only expected to hold good when $\Omega\theta \log(\Omega)/\epsilon^2 \to 0$. In other words, those results can only have biological relevance if in reality $\Omega\theta \log(\Omega)/\epsilon$, respectively $\Omega\theta \log(\Omega)/\epsilon^2$, are sufficiently small.

As a final point we mention that at very small distances from an evolutionary point attractor the framework breaks down all the way. As soon as evolution has come sufficiently near to such an attractor new mutants are selectively almost neutral, so that on this scale the scene will be effectively dominated by demographic stochastic fluctuations.

8.3 Some directions for further research

We see at least two immediate directions for further progress. First of all the underpinning and/or modification of our present assumptions, as far as these are based on community dynamical arguments, should be further explored. Two immediate research problems are (i) the exploration of the continuity assumption S2, for example by elaborating the bifurcation patterns of community equilibria in some appropriately chosen general ODE framework, (ii) the modification of our assumptions P1a and K to account for the occurrence of attracting heteroclinic networks. The second, and ultimately most interesting, topic is the development of a bifurcation theory for Evolutionarily Singular Strategies (but to get started we need a better insight in the potential for generalizing assumption **S2b**).

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