Dynamical Systems: Physics and Numerical Analysis

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1. Introduction

Since it is impossible to do justice to the whole of nonlinear dynamics and chaos in one chapter we shall give a broad-brush overview, but with emphasis on two aspects of the subject not normally given much attention in textbooks on dynamical systems — the emergence of low-degree-of-freedom dynamical systems as a description on a macroscopic scale of systems with large numbers of elements on a microscopic scale, and the numerical analysis of dynamical systems. These are related, as computational approaches can give much new insight in the field of complex systems. This chapter can be read on two levels — on the one hand we endeavour to give heuristic arguments and physical motivations so that the beginner should be able to get a feel for the subject, but on the other hand we also give a flavour of the rigorous mathematical approach and give references to the mathematical literature.

Note: References to sections in this chapter are indicated using the § symbol, words defined in the text are indicated by italics when they are first defined, and words defined in the glossary of this chapter are indicated in bold type when they first occur.

1.1. Chaos — the dynamical systems approach

The insight that has caused the great upsurge in interest in “chaos theory” in recent years [for an introductory overview and reprints of original papers, see Hao (1989)] is that complex behaviour may arise from simple mathematical models. The models we have in mind are dynamical systems — sets of equations describing the deterministic evolution, with respect to time or a time-like parameter, of a number of dynamical variables (see §2) forming a vector in a finite or infinite-dimensional state or phase space. The time variable may be continuous, so that the dynamical system is a system, first
order in time, of ordinary differential equations (ODEs) in the finite-dimensional case, or partial differential equations (PDEs) in the infinite-dimensional case. Alternatively the time variable may be \emph{discrete}, so that the dynamical system is an iterated \emph{map}.

The use of the word \emph{chaos} is usually taken nowadays to imply (a) irregular behaviour not driven by externally imposed random noise; and (b) that the description of the irregular behaviour can be reduced to a low-dimensional dynamical system (even if the original physical system is infinite-dimensional). In this chapter we shall restrict consideration to "pure" chaos in the sense of (a) above, but we caution that a full theory of complex systems requires dynamical systems theory to be extended by including "noise" terms representing stochastic fluctuations (Haken, 1983, p. 315).

For mathematical texts on dynamical systems theory the reader is referred to such books as those of Guckenheimer & Holmes (1983), Devaney (1989) and Arrowsmith & Place (1990). Books on nonlinear dynamics oriented more toward those who are not professional mathematicians are Arrowsmith & Place (1990), Lichtenberg & Lieberman (1992), Moon (1992) and Ott (1993).

Low-dimensional dynamical systems may exhibit complex, chaotic behaviour, but if we mean by "complex system" a system with many interacting components, we may ask is low-dimensional dynamical systems theory really relevant to complex systems theory? We answer this in the affirmative by considering systems with a large or infinite number of degrees of freedom and showing how it can happen that behaviour in such complex systems can often be described by a reduced dynamical system with a small number of degrees of freedom. We take as our paradigm the development of organised collective motion in fluids, as this problem has been intensively studied by physicists, engineers and mathematicians for many years (though there is still much to understand).

A powerful influence on the spread of the field of nonlinear dynamics beyond a handful of mathematicians capable of visualising complex behaviour in the mind's eye has been the advent of easy-to-use computers and computer graphics. This has allowed a much wider community of scientists to grasp the concepts of low-dimensional dynamical systems theory, and to apply them to practical problems. In turn the ability to perform computer experiments has stimulated many new theoretical developments.

Another area, within the fluid dynamics paradigm referred to above, in which computation has shed new light on old problems is in the simulation of liquids, gases and plasmas using "particle-pushing" or \emph{molecular dynamics} methods. In this approach supercomputers are used to advance the equations of motion of a large number of particles (\textsuperscript{[2,8]}) in an effort to model the actual real-world situation in which we know that the seemingly continuous behaviour of matter on a macroscopic scale is in fact the result of the motion of an enormous number, \( N \) say, of particles; where \( N \) is proportional to Avogadro's number, \( 6 \times 10^{23} \) molecules per mole. No conceivable supercomputer can of course handle numbers of degrees of freedom of this order, but, by using cunning numerical tricks and by being careful with the interpretation of results, sufficient numbers of particles often can be followed to obtain physically relevant macroscopic information. However it is through the ability to obtain \emph{microscopic} diagnostic information easily from a numerical simulation that this technique can lead to new insights into the nature of complex systems.

In this chapter we provide an overview of dynamical systems theory with an emphasis on \emph{numerical analysis}. That is, we introduce some of the most important concepts in dynamical systems theory in a mathematical but constructive way, suitable for numer-

\footnote{Chaos is sometimes called "intrinsic stochasticity", but the word "stochastic" is better reserved for truly random phenomena.}
tical implementation, and we also discuss error analysis ([3]) and introduce the concept of shadowing ([9]). This provides the mathematical underpinning for the computer experimentation in which we encourage the reader to engage while reading [2], or other dynamical systems texts. Two excellent interactive graphical computer programs which allow users access to the source code, so that they may provide their own dynamical systems in addition to the default ones, are the Unix X11 code ds tool (Guckenheimer et al., 1992) and the DOS/Unix X11 code dynamics by Yorke & Kostelich whose use is described in Nusse & Yorke (1993). Also very useful are general purpose algebra, computation and graphics packages like Mathematica (Wolfram, 1991), Matlab (Moler et al., 1990) or Maple (Char et al., 1991), which provide facilities for such things as two-dimensional arrow plots to depict vector fields.

In the next three subsections of this introduction we attempt to explain the paradox of how complex systems may sometimes be described by low-dimensional dynamical systems. This is of interest not only to understand the genesis of dynamical systems, but because we believe dynamical systems theory itself casts light on the nature of physical theory by introducing the concept of inertial manifolds ([8] and related techniques for obtaining a reduced description of the long-time behaviour of a system. The basis for such reductions has been called the limiting principle by Haken (1978; 1983), who has emphasised its key role in complex systems theory (called by him synergistics).

1.2. Conservative dynamical systems

The basic dynamical equations of physics are Hamiltonian and consequently conserve phase space volume—see classic texts like Landau & Lifshitz (1971) and Goldstein (1980) or more modern ones discussing dynamics on manifolds, such as Arnold (1988) or Schek (1980). They also exhibit continuous symmetries such as translation invariance in space (giving rise to momentum conservation) and in time (giving rise to energy conservation), and discrete symmetries such as parity and time-reversal invariance (Sudarshan & Mukunda, 1974).

Because of the fundamental nature of Hamiltonian dynamical systems, their nonlinear properties have been much studied in recent years [see the reprint collection of Mackay & Meiss (1987)]. It is now realised that the emphasis in the classic texts on problems that could be solved by action-angle transformations (integrable systems) was misleading, in that a typical Hamiltonian will not have a phase space foliated by invariant tori ([1,3,5,24], as is the case if an action-angle transformation exists, but will have at least some regions of chaotic motion. In these regions there exists a time scale (the inverse of the maximum Lyapunov exponent, see [6]) over which small initial errors in position or velocity amplify exponentially, so that, on a timescale long compared with this Lyapunov scale, the motion is essentially unpredictable.

1.3. Dissipative dynamical systems

There are some large-scale physical systems, such as the solar system, which are well described as low-dimensional Hamiltonian dynamical systems. However many problems of physics (let alone chemistry or biology) involve far too many degrees of freedom for analysis from first principles as a Hamiltonian dynamical system to be practicable. Nevertheless, a low-dimensional dynamical system (typically not Hamiltonian) is often a valid physical description over some macroscopic range of length and time scales. That is, new physics appears when we reframe on larger scales than those of elementary particle physics or atomic physics where (quantum) Hamiltonian dynamics reign supreme. The essentially emergent nature of physical theory on different scales has been emphasised,
and contrasted with the traditional reductionist approach, by the distinguished physicists Anderson (1972) and Schwaber (1983).

How may we understand this loss of the stupendous number of degrees of freedom in the microscopic description and their replacement with a relatively few nontrivial degrees of freedom on a macroscopic scale? The main mechanism by which simplicity can emerge from complexity is irreversibility. Since Boltzmann's work around the turn of the century (Lebowitz, 1991a; Lebowitz, 1991b) we have understood this as arising from the inherently coarse-grained nature of macroscopic observations, in which many microstates are projected onto one macrostate and a statistical or probabilistic description must be adopted, so that knowledge of the initial conditions is lost. The theory describing the evolution of probability densities or distribution functions in phase space, and the derivation from them of macroscopic transport coefficients, is at the core of non-equilibrium statistical mechanics.

One might expect modern chaos theory to shed new light on the origin of irreversibility, and indeed an entropy (the Kolmogorov-Sinai entropy — see [6]) which measures rate of information loss is used in dynamical systems theory. However the relation of this entropy rate to dissipation in physical systems is a surprisingly subtle and controversial question. In fact, on the basis of what is known in the rigorous mathematical literature (Lanford, 1981), Lebowitz (1991a) states that the essential features of irreversibility do not depend on “the positivity of Lyapunov exponents, ergodicity or mixing”.

On the other hand, a clear and practical relation between Lyapunov exponents and viscosity has been found (Evans et al., 1990; Evans et al., 1992) for a “thermostated” quasi-Hamiltonian system developed to allow molecular dynamics computations of stressed systems (e.g., shear flows) to be carried out without having to introduce boundaries to remove the heat generated. This thermostated Hamiltonian is discussed in §2.8. The “thermostated” is spatially distributed for computational convenience and has the remarkable effect of producing a strange attractor in the phase space of an otherwise Hamiltonian system (Morris, 1987).

The relevance of this result to the more realistic case where heat is removed at the boundaries is a topic of hot debate [literally! — see pp. 327-329] of Marchal and Héran (1992)]. As stated by (Cohen, 1992) “The relation between kinetic theory and the theory of dynamical systems has hardly been developed”. A first step in this direction starting from the low-dimensional dynamical systems and the study of transport in area-preserving maps (MacKay et al., 1985), and Wiggins (1992) has begun to extend this into a theory for multi-dimensional Hamiltonian systems.

Another area in which our modern understanding of nonlinear dynamics, combined with computation, raises fundamental issues in the field of statistical mechanics is the question of the compatibility between the Kolmogorov-Arnold-Moser theorem (KAM theorem — see [2,4]) and the “ergodic hypothesis” at the heart of equilibrium statistical mechanics. The ergodic hypothesis is the assumption that the state vector describing an isolated many body system wanders in time over the entire “energy-surface” — the set of points in phase space with the same energy. The KAM theorem, on the other hand, asserts that, under appropriate conditions, a finite fraction of orbits is confined to a more restricted region than the entire energy surface. It was the failure to confirm the ergodic hypothesis in a computational “experiment” by Fermi, Pasta and Ulam (1955) which led eventually to the discovery of the theory of solitons (Zabusky & Kruskal, 1965). Current knowledge of the scaling with number of particles of the chaotic region of phase space is reviewed in Lichtenberg and Lieberman (1992, §6.5).

Irreversibility allows the observable effects of the many-body, microscopic degrees of freedom to damp out on a short timescale. Just what level of macroscopic description is
used depends on the problem. If the time and length scales of the physical experiment are comparable with the statistical relaxation scales (inverse collision frequencies and mean free paths) then we must use a kinetic description.

Kinetic theory works with PDEs describing the evolution of single-particle distribution functions — the probability of finding a particle species in its 6-dimensional phase space of position and velocity at time $t$. This is to be contrasted with the $6N$-dimensional phase space of the complete dynamical description of the system (assuming classical mechanics is an appropriate description at the microscopic level). Thus for kinetic theory to work we need to assume that all the information we need to know about the $N$-body system is contained in the single-particle distribution function. This is the hypothesis behind Bogoliubov's infinite hierarchy of equations for many-particle distribution functions (Montgomery & Tidman, 1964, Ch. 5) — after an initial transient all many-particle correlation functions are slaved to the single particle distribution function, so that a kinetic equation such as the Boltzmann equation can be derived. Another approach is the projection operator formalism (Zwanzig, 1964) [reprinted with many related articles in Oppenheim, Shuler & Weiss (1977)] for deriving the "master equation" or generalised kinetic equation. Also Muncaster (Muncaster, 1982) has developed a general formalism for deriving coarse-grained theories from fine-grained theories and has discussed it in relation to the theory of attracting invariant manifolds (see §§5.6 and 8).

If the time and length scales of the physical experiment are long compared with the statistical relaxation scales the description may be reduced further using the Chapman-Enskog method (Chapman & Cowling, 1930) to derive fluid equations. These are still PDEs but are defined on the ordinary three-dimensional space of position (plus time of course). The loss of information about the microscopic behavior due to coarse graining now shows up in the form of transport coefficients, such as viscosity, which lead to entropy increase. These dissipative terms tend to damp out short-wavelength structure, and thus lead to a contraction of volume elements in the phase space of Fourier amplitudes of excitations of the fluid. This contraction of phase-space volume is a characteristic signature of dissipation, and is to be contrasted with the conserved phase space of the microscopic Hamiltonian description (without thermostatting terms).

If the boundaries of the system are sufficiently close to mutual thermodynamic equilibrium, the system will relax to a simple equilibrium state, but if the system is bordered by regions sufficiently far from mutual thermodynamic equilibrium, spontaneous symmetry breaking of the simple state can occur via one or more bifurcations (see §7.2), and new nontrivial degrees of freedom can thus emerge. These are driven by the input of energy at low entropy (e.g. heat from the hotter parts of the boundary) and its removal at a higher entropy (from the colder parts).

The classic example of this is the onset of Rayleigh-Bénard convection rolls in a fluid between two plates when the temperature of the lower plate exceeds that of the upper by a critical amount (Swinney & Goldblatt, 1988). The moral we draw from this is that self-organisation occurs in open systems through which energy is flowing. For instance the occurrence of life itself can be thought of as a self-organising phenomenon driven by the temperature difference between the Sun and the Earth. The importance of nonlinear non-equilibrium thermodynamics for complex systems theory has been emphasised by Prigogine (Prigogine & Seegers, 1985).

It should also be remarked that the low-entropy energy input need not be in the form of heat; for instance electrical energy can drive magnetic tearing instabilities which destroy...
the translational symmetry of a plasma current sheet (Parker et al., 1990; Grauer, 1989; Wesson, 1992).

In dynamical systems terms the nontrivial degrees of freedom are coordinates on a low-dimensional "inertial manifold" (Temam, 1988) which all orbits approach asymptotically at large times so that the attractor(s) (14) of the system are embedded within it. The damped degrees of freedom have a permanent excitation, but only as a forced, adiabatic response to the motion on the invariant manifold — they are "slaves" to the "master" coordinates on the invariant manifold (Roberts, 1990). The slave modes in turn react nonlinearly back on the master modes to produce a renormalised vector field in the reduced dynamical system of the master modes (8, see also Ch. 7). The master coordinates are also called "order parameters" (Haken, 1978; Haken, 1983) or "central modes" (Manneville, 1980).

In summary, we have put forward the view that self-organised dynamics is the result of a competition between the enslaving effect of irreversible dissipation and the tendency of low-entropy energy input to produce new master modes via symmetry-breaking bifurcations.

1.4. Spatio-temporal chaos

We have already remarked that PDEs first order in time are (infinite-dimensional) dynamical systems, so the study of systems distributed in space is included in dynamical systems theory. Furthermore the existence of a centre (§5.8) or inertial manifold (§8) can make the long-time behaviour describable by a low-dimensional dynamical system. This system may exhibit irregular behaviour in time, but not in space — temporal chaos, or may be irregular in both time and space — spatio-temporal chaos.

The field of spatio-temporal chaos is not as mature as that of temporal chaos, but includes many interesting aspects of complex system theory — pattern formation, lattice dynamics, cellular automata, Lagrangian chaos. An early general review is that of Crutchfield and Kaneko (1987), while a review of more recent work can be found in Chapter 8 of Moon (1992). A much more complete treatment of spatio-temporal chaos in fluids is to be found in Manneville (1980).

1.5. I want dynamics — Why study numerics?

The study of dynamical systems has been going on for at least a century now starting with Poincaré (1892). Most of this work has been done in terms of topology and geometry — much of it "hard" analysis. On the other hand applications to any real situations suffer from the problem that analytical solutions of the governing differential or difference equations are either impossible to find or give little understanding about the existence or non-existence of chaos. Certainly computers have been used to study a great many phenomena arising from chaotic and other dynamical systems. This is the way the fractals that are used to decorate offices and bedroom walls are generated. Furthermore, these computations are not exact — they are almost always done using floating point arithmetic.

There are a number of issues that arise from these computations which are difficult to resolve and involve a great deal of sophisticated mathematics. The first point that should be made is that in dynamical systems, trajectories remain bounded, and yet diverge exponentially fast (until they are no longer close). Because of the finite precision of floating point arithmetic, numerically computed trajectories are constantly being perturbed. And these perturbations lead to exponentially growing errors in the solution. Very quickly the errors will swamp the trajectory itself, and the errors will be of about the same size as the features of the trajectory — thus there will be no significant digits
in the numerically computed trajectories. Yet, the results that come out of simulations of the Lorenz equations or any other particular chaotic equations are remarkably independent of how the equations have been discretised, or how they have been implemented. Why is this? This question leads to some interesting and deep problems in analysis, both numerical and analytical.

One of the ideas that has come out of this work is the idea of shadowing [2]; that is, computed solutions of an iteration really satisfy \[\|y_{n+1} - g(y_n)\| < \delta\] for some small \(\delta > 0\). These \(\epsilon\)-pseudo-orbits are \(\epsilon\)-shadowed by some exact solution \(x_\epsilon\) where \(\|x_\epsilon - y_n\| < \epsilon\). Given a \(\epsilon\) pseudo-orbit we want to find \(\epsilon > 0\) for which there is an \(\epsilon\) shadow. Sometimes this shadowing radius can be numerically computed for a particular trajectory.

Another way in which numerical analysis is of use is in computing and analysing objects that organise the long-term dynamics of the system. The objects might be equilibrium points, periodic trajectories, or more exotic objects like homoclinic orbits, and invariant tori. These structures often give a great deal of information about the structure of the dynamics. For example, homoclinic orbits are orbits that approach the same point both as time goes to \(+\infty\) and as time goes backward to \(-\infty\). Usually these give rise to complicated dynamics (chaos), a fact which was first discovered by Henri Poincaré (1892). Invariant tori often arise in Hamiltonian dynamics. These are tori for which trajectories that start on any torus remain on that torus for all time. Knowledge of the behaviour of the trajectories on the torus can be used to analyse the stability or otherwise of the dynamical system.

Bifurcations [7.1] can also be analysed numerically, and branches of solutions can be followed using continuation methods [7.3]. These are mathematical techniques for tracking, as a parameter is varied, objects such as equilibrium points or periodic orbits from simple cases where the solutions are easy to find to highly nonlinear cases where solutions would otherwise be very difficult to locate. Continuation methods can also be used for calculating homoclinic and heteroclinic orbits [7.4].

Numerical analysis can also be used for computing quantities of interest in the study of dynamical systems. These include the dimensions of fractal attractors [4.2], Lyapunov exponents [6] and the entropy (which gives information on the rate at which the system loses information about where it started — see [6]).

A book which covers many questions about numerical algorithms for nonlinear dynamics and chaos is Parker & Chua (1989). It should be remembered that there is great deal that can be said about, or used to study, dynamical systems and related computations. So there are many topics that go well beyond this chapter, or beyond any one textbook for that matter. The bibliography should provide you with at least a start in discovering the many questions and (incomplete) answers there are about chaotic dynamics.

2. Dynamical systems

Dynamical systems deal with the evolution of sets of dynamical variables, which can be any quantities whatever needed to describe the system of interest. For example, in physics they may be the positions and velocities of a set of particles, whereas in zoology they may be the populations of the various species in an ecosystem. To unify the description of such diverse systems we adopt a somewhat abstract, mathematical approach and form the variables into a vector of arbitrary length, called the state vector.

Before we start our journey with dynamical systems we need some notation and jargon to describe the path we take and the views we see. To start with, the two types of dynamical systems we deal with are continuous time systems described by differential
equations, and discrete time systems described by difference equations or iterations of maps. An autonomous continuous time system describing the state vector $x = x(t)$ evolving under the influence of the vector field $f(x)$ is described by an ordinary differential equation (ODE)

$$\dot{x} \equiv \frac{dx}{dt} = f(x)$$

and a discrete time system describing the iterates $x = x_i$ (integer $i$ being the “time”) under a mapping $g$ is described by

$$x_{i+1} = g(x_i),$$

where in both cases $x$ moves in an $n$-dimensional phase space, $X$ [which can be the space $\mathbb{R}^n$ (see Glossary), or, more generally, an $n$-dimensional differentiable manifold (Arrowsmith & Place, 1990)].

A driven, non-autonomous system is defined in the same way, but with $f$ a function of $t$. Such a system can always be made autonomous by introducing a new dependent variable $\tau$, say, such that $\dot{\tau} = 1$, with $\tau = 0$ at $t = 0$, thus increasing the dimension of the state space by one. Since the restriction to autonomous systems therefore entails no loss of generality, the formal theory of dynamical systems is usually developed under this restriction and we shall do likewise unless otherwise specified.

Continuous time systems define flows, which are functions

$$\varphi : X \times \mathbb{R} \to X,$$

evolving initial positions $x_0$ to their values at time $t$: $\varphi(x_0, t) = x(t)$, with $\dot{x} = f(x)$ and $x(0) = x_0$. These flows have the following properties (assuming, as usual, the system to be autonomous): for all $x \in X$ and $t, s \in \mathbb{R}$,

$$\varphi(x, 0) = x,$$

$$\varphi(\varphi(x, t), s) = \varphi(x, t + s).$$

In some systems such as PDEs we might have to restrict the time argument of the flow to be non-negative (see §2.8). Such a restriction gives rise to semiflows; these have the above properties except that we restrict $t, s$ to be $\geq 0$.

In the discrete time case, if $g$ is smooth and has an inverse function which is also smooth, then $g$ is, by definition, a diffeomorphism if it is not a diffeomorphism (or we don’t know if it is or not), we use the more general term map. The function $\varphi(\cdot, t)$ for an ODE is always a diffeomorphism (but not for a PDE when $\varphi$ is a semi-flow).

Studying flows, rather than the differential equations which generate them, unifies the continuous time and discrete time cases. Indeed we can discover a discrete-time dynamical system in a continuous-time one by “stroking” it periodically: simply take $g(x) = \varphi(x, T)$, where $T$ is the sampling period. This is particularly natural in the case of a non-autonomous system with $T$-periodic time dependence. As argued above, an $n$-dimensional non-autonomous system is equivalent to an $(n + 1)$-dimensional autonomous one, and we have just shown that it generates an $n$-dimensional discrete time system.

This illustrates the close connection between $n$-dimensional discrete time systems and $(n + 1)$-dimensional autonomous continuous time systems.

For notational convenience, we will use the same symbol $\varphi$ for iterated diffeomorphisms and iterated maps, but will use integers (respectively, non-negative integers) as the “time” argument:

$$\varphi(x, i+1) = \varphi(\varphi(x, i), i), i \text{ integer}.$$  

Although we are concerned with nonlinear systems, the truth is that most of the arsenal of mathematics only works against linear systems. Thus the best strategy is almost always to build up a knowledge of the nonlinear system by finding related linear systems to study. This means that we shall often be linearising the dynamical system.
about an orbit, say \( y(t) \), which is assumed known (e.g., it may be an equilibrium, or fixed point, \( y = \text{const} \)). If \( \xi \) is a perturbation away from the known orbit, i.e., if \( x = y + \xi \), then to linear order \( \xi \) obeys the equation found by Taylor expansion about \( y \\
abla f(y) \xi \\
or
\\xi_{n+1} = \nabla f(y) \xi_n,
\\end{align*}
where we use the notation \( \nabla f(x) \) for the Jacobian matrix whose element in the \( i \)th row and \( j \)th column is \( \partial f_i / \partial x_j \); \( i \) and \( j \) being indices indicating the components of the vectors \( f \) and \( x \), respectively.

In the remainder of this section we give representative examples of the various types of dynamical systems.

2.1. A one-dimensional map

Perhaps the best-known map is the “discrete logistic map” on the unit interval \([0, 1]\).

This is given by \( x_{n+1} = \lambda x_n (1 - x_n) \) where \( 0 \leq \lambda \leq 4 \). The behaviour of this map for various values of \( \lambda \) runs the range from having a single stable fixed point (\( x = 0 \) for \( 0 \leq \lambda \leq 1 \)) through a number of bifurcations, and eventually becomes chaotic by a cascade of period doubling bifurcations. For \( \lambda > 1 \) there are two fixed points: \( x = 0 \), which is unstable, and \( x = 1 - 1/\lambda \), which is stable for \( 1 < \lambda \leq 3 \). The first period doubling bifurcation occurs at \( \lambda = 3 \). The fixed point at \( x = 1 - 1/\lambda \) becomes unstable. There follows a sequence of period doubling bifurcations which are progressively closer together. In fact if the \( k \)th period doubling bifurcation occurs at \( \lambda = \mu_k \), then \( (\mu_k - \mu_{k-1})/(\mu_{k+1} - \mu_k) \rightarrow 4.669201609 \cdots \) which is known as Feigenbaum’s constant (Feigenbaum, 1978).

There is an infinite number of period doubling bifurcations in the region \( \lambda < 3.569944 \cdots \). This sequence of period doubling bifurcations is called a period doubling cascade, and is typical of many dynamical systems. Immediately after the period doubling cascade is the onset of chaos (Devaney, 1989; Block & Coppel, 1982). This chaotic regime is interrupted by occasional windows where there is a stable periodic orbit. These periodic orbits also undergo a period doubling cascade to return to chaotic behaviour. Finally at \( \lambda = 4 \) the behaviour is chaotic and the attractor has expanded to fill the entire interval \([0, 1]\).

2.2. A one-dimensional diffeomorphism

Maps \( g : S^1 \rightarrow S^1 \) of the circle onto itself form an important area of study in dynamical systems theory because they form a prototype for the toroidal attractors and invariant surfaces occurring in higher dimensional systems. One of the most important properties of iterates of these maps is the average rate of rotation, or rotation number, \( \alpha = \rho(g) \), and one of the most important questions is “under what circumstances can a change of variable (conjugacy) be found such that the map becomes the rigid rotation \( f(\theta) = \theta + \alpha \)?”

A standard example, whose numerical implementation is easy, is the \( \Phi \) circle map (Arrowsmith & Place, 1990, p. 248)

\[
g(\theta) = \alpha + \theta + \epsilon \sin \theta.
\]

† Note that the order of the indices is reversed from what would be assumed in 3D tensor dyadic notation — in the above equations, \( \xi \) is contracted with the \( \nabla \) operator. Note also that the symbol \( \rho \) is often used instead of \( \nabla \).
For $|\epsilon| < 1$ this is a diffeomorphism, and chaotic behaviour does not occur in one-dimensional diffeomorphisms (all attractors are simple fixed points or periodic orbits). However, for $|\epsilon| > 1$ it is "just a map" because $\gamma$ no longer increases monotonically with $\theta$. This causes folding over of the image of a set and chaos can occur. The transition point $\epsilon = 1$ is often studied as an example of critical behaviour (Lichtenberg & Lieberman, 1992, p. 529), for which universal scaling constants can be found by renormalisation group methods (Delbourgo, 1992).

2.3. A dissipative two-dimensional diffeomorphism

The map $(x', y') = g(x, y)$:

\[ x' = y + 1 - ax^2, \]
\[ y' = bx \]

was introduced by Hénon (Hénon, 1976). Its Jacobian determinant is a constant, \( \text{det } g = -a \neq 0 \), so the map can be inverted uniquely and is hence a diffeomorphism. For $|\epsilon| < 1$ the Hénon map contracts each element of phase space, and can therefore be used to model a dissipative system. The case $a = 1.4$, $b = 0.3$ was shown by Hénon to give rise to a fractal attractor.

2.4. An area-preserving diffeomorphism

The return map taking a Poincaré section of the energy surface of a two-degree of freedom autonomous Hamiltonian system back to itself, or the stroboscopic period-map of a periodically forced one-degree of freedom Hamiltonian system ([2.7]) can be shown to preserve the area of an infinitesimal quadrilateral (Meiss, 1992). Since flows of finite-dimensional dynamical systems are always invertible, and smooth if the vector field is smooth, these area-preserving maps are in fact diffeomorphisms.

The most commonly studied area-preserving diffeomorphism is probably the Taylor-Chirikov or Standard Map $(x', y') = g(x, y)$, where

\[ x' = x + y \mod 1, \]
\[ y' = y - \frac{k}{2\pi}\sin 2\pi x. \]

The first equation has been written in an implicit form purely for compactness — $y'$ can be eliminated immediately in favour of $x$ and $y$ using the second equation. Conversely, the reader can easily verify that the inverse map can be written down explicitly, verifying that it is indeed a diffeomorphism. Area preservation can be demonstrated by showing that the Jacobian determinant, $\text{det } g$, is unity.

As defined above, the phase space is topologically cylindrical, with $x$ the angle around the cylinder (in units of $2\pi$ radians). There is also a periodicity in the $x$-direction and other symmetries (Dewar & Meiss, 1992; Roberts & Quispel, 1992). When the nonlinearity parameter $k$ is zero, the map is integrable — the phase space is composed entirely of invariant circles $y = \text{const}$ encircling the cylinder (i.e. "rotational" circles) and there is no chaos. As $k$ is increased from 0, it is found that the circles for which the rotation number $y$ was a rational fraction immediately evaporate into a complicated structure, known as an island chain, of periodic orbits surrounded by invariant, but not rotational, circles, chaotic regions, and island chains (forming an infinite hierarchy of islands within islands).

On the other hand, the celebrated Kolmogorov-Arnold-Moser (KAM) theorem predicts that, for sufficiently small $k$, most of the rotational invariant circles with irrational rotation numbers will sur-
vive, though deformed, as curves (still topologically rotational circles, or 1-ori) invariant under the map. These KAM curves act as barriers to chaotic diffusion in $y$, but the last of the original invariant circles are destroyed at $k = 0.971635400 \cdots$ (Greene, 1979). These circles have rotation numbers of $\gamma^{-1} = 0.38196 \cdots$ and $\gamma^{-1} = 1 - \gamma^{-1} = 0.61802 \cdots$, where $\gamma \equiv (\sqrt{5} - 1)/2$. The number $\gamma^{-1} \equiv (\sqrt{5} - 1)/2$, known as the "golden mean", is the number that is worst approximated by rationals, and thus gives rise to the KAM curves least affected by the resonances which lead to islands (Meiss, 1992).

In Fig. 1 we show the phase space of the Standard Map at the critical nonlinearity for globally connected chaos, $k = 0.971635400 \cdots$, illustrating the islands arising from the unperturbed circles with rotation numbers $0/1, 1/1, 1/2, 1/3, 2/3, 2/4$. Also shown are the two golden mean KAM curves mentioned above, constructed numerically by minimizing the "quadratic flux" functional of Dewar and Meiss (1992) using nine Fourier modes.

2.5. A two-dimensional continuous-time dynamical system

One of the most studied two-dimensional continuous-time dynamical systems is the van der Pol oscillator. This was based on an electronic vacuum tube circuit devised in the 1920s and analysed by van der Pol (1927). It is given by the 2nd order differential equation

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

This can be made into a two-dimensional system by setting $\epsilon \equiv \dot{x}$. The van der Pol equation then becomes the dynamical system

$$\dot{x} = \epsilon, \quad \dot{\epsilon} = -\epsilon(x^2 - 1)\dot{x} - x.$$
This is an example of an autonomous system with a limit cycle for $\epsilon \neq 0$. The only equilibrium point is the origin $(x, \epsilon) = (0, 0)$. For $\epsilon = 0$ the system reduces to simple harmonic motion, which has an infinite number of periodic orbits, each of which is a circle. For $\epsilon > 0$ a single periodic orbit exists (the limit cycle), which attracts trajectories; for $\epsilon < 0$ there is also a single periodic orbit, which repels trajectories.

Careful asymptotic analysis shows that for small $\epsilon$, the periodic orbit is nearly circular with a radius close to two. For large $\epsilon$ the periodic orbit looks much more distorted (Fig. 2).

2.6. An infinite-dimensional continuous-time dynamical system
We shall consider a simple linear PDE — the diffusion or heat equation with periodic boundary conditions,

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2},$$

where $T(x, t)$ is the temperature at time $t$ (in units such that the thermal conductivity is unity) and position $x$ (in units such that the periodicity length is $2\pi$). To see that this
is a dynamical system, expand $T$ in a Fourier basis

$$T = \sum_{m=-\infty}^{\infty} T_m(t) \exp im\theta$$

Then the infinite-dimensional vector $T$, whose elements are $T_m$ is the state vector and the dynamical system is

$$\dot{T} = -\mathbf{diag}(\lambda_m) T,$$

where $\mathbf{diag}(\lambda_m)$ is the (infinite-dimensional) diagonal matrix with diagonal elements $\lambda_m$.

It is immediately seen that the flow map for this system is given by

$$\phi(t_1, t) = \mathbf{diag}(\exp(-m^2 t_1)) T_1, \quad t \geq 0.$$

Note that the time-reversed heat equation is extremely unstable, and will give infinite temperatures in finite time $t_0$ unless its Fourier coefficients decay faster than $\exp(-m^2 t_0)$ for large $|m|$. This is a very strong restriction on allowable initial conditions, even for arbitrarily small but non-zero $t_0$. Since we do not wish to confine ourselves to such restricted function spaces, $\phi(\cdot, t)$ is defined only for positive $t$ — it is a semiflow.

2.7. One- and $1\frac{1}{2}$-degree of freedom Hamiltonian systems

A 1-degree of freedom mechanical system has only one position coordinate, $q$ say. However the phase space is two-dimensional because, in order to make the equation of motion a first order ODE system we introduce a second dynamical variable, the conjugate momentum, $p$ say, which is defined so that the system of equations (for a non-dissipative system) has the form

$$\dot{q} = \frac{\partial H}{\partial p},$$

$$\dot{p} = -\frac{\partial H}{\partial q},$$

where $H(q, p, t)$ is the Hamiltonian. Normally $H$ is assumed independent of $t$, in which case it is a constant of the motion and no chaos can occur.

To indicate a non-autonomous system, the terminology $1\frac{1}{2}$-degree of freedom system is sometimes used, particularly when the time dependence is periodic. By destroying the constancy of $H$, the time dependence allows chaos to occur. Indeed the stroboscopic map given by the flow during one period is an area-preserving diffeomorphism, as discussed in §2.4.

The physical pendulum Hamiltonian

$$H = \frac{p^2}{2} - \omega^2 \cos \theta,$$

(where $\omega^2 / 2\pi$ is the frequency of small vibrations) is the prototype for developing a qualitative understanding of weakly nonlinear Hamiltonian systems (Lichtenberg & Lieberman, 1992, p. 29).

2.8. $N$-body Hamiltonian systems

The $n$-degree of freedom Hamiltonian dynamical system has exactly the form given above for the 1-degree of freedom system, except that $q$ and $p$ are now $n$-vectors and the phase space is of dimension $2n$. Chaos can occur for $n \geq 1\frac{1}{2}$. In $D$ spatial dimensions an $N$-body system has $n = ND$ degrees of freedom and a phase space of dimension $2ND$. 
The Fermi-Pasta-Ulam experiment (Fermi et al., 1955) was an early attempt at studying an N-body Hamiltonian system computationally. This experiment attempted to simulate the approach to statistical equilibrium of a closed Hamiltonian system — a lattice of coupled oscillators.

To study self-organization in complex systems, on the other hand, we need to simulate a non-equilibrium statistical mechanical problem, one in which the system is being driven by the input of low-entropy energy. Furthermore, to achieve a statistical steady state we need a mechanism for removing an equal amount of energy to that input (and a greater amount of entropy). An ingenious device has been developed for molecular dynamics simulations to achieve this removal in a distributed fashion, rather than at the boundaries of the computational domain (Evans & Morris, 1990). This avoids “wasting” large amounts of computation on boundary layer phenomena, at the expense of a certain artificiality in the dynamical system. For example, to simulate a shear flow with a mean velocity \( \mathbf{u} = \gamma \mathbf{e}_x \), where \( \mathbf{e}_x \) is the unit vector in the \( x \)-direction, the dynamical system

\[
\begin{align*}
\dot{\mathbf{q}}_i &= \frac{\mathbf{p}_i}{m} + \gamma \mathbf{e}_x \cdot \mathbf{q}_i \\
\dot{\mathbf{p}}_i &= \mathbf{F}_i - \gamma \mathbf{e}_x \cdot \mathbf{p}_i - \alpha \mathbf{p}_i
\end{align*}
\]

(Evans et al., 1990) has been used; where \( \mathbf{q}_i \) is the position of the \( i \)th particle, \( \mathbf{u} = \mathbf{p}_i / m \) is its velocity and \( \mathbf{F}_i \) is the sum of the forces from the other particles. The last term, \( -\alpha \mathbf{p}_i \), is the thermostatting term, required to remove the heat generated by the force maintaining the shear flow. It is this term which causes the phase space volume to contract and gives rise to the strange attractor referred to in [1.3 (Hoover, 1992)].

3. Forward vs. backward error

One idea that is very important in numerical analysis is that of backward error analysis. The other kind of error analysis is a forward error analysis. The forward error of a calculation is the difference between what is computed and what would have been computed had there been no error. On the other hand, the backward error is the size in the perturbation in the data of a problem that would have given the computed result had the computations been done exactly.

To obtain estimates or bounds on the errors that are produced in the results of a computation, we need to combine backward error analysis with a perturbation theory for the problem under question. This can take the place of forward error analysis. And it is also often better than using forward error analysis. To illustrate this, suppose we consider solving a system of linear equations \( \mathbf{Ax} = \mathbf{b} \) using Gaussian elimination; we might factor \( \mathbf{A} = \mathbf{LU} \) and obtain large [forward] error bounds on the \( L \) and \( U \) factors, even though \( \| \mathbf{A} - \mathbf{LU} \| \) might be quite small. Unless a great deal of information is included about the structure of the errors, forward error analysis can give gross overestimates of the errors resulting from a computation.

All-in-all, backward error analysis is better than forward error analysis for most classes of computational problems. A related concept, that of shadowing, is discussed in §8.

Not all problems are amenable to backward analysis. There is a number of significant classes of problem for which backward error analyses cannot be done. Often this is associated with a qualitative difference in the behaviour of the computational (perturbed) system and the original system.

Since computations with floating point numbers on computers almost always incur errors due to finite machine precision, lack of backward stability in the mathematical formulation of a problem indicates that simulations cannot be expected to give reasonable
results for that model. On the other hand, in the real world, the differential equations themselves are just approximations, and there is also a great deal of "noise" and other errors. If these unmodelled phenomena can invalidate the model, then the model is inappropriate and should be replaced by one that is backward stable.

3.1. Forward & backward error and dynamical systems

Consider a dynamical system

\[ \dot{x} = f(x), \quad x(0) = x_1, \quad \text{or} \quad x_{n+1} = g(x_n). \]

Forward errors in dynamical systems correspond to the perturbations in the results due to small perturbations in the initial conditions and/or the differential or difference equation(s). Thus if the computed value is \( y(T) \) or \( y_0 \), then the forward error analysis relates \( \| x(T) - y(T) \| \) or \( \| x_n - y_n \| \) to \( \| x_1 - y_1 \| \) and the error per unit time or per iteration, \( \| \eta \| \), defined by

\[ \dot{\eta}(t) = f(\eta(t)) + \eta(t), \quad y_{n+1} = g(y_n) + \eta_n. \]

For stable systems the forward error remains small. For chaotic systems, the forward errors \( \| x_n - y_n \| \) in a trajectory grow exponentially fast. However, objects such as attractors have good backward error properties under certain conditions (such as attracting trajectories exponentially fast). Thus, even though individual trajectories may not be worthwhile objects to compute for chaotic systems, at least for large time intervals, the attractors that they generate are usually much more reliably computed.

For discrete time dynamical systems \( x_{n+1} = g(x_n) \), provided the function evaluation is done in a numerically stable way, the computed iterates \( y_n \) can easily be shown to satisfy

\[ y_{n+1} = g(y_n) + \eta_n, \]

where \( \eta_n \) is small, of the same order as machine epsilon or unit roundoff \( u \). This quantity describes the precision of the floating point arithmetic used by a particular computer or software system. It is usually defined as the smallest number \( u \) such that the computed value “1 + u” is different from 1. For single precision arithmetic this is usually around \( 10^{-7} \), and for double precision using IEEE arithmetic is around \( 10^{-15} \). This single precision usually has a precision of about 6 digits, while IEEE double precision arithmetic has a precision of about 15 digits. The exact value of \( u \) depends on the particular hardware and software used.

For ODEs the problem is a bit more complicated, as we need to use a time stepping scheme of some sort (e.g., Euler, implicit Euler, Runge-Kutta, or a multistep method). Even in exact arithmetic we have to approximate the solution of the ODE. The errors involved in doing a small step of the integration scheme are called local truncation errors. These errors are usually much larger than the roundoff errors; furthermore, they depend smoothly on the current iterate, unlike roundoff errors which can vary unpredictably.

It would be tempting to try to set up a backward error theory for autonomous ODEs assuming exact arithmetic. That is, to write a perturbation of \( f(\cdot, h) \) where \( h \) is the step size, as the flow generated by some perturbation of \( f \). Unfortunately this is not possible if we are looking for autonomous perturbations. Partial results can be found which put most of the errors into an autonomous perturbation of the ODEs, but we cannot put all of the errors into such a perturbation. A discussion of this is given in Sanz-Serna (1972).

However, if we allow non-autonomous perturbations, then we can get a proper backward error theory for ODEs.
4. Attractors and dimensions

If one simulates a dynamical system then usually the system will settle down to wandering around a fairly well-defined (if complicated) set. Such sets are attractors. The formal definition of the attractor of a dynamical system is that a set \( A \subset X \) is an attractor if

**Definition 1.**

- \( A \) is invariant; that is \( \varphi(A,t) = A \) for all \( t \).
- There is an open set \( V \) containing \( A \) such that for any open set \( U \) containing \( A \), there is a \( t_1 \) where \( t > t_1 \) implies \( \varphi(V,t) \subset U \).

Terminology: the union of all such \( V \) is called the basin of attraction of \( A \). The set \( A \) is a global attractor if its basin of attraction is the entire space. On the question of the existence of global attractors, we need only that trajectories be bounded, or approach some compact set, to verify their existence.

4.1. Approximation of attractors

We do not expect numerically computed trajectories to be good approximations to the actual trajectories (at least with the initial conditions that we started with). However, it is easier to believe that the attractors we see coming out of a simulation are close to “the real thing.” To study these questions more closely we need to have some machinery for understanding approximations of sets.

There are some standard metrics for sets, although different situations will require different metrics (just as different problems require different measures of distance). First there is a semi-norm: \( \delta(A,B) \), which gives how far \( A \) is from being a subset of \( B \). More formally,

\[
\delta(A, B) \equiv \sup_{a \in A} d(a, B) \equiv \sup_{a \in A} \inf_{b \in B} d(a, b)
\]

where \( d(x,y) \) is the ordinary distance between the points \( x \) and \( y \). (See the Glossary for \( \inf \) and \( \sup \).) Note:
- \( \delta(A, A) = 0 \),
- \( \delta(A, B) < +\infty \) if \( A \) is bounded & \( B \) nonempty
- if \( A \) and \( B \) are closed then \( \delta(A, B) = 0 \iff A \subseteq B \)
- \( \delta(A, B) = \inf_{\eta > 0} \{ A \subset B + \eta B^1 \} \)

where \( B^1 \) is the (open) unit ball in \( X \). We usually define \( \delta(A, B) = +\infty \) if either \( A \) or \( B \) is empty.

Associated with this is the Hausdorff metric given by

\[
d_H(A, B) = \max\{\delta(A, B), \delta(B, A)\}.
\]

Set valued functions \( A(\alpha) \) are said to be **upper semi-continuous** if

\[
\lim_{\alpha \to \beta} \delta(A(\alpha), A(\beta)) = 0;
\]

**lower semi-continuous** if

\[
\lim_{\alpha \to \beta} \delta(A(\beta), A(\alpha)) = 0;
\]

and **continuous** if

\[
\lim_{\alpha \to \beta} d_H(A(\alpha), A(\beta)) = 0.
\]

While we would like to get continuity of the attractors with respect to perturbations, the best that can be done in general is only upper semi-continuity: Let \( \varphi \) be the exact flow, and \( \varphi_h \) a perturbation to it for small \( h \).
Theorem 1. Suppose that $A$ is the global attractor of a dynamical system and that we have a numerical process with attractor $A_h$ where $\|\varphi(x, 1) - \varphi_h(x, 1)\| \to 0$ as $h \downarrow 0$ and the $A_h$ lie in a common compact set. Then $\delta(A_h, A) \to 0$ as $h \downarrow 0$.

Furthermore, if $\|\varphi(x, 1) - \varphi_A(x, 1)\| = O(h^\rho)$ and $A$ attracts trajectories exponentially fast, then $\delta(A_h, A) = O(h^\rho)$.

A proof can be found in, for example, Kloeden and Lorenz (1986), or Hale, Lin and Raugel (1988). The basic idea of the proof is described below. Consider a region $U$ around $A$ which is attracted to $A$ under the unperturbed flow. Then for any region $A(\epsilon)$ containing all points within distance $\epsilon > 0$ of $A$, there is finite time $T$ (depending on $\epsilon$) after which all the points of $U$ have been mapped into $A(\epsilon)$ by the unperturbed flow.

Note that we choose $\epsilon$ small enough so that $A(2\epsilon) \subseteq U$. For $h$ sufficiently small the perturbed flow $\varphi_h(x, T)$ is within $\epsilon$ of the unperturbed flow $\varphi(x, T)$ for all $x$ in $U$, since the time $T$ is independent of $h$. So after time $T$ under the perturbed flow, the trajectories starting in $U$ lie within $A(3\epsilon) \subseteq U$, and the same argument can be applied to show that for any $x$ in $U$, $\varphi_h(x, 2T)$ is in $A(4\epsilon)$, and by induction, so is $\varphi_h(x, kT)$ for $k = 1, 2, 3, \ldots$.

To get the $O(h^\rho)$ estimate of the error, choose $T$ to be large enough that points in a neighbourhood have the distance to the exact attractor halved. Then the same argument goes through, but this time it also gives an estimate of the value of $\epsilon$. Full continuity results can be proven if we assume much stronger conditions. Raugel and Hale (1989) have proven lower semi-continuity as well for gradient systems.

One thing should be pointed out: it is rather unfair to expect that a single trajectory should flush out the entire global attractor. Of course, if an attractor has several disconnected parts and does not map points in one component into the other, then a single orbit can only give information about one component of the global attractor.

Sometimes though, numerical orbits fail badly to give sensitive information about attractors. One simple example, which gives a warning to us all, is the tent map (Fig. 3)

$$g(x) = \begin{cases} \alpha x & 0 \leq x < 1/2 \\ \alpha(1-x) & 1/2 \leq x < 1 \end{cases}$$

It can be proven quite easily that for $2 \geq \alpha > 1$, this has chaotic orbits and that for $\alpha = 2$ the attractor of the map is the whole interval $[0, 1]$. But if $\alpha = 2$, on a computer the trajectories will quickly end up at zero. (You can try this yourself, to see that it
happens.) But zero is not even an attracting fixed point. Why? The answer is that if you consider what is happening from the point of view of the machine’s arithmetic, every iteration effectively shifts the bits of the mantissa left. [The operation of forming \((1 - x)\) can be thought of basically as inverting the bits of the mantissa.] When all bits have been shifted off, the result is zero.

By the way, one of the easiest ways to show that this map with \(\alpha = 2\) is chaotic is precisely in terms of bit shifting ([Devaney, 1989, pp. 48–52]).

4.2. Fractals and approximating dimensions

Assuming that we have a decent approximation for the attractor we will often find that it is a rather complicated self-similar object. Such objects are often referred to as fractals; this name was invented by Benoît Mandelbrot because the sets have fractional (Hausdorff) dimension.

The notion of the Hausdorff dimension of a fractal is discussed in detail in sections 3A and 4.6 of J. Hutchinson’s article “Deterministic and random fractals” in this book. It should be noted that the Hausdorff dimension is associated with a \(d\)-dimensional volume measure \(\mathcal{H}^d(E)\) of a set \(E\), as described in Hutchinson’s article.

This is one of a number of definitions of dimension that are used in dynamical systems theory. From a theoretical perspective the Hausdorff dimension is very useful as it is based on a true measure. However, nobody knows how to calculate this from data obtained from a simulation, so it (so far) does not have much practical significance.

A related version of dimension is called the fractal dimension or the capacity dimension of a set \(A\), denoted \(\dim_f A\). Instead of taking the sum of \((\text{diam } U_i)^d\) we impose the condition that \(\text{diam } U_i \leq \epsilon\) and replace the sum by \(N(\epsilon)^d\) where \(N(\epsilon)\) is the (minimum) number of sets in the covering. The procedure for defining the “dimension” apply. However, the resulting “measure” is not a true measure — it fails to have countable additivity (see Hutchinson’s article “Deterministic and random fractals”, [4, 1]).

A simpler formula can be used than the above:

\[
\dim_f A = \limsup_{\epsilon \to 0} \frac{\log N(\epsilon)}{\log(1/\epsilon)}
\]

For the meaning of \(\limsup\) see the Glossary.

Computational methods can be developed for estimating the fractal dimension; the commonest is the box-counting method.

The sort of data that is obtained from a simulation is a series of points \(x_1, x_2, x_3, \ldots \in \mathbb{R}^n\). These are assumed to belong to some known rectangular region \(\{ x \in \mathbb{R}^n | l_i \leq x_i \leq u_i \}\) where \(l_i\) and \(u_i\) are, respectively, lower and upper bounds. The rectangular region is subdivided into 2\(^n\) boxes (halving each dimension — see Fig. 4). The boxes are marked according to whether or not one of the points \(x_k\) belongs to the box.

This subdivision can be done recursively, giving a hierarchy of sets of marked boxes. The boxes cover the set \(\{ x_1, x_2, x_3, \ldots \}\) and as we go to finer and finer subdivisions of the original rectangle, we get better approximations to the actual set.

More formally, if \(A_k\) is the union of marked boxes after \(k\) subdivisions, then

\[
[x_1, x_2, x_3, \ldots] = A = \bigcap_{k \geq 1} A_k
\]

If we set \(N_k\) to be the number of marked boxes on the level of \(A_k\), then

\[
\dim_f A = \limsup_{k \to \infty} \frac{\log N_k}{k \log 2}
\]

While this limit can be estimated directly by looking at the ratio for large \(k\) (that is,
at fine subdivisions), it is better in practice to fit a line of the form \( \log N_k = a + b \log k \) and to get estimates of \( a \) and \( b \). Care should be taken to limit the maximum value of \( k \) for such a fit depending on the amount of data. One heuristic that you might use, is that at the finest sub-division there should be an average of several points (say \( > 2 \)) per box. With this maximum value of \( k \), you should pick a minimum value of \( k \) over which the fit should be done. This is a compromise between taking \( k_{\text{min}} \) close to \( k_{\text{max}} \) to get close to the limit, and choosing \( k_{\text{min}} \) small so as to kill some of the noise by fitting over a number of points. You could, for example, take \( k_{\text{max}} = k_{\text{max}}/2 \). More sophisticated analysis of the effects of finite amounts of data, and how to deal with it, can be found in (Hunt, 1990).

4.3. Other estimates of dimension & their relationships

Before we consider other “dimensions”, we should first note a basic relationship between the Hausdorff dimension and the fractal dimension. In the former, the basic formula are the same except that the infimum is taken over all covers of the set \( A \), while for the latter, the infimum is taken over all covers with diameter \( c \). Thus, for any \( A \),

\[
\dim_P A \geq \dim_H A.
\]

They can and do differ. One of the simpler examples where they differ is the set \( B_1 = \{0, 1, 1/2, 1/3, 1/4, \ldots \} \). (Note: this set is closed and can be generated in an obvious way.) In fact, \( \dim_P B_1 = 1/2 \), while \( \dim_H B_1 = 0 \). The latter follows from the fact that the set is countable. The former is an exercise for the reader!

There is a generalised class of such examples \( B_\alpha = \{0, 1, 1/2^\alpha, 1/3^\alpha, 1/4^\alpha, \ldots \} \) for \( \alpha > 0 \). \( B_\alpha \) has fractal dimension \( 1/(1+\alpha) \), but has Hausdorff dimension zero. On the other hand, convergent geometric sequences have both fractal and Hausdorff dimension zero.

These simple observations have implications for estimating the dimensions of attractors. It is common practice to chop off the leading part of the sequence of iterates of a chaotic dynamical system before using them to estimate dimensions. This is almost always appropriate, but if the rate of convergence to the attractor is slower than geometric or exponential, the fractal dimension may still be inflated above the true fractal dimension of the attractor.

As noted above there are a number of definitions of “dimension”, some of which have been invented by people coming to fractals and chaotic systems from different directions:

**Correlation dimension** Suppose that we have generated \( N \) points of an iteration \( x_1, x_2, x_3, \ldots, x_{N-1} \). For each point \( x_i \) count the number of points within a radius of \( \epsilon > 0 \) and call this \( N_i(\epsilon) \). The average ratio \( N_i(\epsilon)/N \), where \( N \) is large and fixed, should
behave like $e^d$ for some exponent $d$ — this $d$ is the correlation dimension. More formally,

$$\dim c = \limsup_{N \to \infty} \limsup_{\epsilon \to 0} \frac{\log(\sum_{i} N^{-1} \chi_{B_i}(c))}{\log \epsilon}$$

We have not written $\dim_{Haus} A$ because it is not really the dimension of a set so much as being the dimension of a probability measure. For a probability measure $\mu$, the ratio $N_i(\epsilon)/N$ corresponds to the probability of being within distance $\epsilon$ of $z_i$, $\mu(z_i + \epsilon B_i) (B_i$ is the unit ball). Thus we get

$$\dim_{Haus} \mu = \limsup_{\epsilon \to 0} \frac{\log \int \mu(z + \epsilon B) \, d\mu(z)}{\log \epsilon}$$

If the measure is the appropriate Hausdorff measure normalised onto the attractor, then the fractal dimension and the correlation dimensions are identical.

**Information dimension**

This is more like computing the fractal dimension by the box-counting method, except that this time we assign probabilities to each box. At each level instead of using $\log N_i$ we use $I_k = -\sum_i p_i \log p_i$ where $i$ is an index that ranges over all boxes on level $k$. Like the correlation dimension this is really a dimension for a probability measure. More formally, the dimension is given by

$$\dim_{Info} \mu = \limsup_{k \to \infty} \frac{I_k}{k \log 2}$$

Equivalent definitions can be given in terms of general (measurable) covers of the attractor.

If $\mu$ is a probability measure with bounded support $A \subset \mathbb{R}^n$ we have the inequalities

$$\dim_{Haus} A \leq \dim_{Info} \mu \leq \dim_{Haus} A$$

**Lyapunov dimension**

This “dimension” really belongs in a separate section as it is really a bound on the Hausdorff dimension of an attractor that is computed essentially from the dynamical system and one or more trajectories. More will be said on this in §6.

### 4.4. Amount of data

One of the difficulties that must be faced with any method for estimating dimensions is that of limited data. This is particularly important with box-counting and related methods. To get even a rough estimate of the dimension you should get at least hundreds, and usually thousands of points. In practice, for low dimensional attractors and sets, it is our experience that we can get errors of a few percent by using upwards of $\sim 10^4$ points.

For higher dimensional attractors (dimension $> -\frac{1}{2}$, say), the amount of data needed grows somewhat faster.

### 4.5. Time-series and embeddings

In recent times, seeing that many deterministic systems are chaotic, and appear to be random but are not, there has been a surge of interest in analysing data to see if we can determine whether or not it is (mostly) stochastic or (mostly) deterministic (but possibly chaotic). This leads to the world of “chaotic time-series”.

If one knew the full state vector then one could quickly determine if a system was stochastic or deterministic — wait until identical (or nearly identical) states re-occurred.
and look at the difference in the outputs. Deterministic systems will not look random over short time intervals, so randomness can easily be detected or ruled out.

Consider the situation where there is a stream of data coming from some "real world" process, such as a sunspot data, population data, weather (temperatures, rainfall) or the Dow Jones index of the New York Stock Exchange. The problem is to understand what kind of process has generated the data. In a situation like this, not only is the state vector of the process not measurable, we do not even know what dimension it is! Often more information taken at each sampling time will give much more information about the process. For example, other data from the sun might help understand the sunspot cycle, age structure is needed for accurate population prediction and analysis, pressures are useful as well as temperatures in analysing the weather, and a selection of "key stocks" may give greater insight to the behaviour of stockbrokers. This corresponds to taking a (short) vector of measurements at once. As always with data collection, collecting data can be expensive, as well as the cost of analysing it. A good understanding of the fundamentals of the system should help guide how much and what sort of data is collected. The problem is, given this data, to reconstruct the dynamics of the system, and to obtain further information about, for example, the fractal dimensions of attractors.

A thorough article on this topic is Embedology by Sauer, Yorke and Casdagli (1991). See also the review and reprint collection (Ott, et al., 1994). Previous work in this area was done by Takens (1981).

We start with a set \( A \subseteq \mathbb{R}^N \) (\( A \) and \( N \) are both unknown) which is bounded. We assume that there is a measurement function \( h: \mathbb{R}^N \rightarrow \mathbb{R}^m \). We also assume that \( A \) is an invariant set (such as an attractor) for a map \( g: \mathbb{R}^N \rightarrow \mathbb{R}^N \). Sometimes we might have a set (which does not come from a dynamical system) and we just wish to determine its dimension. In this case we just have a measurement function \( h \) but no map \( g \).

The following results are taken principally from Sauer et al. (1991), whose main results are generalisations of Whitney's embedding theorem (Guilleman & Pollack, 1974, §1.8). To state this we need to define what it means for a property or set to be generic. First, consider \( \mathbb{R}^m \) for any finite \( m \). On this space we have the Lebesgue measure \( \mu_{\mathbb{R}^m} \) which measures the volumes of sets. It is translation invariant and finite for bounded (measurable) sets. A set \( E \) is a null set if its Lebesgue measure \( \mu_{\mathbb{R}^m}(E) \), or \( m \)-dimensional volume, is zero. A property is said to hold almost everywhere if the set of exceptions is a null set.

These definitions are usually appropriate for finite dimensional spaces, but for function spaces we cannot define measures in an easy or natural way. While there are some more generally applicable approaches: one is to say that a set is generic if it is open and dense (i.e. its closure is the entire space). Some people define a set to be generic if it is the countable intersection of open dense sets. In \( \mathbb{R}^m \), the two concepts of a property being generic and holding almost everywhere are actually not comparable: neither implies the other. However, if a property is either generic or holds almost everywhere, there is at least something that satisfies the condition - and as close to any given point as you wish.

Sauer, Yorke and Casdagli (1991) define a generalisation of "almost everywhere" which they call prevalence. A set \( S \) in a vector space \( X \) is called prevalent if there is a finite dimensional subspace \( V \) where for every \( x \in X \) and almost every \( \epsilon \in V \) the point \( x + \epsilon \) lies in \( S \).

For sets \( X \) and \( Y \), an embedding is a smooth map \( f: X \rightarrow Y \) where \( f \) has a smooth inverse on the image \( f(X) \). The importance of this idea is that often a set can be embedded in a higher dimensional space in a way that preserves the "shape" of the set. For example, a circle can be embedded in three-dimensional space in a knotted way as
shown in Fig. 5. The main embedding theorem is due to Whitney, and it and related concepts are described in books on differential topology such as Guillemin and Pollack (1974). The Whitney theorem states that if the dimension of a smooth manifold $X$ is $k$, then a generic set of smooth maps $f: X \to \mathbb{R}^{k+1}$ embeds $X$ in $\mathbb{R}^{k+1}$. This means that for manifolds, provided the dimension of the manifold is strictly less than half of the space into which we wish to embed it, almost any smooth function will do.

This result was modified by Sauer et al. (1991) in terms of prevalence:

**Theorem 2.** If $A$ is a smooth manifold of dimension $d$, the set of smooth maps $h: A \to \mathbb{R}^m$ which are embeddings is prevalent if $m > 2d$.

To understand these embedding theorems, the following fact is crucial. If there are two hyperplanes in $\mathbb{R}^m$ where the first has dimension $k$ and the second has dimension $l$ where $k + l < m$, then almost always the hyperplanes will not touch. A simple example to consider is a pair of lines in three-dimensional space. If they do touch, then bringing one of the lines will almost always break the contact. Why is this? For a point to lie on the $k$ dimensional hyperplane is equivalent to that vector satisfying a collection of $m - k$ equations. Similarly for the $l$ dimensional hyperplane. For a point to lie on both hyperplanes requires satisfying $(m - k) + (m - l)$ equations with just $m$ unknowns (which are the co-ordinates of the point in $\mathbb{R}^m$). If $k + l < m$, then there are more equations than unknowns, and the system cannot be expected to be solvable in general.

For studying embeddings, the main problem is when the manifold intersects itself in the embedding space. Since the manifold is smooth, it can be approximated by hyperplanes near the point(s) of intersection, and these hyperplanes have the same dimension as the manifold, $k$. If $2k < m$, then almost any perturbation of the original function will separate the two parts of the same manifold, and the self-intersection will be eliminated—this is the essence of the Whitney embedding theorem.

Sauer et al. (1991) went on to prove a related result for the fractal dimension of a set. Note that an immersion is a smooth map on a manifold whose gradient is one to one on the tangent plane of that manifold.

**Theorem 3.** If $A$ is a bounded set with fractal dimension $d$, then the set of smooth maps $h: \mathbb{R}^N \to \mathbb{R}^m$ satisfying

(a) $h$ is one to one on $A$,
(b) $h$ is an immersion on any smooth manifold in $A$, is prevalent if $m > 2d$.

In practice, we often have just one measurement! (So $h: \mathbb{R}^N \to \mathbb{R}$.) In this case, we have to use a number of measurements to build up an idea of what the state was at the beginning of the series of measurements. However, if we take a long enough sequence we can recreate an diffeomorphic image of the fractal set $A$: 

![Figure 5. Knotted circle, which can be embedded in three-dimensional space but not in two-dimensional space.](image-url)
Theorem 4. Suppose that \( g \) is a diffeomorphism and that \( A \) is a compact set in \( \mathbb{R}^N \) with fractal dimension \( d \). Assume further that for every positive \( p \leq m \text{ dim} \{ x \mid g^p(x) = x \} < p/2 \) and that \( \nabla(g^p) \mid_x \) has distinct eigenvalues whenever \( g^p(x) \neq x \).

Then for a prevalent set of functions \( h : \mathbb{R}^N \to \mathbb{R} \) the map

\[
F_m(h, g)(x) = (h(x), h(g(x)), h(g^2(x)), \ldots, h(g^m(x)))
\]

is

(a) one to one on \( A \) and
(b) an immersion on every smooth manifold in \( A \).

Once a suitable embedding dimension has been found, parametric models of the local behaviour can be estimated to give a "model" dynamical system that represents the data (Abarbanel et al., 1993).

The standard technique for getting the fractal dimension of an attractor from time series \( y_0, y_1, y_2, \ldots \) is to construct short vectors containing \( m \) successive values of the \( y_k \). The value \( m \) is the embedding dimension that is used. These vectors are\( x_1 = [y_0, y_1, \ldots, y_m], x_2 = [y_1, y_2, \ldots, y_m], x_3 = [y_2, y_3, \ldots, y_m], \ldots \) etc. The vectors \( x_1, x_2, x_3, \ldots \in \mathbb{R}^m \) are then used as the input data for a fractal-dimension estimating algorithm.

The fractal dimension can then be estimated for \( m = 1, 2, 3, \ldots \). Since the fractal dimension of \( \{ x_1, x_2, x_3, \ldots \} \) is (usually) the minimum of \( m \) and the fractal dimension of the underlying attractor, if \( m \) is large enough, then the fractal dimension of \( \{ x_1, x_2, x_3, \ldots \} \) is the fractal dimension of the attractor.

The main requirement for reconstructing the dynamics of a system is that the embedding dimension must be greater than twice the fractal dimension of the attractor(s) of the system. What should the embedding dimension be if we do not wish to reconstruct the dynamics, but just to estimate the fractal dimension of the attractor? The general conclusion is that it is only necessary to have the embedding dimension \( \geq \) the dimension of the attractor(s). However, there are some questions regarding the mathematical validity of this answer.

To preserve the Hausdorff dimension it has been proven that the embedding dimension \( m \) just needs to be \( \geq \) the Hausdorff dimension of the attractor (Sauer & Yorke, 1991). However, the corresponding result for the fractal dimensions is not true (Sauer & Yorke, 1991). This is not entirely satisfactory, even though for most practical situations the Hausdorff and fractal dimensions are the same.

As with all dimension estimation techniques for fractals, care must be taken with offsetting the resolution (the \( \epsilon \) used in the estimates) with the amount of data available, and the embedding dimension \( m \). Asymptotically you need \( O(\epsilon^{-d}) \) data points where \( d \) is the fractal dimension — and more data is better than less. Also, as the embedding dimension increases, the amount of data also needs to increase, although perhaps not as quickly. To get reasonable estimates, \( 10^4 \) to \( 10^5 \) data points would be needed; but more would not be unwelcome, especially if you wish to have confidence in the results.

To illustrate these points, Fig. 6 shows some plots of box counts against \( \text{log}_2(1/\epsilon) \) from a box-counting algorithm for data obtained from the Henon map. Standard parameter values were used: \( a = 1.4 \) and \( b = 0.3 \). The fractal dimension of the attractor of the Henon map is estimated to be \( \approx 1.25 \) from the same box-counting approach, using \( 10^5 \) points.

For these graphs, the first coordinate was used as the "measured" quantity from which to estimate fractal dimensions. The main point of these graphs is the amount of data needed to obtain reliable results, and the effect of the embedding dimension. Each graph
shows a plot of the logarithm of the box count against the logarithm of the resolution used in the box counting for $N$ data points. The fractal dimension is estimated by the slope of the linear part of the curves. The different curves in each graph correspond to different embedding dimensions. The lowest curve is for $m = 1$; the curve above that is the curve for $m = 2$; the curve above that is for $m = 3$, and so on.

For a large amount of data (see the $N = 100 000$ graph), the linear part is quite clear, and good estimates can be obtained for the fractal dimension. Note that the slope of the curve for $m = 1$ is exactly one; an embedding dimension of one is clearly too small.

For the graph with $N = 10 000$ data points it can be seen that for $m = 3$ and $m = 4$ the slopes are starting to drop off at the finer resolutions. The curve for $m = 2$ would give the best estimate of the fractal dimension. These effects are even more pronounced in the graph for $N = 1000$ data points. With only $N = 100$ data points it has become very difficult to identify a linear region in any of the curves, and is worse for larger values of $m$.

Clearly, the amount of data needs to be related to both the resolution used, and the embedding dimension. It should also be clear that a great deal of data is needed for obtaining truly reliable results for fractal dimensions.

The problems of limited data are more extensively discussed in several articles (Hunt, 1990; Ramsey & Yuan, 1990; Tong, 1992). Comments on the harder task of reconstructing the dynamics of a system from time series can be found in Cudaghi et al. (1991) and Kostelich (1992).
4.6. Random or chaotic?

One question that arises repeatedly is the question of whether apparently “noisy” systems are stochastic or are deterministic chaotic systems. Of course, a system could be a combination of the two with truly random noise driving a chaotic system. Trying to answer the question as to whether a system is chaotic from time series data is extremely challenging one in practice. For a truly random process and an infinite amount of data, the fractal dimension of the data embedded into $\mathbb{R}^m$ is $m$, as independent random vectors will slowly fill up all of the space. In principle this hypothesis can be tested by embedding and estimating the fractal dimensions. If the estimates of the fractal dimensions for different $m$ increase without bound as $m$ increases, then the system is stochastic, since for a chaotic system, the fractal dimensions of embeddings are bounded.

The practical limitation of this approach is that the amount of data needed to do this increases exponentially in $m$. An alternative approach has been involves trying to obtain stochastic systems with no chaotic component that mimic the statistical behaviour of the time series data. Such a stochastic system is called a surrogate (Theiler et al., 1992) (see Fig. 7).

One simple example of a surrogate system for a time series is obtained as follows. Take a Fourier transform of the time series data, and save the magnitudes of the Fourier components. The idea is that the frequency components of the original data are preserved if white noise is passed through a filter with a frequency response which is identical to the spectrum (or periodogram) of the original data. Such a statistical system is linear, and is clearly not chaotic. To obtain a sample output of such a linear system, for each frequency component independently choose random numbers $a$ and $\theta$ from a Gaussian distribution with mean zero and standard deviation 1. Multiply the corresponding component of the Fourier transform of the original data by $a + it$ ($i = \sqrt{-1}$), take the inverse Fourier transform of the result, and ignore the imaginary part of the result. This is the result of filtering white noise in a way that mimics the original data, but in a way that is in no way chaotic. If the test used to distinguish between chaotic and stochastic systems cannot distinguish the surrogate from the original in a statistical sense, then there is no reason to claim that the system is actually chaotic. This “surrogate test” is stronger than the “fractal dimensions test” on its own, and can help to identify problems in the latter test due to insufficient data.

5. Stable, unstable & centre subspaces & manifolds

Equilibrium points (also called fixed points) are of course very important for understanding a dynamical system, and help to organise its behaviour. Indeed, this is a
standard mathematical approach: find the equilibrium points; determine the behaviour near them, and use this information to explore the behaviour away from equilibrium. This is a fruitful approach whether the system is well-behaved or chaotic. Let us look at an equilibrium point $x^*$. For concreteness, consider the dynamical system

$$ \frac{dx}{dt} = f(x) \quad \text{or} \quad x_{n+1} = g(x_n), $$

with $x \in \mathbb{R}^m$, so that $f(x^*) = 0$ or $g(x^*) = x^*$. The first way to obtain information about the behaviour of the system near an equilibrium point is to consider the linearisation about $x^*$: Write $x = x^* + y$, where, to linear order,

$$ \dot{y} = \nabla f(x^*) y \quad \text{or} \quad y_{n+1} = \nabla g(x^*) y_n. $$

Determining whether the linear system is stable is a matter of looking at the eigenvalues of the matrix $\nabla f(x^*)$ or of $\nabla g(x^*)$. If $\lambda$ is an eigenvalue of $\nabla f(x^*)$ with an eigenvector $z$, then $\nabla f(x^*) z = \lambda z$. Then we can look for solutions of $\dot{y} = \nabla f(x^*) y$ of the form $y(t) = \psi(t) e^{\lambda t}$. Substituting this gives

$$ \dot{\psi}(t) = \lambda \psi(t) \quad \text{and hence} \quad \psi(t) = e^{\lambda t} \psi(0). $$

If the real part of $\lambda$ is negative, then $e^{\lambda t}$ goes to zero as $t \to -\infty$; if the real part of $\lambda$ is positive, then the size of $e^{\lambda t}$ goes to infinity as $t \to +\infty$. A sufficient condition for $x^*$ to be a stable equilibrium for $\dot{x} = f(x)$ is that all eigenvalues of $\nabla f(x^*)$ have negative real part. Furthermore, if any eigenvalue has positive real part, then the original nonlinear system is unstable at $x^*$.

A similar analysis can be made for the discrete time system $x_{n+1} = g(x_n)$ and its linearisation $y_{n+1} = \nabla g(x^*) y_n$. Suppose, instead that $z$ is an eigenvector of $\nabla g(x^*)$ with eigenvalue $\lambda$:

$$ \nabla g(x^*) z = \lambda z.$$

Then there are solutions of the linearised system with $y_n = \psi_n z$. The equation for the $\psi_n$ is then $\psi_{n+1} = \lambda \psi_n$, which has the solution $\psi_n = \lambda^n \psi_1$. This decays to zero if $|\lambda| < 1$, and grows (to infinity) if $|\lambda| > 1$. Thus the nonlinear discrete-time system is stable if all eigenvalues have magnitude less than one, and unstable if some eigenvalue has magnitude greater than one.

If eigenvalues lie on the stability boundary (Re $\lambda = 0$ — imaginary axis — for the ODE, or |$\lambda$| = 1 — unit circle — for the discrete-time case) then the analysis of the linearised system is not sufficient to determine the local behaviour of the system. In the alternative case, where no eigenvalue lies on the stability boundary, the local behaviour about $x^*$ can be determined from the linearised analysis. Such fixed points are called hyperbolic. These systems also exhibit the property of structural stability around $x^*$: that is, small changes to the dynamical system (i.e. perturbing $f$ or $g$) will not change the [topological] structure of the behaviour near $x^*$. Equilibrium points which are not hyperbolic are usually associated with bifurcations (see §7) where the local behaviour can change its structure with arbitrarily small perturbations.

From the nature of the linearised flow, it is clear that there are some directions in which the flow is attracted exponentially toward the equilibrium point and others in which it is repelled exponentially, so that the qualitative nature of the flow is as depicted in Fig. 8.

Associated with an equilibrium point $x^*$ are its stable and unstable sets which are

$$ W^s(x^*) = \{ x \mid \varphi(x, t) \to x^* \text{ as } t \to +\infty \} $$

and

$$ W^u(x^*) = \{ x \mid \varphi(x, t) \to x^* \text{ as } t \to -\infty \} $$
respectively. If \( x^* \) is a hyperbolic equilibrium point, then these turn out to be smooth manifolds — the stable and unstable manifolds, respectively.

The set of tangent vectors of a smooth manifold form a linear subspace known as the tangent plane or tangent space. This tangent plane at a point gives the best linear approximation of the manifold nearby to the point. The tangent spaces to \( W'(x^*) \) and \( W^n(x^*) \) are denoted \( V'(x^*) \) and \( V^n(x^*) \) respectively. [Alternatively, we may just use \( V' \) and \( V^n \) if \( x^* \) is understood.]

These subspaces are just the eigenspaces associated with the stable and unstable eigenvalues respectively. Clearly, \( V' + V^n = \mathbb{R}^n \) and \( V' \cap V^n = \{0\} \). In order to start computing representations of the stable and unstable manifolds we need to get the stable and unstable subspaces.

5.1. Computing the stable and unstable subspaces

One way to get \( V' \) and \( V^n \) is to compute the (generalised) eigenvectors for the stable and unstable eigenvalues. To begin with, there may not be as many eigenvectors as the dimension as the space you are working in. In this case the matrix cannot be put into diagonal form. Thus, finding all of the eigenvectors may not be sufficient to compute the right subspaces. In most courses on linear algebra, the Jordan canonical form is the standard way to get around this problem. Unfortunately, computing the Jordan canonical form is a numerically unstable process. The most direct indication of this is that the Jordan canonical form is not continuous in the matrix entries.

Consider \[
\begin{pmatrix}
1 & \epsilon \\
0 & 1
\end{pmatrix}
\]
This matrix is not diagonalisable for \( \epsilon \neq 0 \) and has a single Jordan block; but if \( \epsilon = 0 \) then the matrix is trivially diagonalisable. On the other hand
\[
\begin{pmatrix}
1 & 1 \\
0 & 1 + \epsilon
\end{pmatrix}
\]
is diagonalisable for all \( \epsilon \neq 0 \) but has a trivial Jordan block if \( \epsilon = 0 \).

The more stable way of computing eigenspaces is in terms of the Schur decomposition.
(Golub & Van Loan, 1989, §7.1.2). Given a matrix \( A \in \mathbb{C}^{n \times n} \) (where \( \mathbb{C} \) is the complex plane) there is a unitary matrix \( Q \) and an upper triangular matrix \( T \) such that

\[
\overline{Q}^T AQ = T,
\]

where \( \overline{\cdot} \) denotes complex conjugation and \( (\cdot)^T \) denotes the matrix transpose. The eigenvalues of \( A \) are the diagonal entries of \( T \). The eigenvalues can be put in any order using unitary similarity transformations by a Schur decomposition algorithm (Golub & Van Loan, 1989, §7.1.3).

This sorting technique can be used to separate out the eigenvalues. This gives one way of obtaining orthogonal bases for the subspaces:

\[
\begin{bmatrix}
T_{11} & T_{12} \\
0 & T_{22}
\end{bmatrix}
\begin{bmatrix}
\overline{Q}_1^T \\
0
\end{bmatrix} =
\begin{bmatrix}
T_{11} & T_{12} \\
0 & T_{22}
\end{bmatrix}
\begin{bmatrix}
\overline{Q}_1^T \\
0
\end{bmatrix}.
\]

Alternatively, we can give a linear change of coordinates that is well conditioned but splits the matrix:

\[
\begin{bmatrix}
I & X \\
I & I
\end{bmatrix}
\begin{bmatrix}
T_{11} & T_{12} \\
0 & T_{22}
\end{bmatrix}
\begin{bmatrix}
I & X \\
I & I
\end{bmatrix}^{-1} =
\begin{bmatrix}
T_{11} & T_{12} + T_{12}X - XT_{22} \\
0 & T_{22}
\end{bmatrix}.
\]

To obtain the change of coordinates we need to solve the Sylvester equation \( T_{12} = XT_{12} - T_{12}X \) so that the upper-right block on the RHS vanishes. Supposing we have already ordered the Schur decomposition so that the stable eigenvalues are in \( T_{11} \) and the unstable eigenvalues are in \( T_{22} \), then we can solve this system by the Bartels-Stewart method (Golub & Van Loan, 1989, pp. 386–389): Let \( T_{12} \) be \( q \times q \) and \( T_{22} \) be \( p \times p \). The \( q \)th column of \( X = [x_1, \ldots, x_q] \) can be computed by the equation

\[
(T_{12})_q = (T_{12})_q (I - T_{11})^{-1} x_q.
\]

Since \( (T_{12})_q \) is not an eigenvalue of \( T_{11} \), this is a well-conditioned system of equations to solve. Once \( x_q \) is computed, \( x_{q-1} \) can be computed in terms of the \((q-1)\)th column of \( T_{12} \) and \( x_{q-1} \) similarly the remainder of the columns of \( X \) can be computed.

If we write \( Q = [Q_1, Q_2] \) where \( Q_1 \) is \( n \times p \) and \( Q_2 \) is \( n \times q \), then the stable subspace in the original coordinates is span \((Q_1)\), and the unstable subspace is span \((Q_1 + Q_2)X\).

5.2. Equations for the stable manifold

Supposing that we have been able to split the linearisation of the system at the equilibrium point (and so compute bases for the stable and unstable subspaces), we can set up some equations for the stable and unstable manifolds. We will just look at the stable manifold; the unstable manifold is defined in similar fashion, but with time reversed. This works provided the dynamics can be reversed. For ODEs this is just a matter of reversing the signs of the derivatives with respect to time; for diffeomorphisms this requires inverting \( x_{n+1} = g(x_n) \) to \( x_n = g^{-1}(x_{n+1}) \). However in general this is not always possible, for example for maps where \( g^{-1} \) does not exist as a function, or for dissipative PDEs like the heat equation (§2.6) which give rise to semi-flows (§2). We will look at the ODE case here. The case for diffeomorphisms and maps is mostly taken care of by replacing integrals by sums, and exponentials by powers.

The ODEs can be put in the following form by an affine change of variables:

\[
\begin{bmatrix}
\dot{y} \\
\dot{z}
\end{bmatrix} =
\begin{bmatrix}
A & B \\
C & D
\end{bmatrix}
\begin{bmatrix}
y \\
z
\end{bmatrix} + \begin{bmatrix}
F(y, z) \\
G(y, z)
\end{bmatrix},
\]

where \( F(0, 0) = G(0, 0) = 0 \) and \( \nabla F(0, 0) = \nabla G(0, 0) = 0 \). For any \( \epsilon > 0 \) we can find a ball about the origin of radius \( \delta > 0 \) for some \( \delta \) where \( F \) and \( G \) are Lipschitz in this...
neighbourhood with Lipschitz constant \( \epsilon \). It is also assumed that \( F \) and \( G \) have a global Lipschitz constant \( K' \) to ensure that the ODEs are meaningful.

Since \( A \) contains the stable eigenvalues and \( B \) the unstable eigenvalues we have bounds of the form \( \|e^{At}\| \leq Ke^{-\alpha t} \) for \( t \geq 0 \) and \( \|e^{Bt}\| \leq Ke^{\alpha t} \) for \( t \leq 0 \) where \( \alpha > 0 \). The actual value of \( \alpha \) must be less than the smallest real part of an eigenvalue of \( B \), and \(-\alpha\) greater than the largest real part of an eigenvalue of \( A \).

Then we consider the integral equations for a given \( y_1 \)

\[
y(t; y_1) = e^{At} y_1 + \int_0^t e^{A(t-\tau)} F(y(t-\tau), z(t-\tau)) \, d\tau
\]

\[
z(t; y_1) = -\int_0^\infty e^{B(t-\tau)} G(y(\tau), z(\tau)) \, d\tau
\]

It is easy to check that a solution of this integral equation is also a solution to the above ODEs. Provided \( \|y_1\| \) is small enough, then a Picard type iteration (see below) will converge. This is because the operator of \( y^{(m)} \) and \( z^{(m)} \) is a contraction (i.e. the operation reduces distances by a guarantee ratio) for sufficiently small \( y^{(m)} \) and \( z^{(m)} \).

\[
y^{(m+1)}(t; y_1) = e^{At} y_1 + \int_0^t e^{A(t-\tau)} F(y^{(m)}(t-\tau), z^{(m)}(t-\tau)) \, d\tau
\]

\[
z^{(m+1)}(t; y_1) = -\int_0^\infty e^{B(t-\tau)} G(y^{(m)}(\tau), z^{(m)}(\tau)) \, d\tau
\]

For details, see Perko (1991, [2.7]) and Pailis & de Meelo (1982). The reason why this works is that the integrals are arranged so that the exponentials are both decaying.

The stable manifold is given locally in terms of solutions of this integral equation by the parameterisation \( (y_1(\cdot; y_1), z(\cdot; y_1)) \). Once the stable manifold has been locally defined, it can be extended to be a global manifold by solving the reversed time equations.

5.3. Stable and unstable manifolds for maps and diffeomorphisms

Corresponding results can be obtained for stable manifolds for maps and diffeomorphisms.

As with the ODE case we need to split the linearisation of the system by a linear change of coordinates:

\[
\begin{bmatrix}
y_{n+1} \\
z_{n+1}
\end{bmatrix} =
\begin{bmatrix}
A & B \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
y_n \\
z_n
\end{bmatrix} +
\begin{bmatrix}
F(y_n, z_n) \\
G(y_n, z_n)
\end{bmatrix}
\]

where \( F \) and \( G \) satisfy the same conditions as above. The matrix \( A \) contains the stable eigenvalues (with magnitudes less than one) and \( B \) the unstable eigenvalues (with magnitude greater than one). The equations for the stable and unstable manifolds are then given by solving the following equations for a given \( y_1 \):

\[
y_k = A^k y_1 + \sum_{k=1}^{n-1} A^k F(y_{n-k}, z_{n-k})
\]

\[
z_n = -\sum_{k=n+1}^{\infty} B^{n-k} G(y_k, z_k).
\]

We can use a Picard iteration for these equations:

\[
y^{(m+1)}_{n+1} = A^m y_n + \sum_{k=1}^{n-1} A^k F(y^{(m)}_{n-k}, z^{(m)}_{n-k})
\]
\[ z_{n+1}^{m+1} = - \sum_{k=0}^{m} y_{k} G(y_{k}, z_{n}^{m}) \cdot z_{n}^{m} \cdot \hat{z}_{k}^{m} \cdot z_{n}^{m}. \]

With zero initial conditions \( z_{0}^{m} = 0, \hat{z}_{k}^{m} = 0 \) we get convergent sequences \( y^{m} \to y \) and \( z^{m} \to z \) provided \( y \) is small enough. The stable manifold is given by \( z(y) = z_{1} \).

5.4 Stable and unstable manifolds for periodic orbits

Stable and unstable manifolds also exist for periodic orbits, in both the discrete time and continuous time cases, though there are some subtle differences between the two cases.

The discrete time case with diffeomorphisms is the easiest.

Consider a periodic orbit: \( x_{k+1} = g(x_{k}) \) for \( k = 0, \ldots, p - 1 \) and \( x_{1} = g(x_{p-1}) \). We can consider this as being equivalent to the equilibrium case with the diffeomorphism \( G = g^{p} \). The linearisation of this map at \( x_{1} \) is

\[ \nabla G(x_{1}) = \left( \nabla g(x_{p-1}) \nabla g(x_{p-2}) \ldots \nabla g(x_{1}) \right) \nabla g(x_{1})^{-1} = \nabla G(x_{1}) \]

since \( x_{1} = g(x_{p-1}) = x_{2} \), so \( \nabla G(x_{1}) \) and \( \nabla G(x_{2}) \) have the same eigenvalues.

There are computationally suitable algorithms due to Bojanetz, Van Dooren and Golub (1992), who compute the (real) Schur decomposition in factored form. Keeping everything in factored form permits a backward error analysis in terms of the matrix factors.

Each point in the periodic orbit has its own stable and unstable subspaces and manifolds. The subspaces are related through the Jacobian matrices:

\[ V^{\top}(x_{k+1}) = \nabla g(x_{k}) V^{\top}(x_{k}), \quad V^{\top}(x_{k+1}) = V^{\top}(x_{k}) \nabla g(x_{k}). \]

The manifolds are related through the map:

\[ W^{\top}(x_{k+1}) = g(W^{\top}(x_{k})), \quad W^{\top}(x_{k+1}) = g(W^{\top}(x_{k})). \]

The continuous time case is a bit more difficult, and we have to modify the meaning of ‘hyperbolic’ for periodic solution of autonomous ODEs. In this case we have \( \dot{x} = f(x) \) and \( x(0) = x(T) \) where \( T > 0 \) is the period of the orbit. However, the map \( x \mapsto f(x, T) \) is not hyperbolic at \( x(0) \). The reason is that \( \nabla f(x(0), T) \) has an eigenvalue 1 with the eigenvector \( f(x(0)) \). The way to prove the existence of stable and unstable manifolds is to set up a local Poincaré section at \( x(0) \) perpendicular to (or at least not tangential to) \( f(x(0)) \), provided only one simple eigenvalue of \( \nabla f(x(0), T) \) is on the unit circle.

Stable and unstable manifolds for the local Poincaré map at \( x(0) \) can then be set up, and then these manifolds can be transferred to all the other points in the periodic orbit by the maps \( x \mapsto f(x, t) \) for \( 0 < t < T \). As with the the discrete time case, \( \nabla f(x(t), T) \) does change with \( t \), but the eigenvalues do not change.
5.5. Hyperbolicity for attractors

So far stable and unstable manifolds and the concept of hyperbolicity have been defined for equilibria and periodic orbits. This can be generalised to general (fractal) invariant sets. The notion of an invariant set being hyperbolic is closely related to the idea of exponential dichotomies (Coppel, 1978), where a linear system can be split into parts, one of which is exponentially growing, and the other is exponentially decaying. Hyperbolicity of a dynamical system means that the linearisation about any trajectory has an exponential dichotomy whose constants are independent of the trajectory. Where a system has exponential dichotomies it turns out that two point boundary value problems are well conditioned, even if the corresponding initial value problems are not.

Another reference which ties together exponential dichotomies and related topics is Palmer (1988).

Hyperbolicity is important in many studies of dynamics. One example is Smale’s axiom A (Smale, 1980). Another is in shadowing, which we treat later.

The idea of hyperbolicity is that each point has a pair of subspaces of which one contains the exponentially growing modes, and the other contains the exponentially decaying modes. To use this, it is usual to consider the exponentially decaying modes forward in time, and the exponentially growing modes backwards in time. An invariant set $A$ of a discrete time dynamical system $g: \mathbb{R}^n \to \mathbb{R}^n$ is hyperbolic if for each $x \in A$ there is a splitting $\mathbb{R}^n = V^s(x) + V^u(x)$ and constants $K > 0$ and $\alpha < 1$ such that

- $V^s(x)$ and $V^u(x)$ are both continuous in $x$ in the sense that $dU(V^s(x) \cap B_1, V^u(y) \cap B_1) \to 0$ as $x \to y$ where $B_1$ is the usual unit ball.
- $\nabla g(x) V^s(x) = V^s(g(x))$ and $\nabla g(x) V^u(x) = V^u(g(x))$.
- If $P^s(x)$ and $P^u(x)$ are the projections onto $V^s(x)$ and $V^u(x)$ respectively, then

$$\|P^s(y^k(x))P^s(x)\| \leq K\alpha^k,$$

$$\|P^u(y^k(x))P^u(x)\| \leq K\alpha^k$$

for all $k \geq 0$.

The projections are completely specified with the additional condition that $P^s(x) + P^u(x) = I$ for all $x$. An analogous definition applies to autonomous continuous time systems, although it must be modified to take account of the (simple) eigenvalue of $\nabla x\varphi(x, t)$ of 1. This simple eigenvalue, at least for periodic trajectories, corresponds to the direction of motion for the ODE. The behaviour of most concern regarding continuous-time systems is the behaviour orthogonal to the direction of travel.

To illustrate the use of hyperbolicity, consider axiom A diffeomorphisms:

**Definition 2.** A diffeomorphism $g: \mathbb{R}^n \to \mathbb{R}^n$ satisfies axiom A if the non-wandering set:

$$\Omega = \{x \ | \text{for every open } U \text{ containing } x, g^k(U) \cap U \neq \emptyset \text{ for some } k \neq 0\}$$

is hyperbolic and is the closure of a set of periodic orbits.

[See Smale (1980, §1.1).] If an attractor $A$ is hyperbolic, is the closure of a set of periodic orbits, and has a dense orbit, then the flow on $A$ is structurally stable. It is usually thought that the attractors that appear in numerical simulations for, say, Lorenz’ equations, are structurally stable. Theorems such as this are sometimes used to explain why attractors obtained by simulations so often appear to be quite robust, not only to numerical errors, but also to quite large changes in parameters. Unfortunately, the theoretical situation is rather unsatisfactory. On the one hand the theoretical tools assume the existence of structures such as hyperbolicity. On the other hand, the existence
of these structures has been verified only for specialised cases. For “real” problems the situation remains unclear in spite of considerable numerical analysis and computational work.

5.6. Non-hyperbolic fixed points — centre manifolds

Although the case where the fixed point $z^*$ is hyperbolic is generic, the non-hyperbolic case is important because it occurs at bifurcations (see §7). Thus, consider the case in which one or more of the real parts of the eigenvalues of $\nabla f(z^*)$ is zero, or one or more of the eigenvalues of $\nabla g(z^*)$ is on the unit circle. Associated with these eigenvalues there is then a centre subspace $V^c(z^*)$, in addition to the stable and unstable subspaces $V^s(z^*)$ and $V^u(z^*)$. $V^c(z^*)$ is tangent to an invariant manifold, $W^c(z^*)$ (Carr, 1981; Guckenheimer & Holmes, 1983; Shub, 1987), at least locally, but this centre manifold is not unique — there is typically an infinity of centre manifolds of any given degree of differentiability which become exponentially close in the neighbourhood of $z^*$.

For example, consider the two-dimensional dynamical system

$$ (\dot{x}, \dot{y}) = (\pm x, y^2) \, , $$

which generates the flow $\varphi_t(x, y) = (x \exp(-t), \pm y/(1 - y t))$. There is a fixed point at the origin, where the eigenvalues of the Jacobian matrix are $-1$ and $0$.

The vector field $(-x, y^2)$ is plotted in Figure 9, as well as some typical trajectories. All the trajectories in the lower half-plane are tangential to the $x$-axis at the fixed point (the origin). These, taken together with the origin and the positive $y$-axis, all form centre manifolds — cf. Arrowsmith & Place (1990, p. 96).

Notice that the trajectories are all attracted exponentially to any of the centre manifolds (e.g. to the $y$-axis), so that the long-time asymptotic behaviour is one-dimensional, algebraic evolution on a centre manifold. This asymptotic collapse in the dimensionality of a dynamical system is the crucial defining feature of an inertial manifold (see §8). The non-uniqueness of the centre manifold is caused only by exponentially small terms in the long-time limit. In this sense the centre manifolds are asymptotically equivalent, and in applications one often talks of “the” centre manifold.

When there are both stable and unstable manifolds, one also defines two more invariant manifolds, (Shub, 1987) the centre stable and centre unstable manifolds, tangent respectively to $V^s(z^*) \oplus V^u(z^*)$ and $V^u(z^*) \oplus V^s(z^*)$. The centre manifold is then the intersection of these. In applications one is primarily concerned however with stable fixed points.

The question of stability of a non-hyperbolic fixed point is much subtler than in the hyperbolic case since it is no longer sufficient for stability that $V^s(z^*) = \emptyset$. However [[Carr, 1981], Theorem 2(a)] in this case stability can be completely determined by restricting consideration to dynamics on one of the centre manifolds. This can be a very important simplification since the centre manifold may be of much lower dimension than the original dynamical system (which may even be infinite-dimensional).

In these delicate cases it is necessary to have a definition of stability that is not based on exponential divergence or contraction. Instead we use stability in the sense of Lyapunov:

Definition 3. A fixed point, $z^*$, of a flow $\varphi_t$ is said to be stable if for every neighbourhood $N$ of $z^*$, there is a neighbourhood $N^* \subseteq N$ of $z^*$ such that, if $z \in N^*$, then $\varphi_t(z) \in N$ for all $t > 0$.

Typically a stable fixed point $z^*$ has a stable manifold on which exponential attraction toward $z^*$ occurs, but Lyapunov stability does not imply that most orbits are attracted toward $z^*$, merely that they are not repelled from $z^*$. However any solution of a sta-
The dynamical system (started sufficiently close to \( x^* \)) is attracted toward the centre manifold, i.e. it approaches some solution on the chosen centre manifold with an error decaying exponentially as time increases (Carr, 1981). Thus, apart from losing initial transients, we can understand the general dynamics completely by restricting attention to motion on the centre manifold. Note that the motion on the centre manifold can in principle be arbitrarily complicated. The centre manifold is a particular case of an inertial manifold (see §8), appropriate to parameter ranges close to bifurcation points.

Applications of centre-manifold theory to spatio-temporal chaos can be found in Eckmann and Procaccia (1991) and Roberts (1992). Both papers discuss model equations for convection in which several convective rolls with close wavevector can be simultaneously linearly unstable, and interact nonlinearly, so that interference can produce “defects” which move chaotically. The former assumes a small aspect ratio (convection in a channel of finite width) while the latter assumes an aspect ratio of order unity. In this case the dimension of the centre manifold tends to infinity as the size of the box tends to infinity; Roberts (1992) argues that a simplified PDE can be derived whose centre manifold is the same as that of the original system and which approximates the dynamics more accurately than previous attempts. This is supported by numerical calculation in a box of finite size using a spectral method (projection of the PDE onto a finite Fourier basis).

6. Lyapunov exponents

Lyapunov exponents (Temam, 1988) describe the long term exponential rates at which the dynamical system stretches and squeezes sets. They provide considerable information about the behaviour of the system and can be used to estimate, amongst other things, the Hausdorff dimension of the attractor, the entropy rate, and estimates of the prediction...
horizon. In fact, one definition of chaos is simply that there is a positive Lyapunov exponent (and bounded trajectories).

The paper by Eckmann and Ruelle (1985) gives considerable information about Lyapunov exponents, including some information about how to estimate them. See also Ruelle (1989, Ch. 9).

To define the Lyapunov exponent for a trajectory with initial state \( x_i \), consider the Jacobian matrix \( \Phi(t) = \nabla_x \phi(x_i, t) \). The \( i \)th Lyapunov exponent is given by

\[
\lambda_i = \limsup_{t \to \infty} \frac{\log \| \Phi(t) \|}{t}.
\]

where \( \sigma_i(A) \) is the \( i \)th largest singular value of the matrix \( A \) (for \( \lim \sup \) see the Glossary). The singular values are just the square roots of the eigenvalues of \( A^T A \). (The matrix \( A^T A \) is positive semi-definite so the square roots of its eigenvalues are real and non-negative, and thus make sense.)

Dynamical systems where the above \( \limsup \) can be replaced with just \( \lim \) are called normal. It is believed that most dynamical systems are normal on the basis of numerical simulations.

If we consider a small sphere about \( x_i \), then its image at time \( t \) is (very nearly) a small ellipse. The singular values are the ratios of the semi-major axes of this ellipse to the radius of the initial sphere. Thus the Lyapunov exponents measure the (exponential) rates of stretching and squeezing.

A bound on the Hausdorff dimension of an invariant set \( A \) generated by a trajectory can be found in terms of the Lyapunov exponents \( \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n \). Let \( j \) be the largest index where \( \lambda_1 + \lambda_2 + \ldots + \lambda_j > 0 \). (We take \( \lambda_{n+1} = -\infty \) to ensure that there is such a \( j \).) Then the Hausdorff dimension of \( A \) is bounded by

\[
\dim_H A \leq j + \frac{\lambda_1 + \lambda_2 + \ldots + \lambda_j}{|\lambda_{j+1}|}.
\]

The quantity on the right is sometimes referred to as the Lyapunov dimension of \( A \).

Lyapunov exponents can also be used to estimate the entropy rate, or Kolmogorov-Sinai entropy (Lichtenberg & Lieberman, 1992, p. 304) of a dynamical system. This rate is the rate at which information about the initial conditions is lost. If we have a dynamical system with bounded trajectories we can imagine carving up the state space into cubes (say) of size \( \epsilon > 0 \). Any trajectory of a map can be followed to within a tolerance of \( \epsilon \) by noting the sequence of cubes that the trajectory touches. The set of all such sequences of boxes of given length \( N \) is clearly finite, and a particular sequence can be described by a string of bits of length \( b(\epsilon, N) \). The limit \( \lim_{N \to \infty} b(\epsilon, N)/N \) is the average number of bits needed to specify a particular trajectory within a tolerance of \( \epsilon \).

The entropy rate of the map is

\[
\rho = \limsup_{N \to \infty} \frac{b(\epsilon, N)}{N \log \epsilon}.
\]

Lyapunov exponents give a way of estimating the entropy. An upper bound for the entropy is given by \( (\lambda_1 + \ldots + \lambda_j)/\log 2 \) where \( j \) is the largest index of a positive Lyapunov exponent.

There are some instances where Lyapunov exponents can be computed very quickly. For example, with constant coefficient systems \( \dot{z} = Az \), the Lyapunov exponents are just the real parts of the eigenvalues of \( A \). Trajectories of autonomous ODEs that are bounded but do not approach equilibrium points must have a zero Lyapunov exponent. This Lyapunov exponent is associated with the direction of the flow, and is related to the eigenvalue 1 of \( \nabla_x \phi(x, T) \) discussed in the last paragraphs of §5 A.
6.1. Computing Lyapunov exponents


In principle the above definition of Lyapunov exponents gives a numerical procedure for computing Lyapunov exponents, at least about a particular trajectory. However, because of the exponential growth and decay of the singular values, the smaller singular values can quickly be lost in the numerical "noise". One way to get around this is to perform the computations in extended precision arithmetic with about \( \log_2 (\sigma_1(\Phi(t)) / \sigma_n(\Phi(t))) \) digits. For a product of several hundred matrices this would require several hundred to thousands of digits. Needless to say, this is a rather expensive way of doing these computations.

There are many other methods which don't require extended precision arithmetic but still give quite accurate results. The best known is described by Eckmann and Ruelle (1985); this method is better known in the numerical analysis literature as treppeniteration. This method does not compute the singular values of the product, but rather what is known as the QR factorisation: the QR factorisation of a matrix \( A \) is a factorisation \( A = QR \) where \( Q \) is orthogonal and \( R \) is upper triangular. This can be computed accurately in a suitable backward error sense. (For details see (Golub & Van Loan, 1989, ch. 5).) The QR factorisation is well known in numerical linear algebra and is widely used for least-squares problems, finding orthonormal bases for null-spaces and as a component of algorithms for computing eigenvalues (Golub & Van Loan, 1989).

Treppeniteration gives a QR factorisation of the product

\[
\nabla_\nu \Phi(x, k) = \nabla g(x_{k-1}) \nabla g(x_{k-2}) \cdots \nabla g(x_1)
\]

as follows. Set \( C_1 = \nabla g(x_1) \) and factorise \( C_1 = Q_1 R_1 \) by the standard QR factorisation. Then form \( C_2 = \nabla g(x_2) Q_1 \), and factorise \( C_2 = Q_2 R_2 \). Repeat the process, forming \( C_3 = \nabla g(x_3) Q_2 \), and factorising \( C_3 = Q_3 R_3 \). Repeating until we reach \( C_k = \nabla g(x_k) Q_{k-1} \) and factorising \( C_k = Q_k R_k \) we have

\[
\nabla_\nu \Phi(x, k) = Q_k R_k R_{k-1} \cdots R_1 R_0 = Q^k R^k.
\]

Since the product of upper triangular matrices is upper triangular, this is a QR factorisation of the product. If we start with a "randomisation" step \( C_1 = \nabla g(x_1) Q_{-1} \) with \( Q_{-1} \) a random orthogonal matrix, then we have the theorem:

**Theorem 5.** For almost all \( Q_{-1} \) the Lyapunov exponents are given by

\[
\lambda_i = \limsup_{k \to \infty} \frac{\log |R_{ii}^k|}{k}
\]

(The original version of treppeniteration sets \( Q_{-1} = I \).) The reason for the initial randomisation step is that the columns of \( Q_{-1} \) may not have non-zero components in the associated Lyapunov directions. Usually this randomisation is ignored as a failure happens only with probability zero in exact arithmetic, and (2) numerical errors usually generate vectors with non-zero components in the right directions.

Note that the diagonal entries of \( R^k \) are just the products of the diagonal entries of the factors, so \( \sigma_{ii}^k = \prod_{j=1}^{k} (R_{ji}) \). Thus

\[
\lambda_i = \limsup_{k \to \infty} \frac{\sum_{j=1}^{k} \log |R_{ji}|}{k}
\]

Treppeniteration has a backward error analysis which can be developed from the
backward error analysis of the ordinary QR factorisation. The computed factorisation \( \tilde{Q}^{(h)} \tilde{R}_k \tilde{R}_{k-1} \ldots \tilde{R}_1 \) satisfies the property that there is an exactly orthogonal matrix \( \tilde{Q}^{(h)} \) near \( \hat{Q}^{(h)} \) where

\[
\tilde{Q}^{(h)} \tilde{R}_k \tilde{R}_{k-1} \ldots \tilde{R}_1
\]

is the exact QR factorisation of

\[
(\nabla y(x_k) + E_k)(\nabla y(x_{k-1}) + E_{k-1}) \ldots (\nabla y(x_1) + E_1)
\]

where \( \|E_k\|_2 = O(h) \|\nabla y(x_0)\|_2 \) where \( h \) is "machine epsilon" or "unit roundoff" \([\text{§3.1}].\) This corresponds to a time-dependent perturbation of the map of size \( O(h) \) relative to the size of \( \nabla y(x) \).

Alternative algorithms for estimating Lyapunov exponents exist, with some tuned for the ODE case. One is based on the \textit{stabilised march} which is used for solving boundary value problems. If \( \dot{x} = f(x(t)) \) then the variational equation is

\[
\Phi'(t) = \nabla f(x(t)) \Phi(t) = A(t) \Phi(t).
\]

The idea is to set up ODEs for the \( Q \) and \( R \) factors of \( \Phi(t) \).

Write \( \Phi(t) = Q(t) R(t) \). Differentiating gives the system

\[
Q'R + QR' = AQR.
\]

Since \( Q(t) \) is orthogonal, \( Q(t)^T Q(t) = I \) for all \( t \). Differentiating this gives

\[
(Q'R + QR')^T Q + Q^T Q'R' = 0.
\]

Thus \( Q(t)^T Q'(t) \) is an antisymmetric matrix \( S(t) \), and \( Q'(t) = Q(t) S(t) \). Hence \( Q S R + Q R = A Q R \). Pre-multiplying by \( Q^T \) and post-multiplying by \( R^{-1} \) gives

\[
S + R R^{-1} = Q^T A Q.
\]

Taking the strict lower triangular part of this matrix ODE gives

\[
s_{i,j}(t) = \sqrt{q_i(t)^T A(t) q_j(t)} \quad \text{for } i > j.
\]

This can be extended to a unique antisymmetric matrix. Thus we have a well-defined ODE for \( R(t) \). As we are really only interested in the diagonal entries of \( R(t) \) we take the diagonal part of the ODE for \( R \). This gives

\[
\frac{d}{dt} \log r_{i,i}(t) = \sqrt{q_i(t)^T A(t) q_i(t)}.
\]

This is clearly just an integration once \( Q(t) \) is computed via \( Q = Q S \).

Care must be taken here to ensure that \( Q \) remains orthogonal, by suitable integration schemes \((\text{Devi et al., 1984})\) or by periodically forcing \( Q(t) \) to be orthogonal. If this is not done, then as the set of orthogonal matrices may be unstable for the ODE for \( Q \), and the method breaks down.

There are also algorithms for computing the \textit{singular value decomposition} (SVD) of a product of matrices. This is the factorisation

\[
A = U \Sigma V^T
\]

where \( U \) and \( V \) are orthogonal matrices and \( \Sigma \) is a diagonal matrix \( \text{diag} \{ \sigma_1, \ldots, \sigma_n \} \) with \( \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \). \((\text{See Gelub and Van Loan} \ 1989, \ [2.5.,8.3.])\) The value \( \sigma_i \) is the \( i \)th singular value of \( A \). Bojanczyk, Everling, Iak and Van Dooren \((1991)\) a method based on Jacobi rotations. Stewart \((1994a, 1994b)\) and Abarbanel \textit{et al.} \((1992)\) give methods based on treppeneration.
Computing SVDs by setting up differential equations for the singular values, analogously to the above method for the QR factorisation, suffers from breakdown when singular values cross over. This breakdown does not occur for the continuous QR factorisation algorithm.

7. Continuation and bifurcation

Continuation is a technique for solving non-linear equations. This is done by embedding the equations in a one-parameter family of equations $H(x, \lambda) = 0$. Starting at one parameter value, a solution can be followed along the curves in $(x, \lambda)$ space, hopefully until a solution of the original problem is found. This technique can be used to follow branches of equilibrium points, periodic solutions and particular trajectories. Where continuation breaks down there are usually bifurcations.

Bifurcations occur in both non-linear equations and in dynamical systems, though what can happen in dynamical systems is usually much richer and more complex. Bifurcations are essentially local phenomena; they are about what happens as a parameter varies in the neighbourhood of a bifurcation point.

The theory of bifurcations is a very rich subject and goes well beyond the scope of this chapter. A good introduction is the review by Crawford (1991). All we can hope to do here is to have a look at some of the simpler and more important bifurcations.

Regarding numerical techniques, two sources are Keller (1987) and Crouzeix and Rapatz (1990).

7.1. Bifurcation jargon

If we picked a random matrix we would that it is non-singular with probability one. This is called the generic case. We might say that matrices are generically non-singular. In dynamical systems theory an equilibrium point $x_1$ of a smooth ODE or map is generically hyperbolic (i.e., with no eigenvalues on the stability boundary --- see §5). What is of interest is what happens when one or more eigenvalues(s) crosses the stability boundary. Where this happens determines the sort of bifurcation.

Often bifurcations are described as being codimension $k$ bifurcations. This means that they (usually) occur on submanifolds of the parameter space with dimension $k$ less than the full dimension. This idea can be made precise for spaces of functions by a similar technique to that used to define prevalence. Another way of understanding the codimension is as the number of parameters that are needed to make the bifurcation happen for some set of parameter values.

The simplest bifurcations are called codimension 1 bifurcations. The next simplest are codimension 2 bifurcations.

If we considered square matrices, almost all matrices are non-singular. But amongst the singular matrices, the matrices with a one-dimensional null space are generic. The matrices with a one-dimensional null space are said to have codimension 1 in the space of all matrices.

The way the solutions change as the parameters vary is called the unfolding of the bifurcation. If all unfoldings are equivalent to a given unfolding, or some subset of it, that unfolding is called universal.

Usually the dimensionality of the bifurcation can be reduced to a few "essential" dimensions by means of a variant of the implicit function theorem. This is called Lyapunov-Schmidt reduction.

The connections between the branches of solutions and their bifurcations is often displayed on a bifurcation diagram, which plots some relevant quantity against a parameter.
Stable branches are usually indicated by solid lines and unstable branches by dotted or dashed lines. An example can be seen in Fig. 10 which represents a fold bifurcation. The top branch is unstable while the bottom branch is stable.

7.2. Some basic bifurcations

These bifurcations are all codimension 1 bifurcations.

Fold bifurcation In dynamical systems terms, this happens when two equilibria collapse and disappear. A universal unfolding for this comes from the equations (for an equilibrium point):

\[ x^2 - \lambda = 0. \]

Here \( x \) is the state variable and \( \lambda \) is the parameter that is being varied. For \( \lambda > 0 \) there are two equilibria at \( +\sqrt{\lambda} \) and at \( -\sqrt{\lambda} \). If we consider the ODE

\[ \dot{x} = x^2 - \lambda \]

the equilibrium at \( -\sqrt{\lambda} \) is stable while the equilibrium at \( +\sqrt{\lambda} \) is unstable. A bifurcation diagram for this is shown in Fig. 10.

Other bifurcations for ODEs and maps come from a single equilibrium when its stability changes. These bifurcations are described in terms of where eigenvalues cross the stability boundary. Generically, only one real eigenvalue or a complex conjugate pair cross the stability boundary at a time. For a system of ODEs the stability boundary is the imaginary axis so either a real eigenvalue crosses the axis at zero, or a complex conjugate pair crosses the imaginary axis. The former case is called a pitchfork bifurcation, the latter a Hopf bifurcation. For maps, there are both pitchfork (one real eigenvalue crossing at one) and Hopf bifurcations (a complex conjugate pair cross the unit circle), but as well there is the possibility of an eigenvalue leaving the unit circle at minus one. This is called a flip bifurcation.

Pitchfork bifurcation This results from a real eigenvalue going through zero (for an ODE) or through one (for a map). This results in the creation of a pair of equilibrium points with opposite stability. A standard example for this is

\[ \dot{x} = -x^3 + \lambda x. \]

For \( \lambda < 0 \) the equilibrium \( x = 0 \) is stable and there are no other equilibria. As \( \lambda \) becomes positive \( x = 0 \) becomes unstable and two stable equilibria arise at \( x = \pm\sqrt{\lambda} \). Alternatively, an unstable equilibrium can become stable while throwing off two new unstable equilibria. An example is the ODE \( \dot{x} = +x^3 + \lambda x \) with \( \lambda \) going from being
positive to negative. Bifurcation diagrams for this is shown in Fig. 11. The direction in
which the “fork” goes (to the right or the left) depends on higher order (cubic) terms.

**Hopf bifurcation** This results from a complex conjugate pair going through the imaginary axis (for an ODE) or through the unit circle (for a map). For autonomous ODEs this results in a new limit cycle with the same stability as the original equilibrium point. The equilibrium point usually changes stability. The period of the new orbit is $2\pi /\omega$ where the eigenvalues cross at $\pm i\omega$. For maps the situation is more complex; there is an invariant circle, and the behaviour on this circle is like a circle map. And with circle maps, whether or not there can be a periodic orbit depends on whether the rotation number is rational or not. Of course the angle of the critical eigenvalues to the real axis is changing continuously with the parameter, so the situation is considerably more subtle here.

An example of a Hopf bifurcation for ODEs is given by the following system:

\[
\begin{align*}
\dot{x} &= -y + x(\lambda - (x^2 + y^2)) \\
\dot{y} &= +x + y(\lambda - (x^2 + y^2)).
\end{align*}
\]

For $\lambda < 0$ the origin is a stable equilibrium and there are no periodic solutions. For $\lambda > 0$ the origin becomes an unstable equilibrium and there is a stable limit cycle which is formed by a circle of radius $\sqrt{\lambda}$. For $\lambda > 0$ the period of the limit cycle of this example is $2\pi$. Of course, in general, the period of the limit cycle will only approach $2\pi /\omega$ as the parameter approaches the bifurcation point.

The bifurcation diagrams associated with Hopf bifurcations are essentially like the pitchfork bifurcation diagrams; often Hopf bifurcation diagrams are drawn in like one-sided pitchfork diagrams.

**Flip bifurcation** This bifurcation can only occur for maps. It occurs when an eigenvalue goes through the unit circle at $-1$. The equilibrium point involved changes stability as the eigenvalue moves in or out of the unit circle, but once the bifurcation point is crossed there is a new orbit of period 2. This is the bifurcation view of why period doubling is so common. (This is especially true in one dimension as then Hopf bifurcation of maps is not possible.) An example of such a map is

\[ x_{n+1} = -(1 + \lambda)x_n + x_n^3 \]

and at the equilibrium point $x = 0$ as $\lambda$ crosses through zero. The periodic orbit for $\lambda > 0$ consists of two points at distance $\approx \sqrt{\lambda}$ from the equilibrium point.

Flip bifurcation diagrams, like Hopf bifurcation diagrams, are often drawn as one-sided pitchfork bifurcations.

**Transcritical bifurcation** Transcritical bifurcations occur when two equilibria or pe-
Transcritical bifurcation. points points cross each other, one stable and the other unstable. As a result, the two equilibria exchange stability. An example of such a bifurcation is

\[ \dot{x} = x(x - \lambda) \]

There are two equilibria for \( \lambda \neq 0 \), which are \( x = 0 \) and \( x = \lambda \). For \( \lambda < 0 \), the equilibrium point \( x = 0 \) is stable and the equilibrium point \( x = \lambda \) is unstable. But for \( \lambda > 0 \), \( x = 0 \) is now unstable and \( x = \lambda \) is stable. This is illustrated in Fig. 12. Note that a combination of a transcritical bifurcation and a fold bifurcation can approximate a pitchfork bifurcation.

7.3. Continuation


Continuation is a technique that is used for solving nonlinear equations. Modern continuation techniques provide globally convergent methods for solving difficult and highly nonlinear equations. They are backed up with considerable theory, and there are a number of software packages available which perform continuation. The package HOMPACK (Watson et al., 1987) is one example of a suite of continuation routines which is publicly available. Continuation software has been incorporated into a number of packages for analysing dynamical systems; these use continuation to get to bifurcation points; the bifurcation is analysed and solution branches are identified; finally, continuation is used to track the behaviour of the different solution branches. This is done, for example, in the AUTO package (Doedel, 1986) and in BIFPACK (Seidel, 1989) and other packages.

The general set up for continuation is that we wish to solve a system of equations \( F(x) = 0, x \in \mathbb{R}^n \), starting from a computationally trivial system \( G(x) = 0 \). The idea is to set up a homotopy between the two problems \( H(x, \lambda) \) where \( 0 \leq \lambda \leq 1 \) with \( H(x, 0) = G(x) \) and \( H(x, 1) = F(x) \). Then we can try to follow the path \( H(x, \lambda) = 0 \) in \( (x, \lambda) \) space, from the trivial solution of \( G(x) = 0 \) (\( \lambda = 0 \) ) to the solution we want, \( F(x) = 0 \) (\( \lambda = 1 \) ). Old style continuation assumed that one could write \( x = x(\lambda) \) and monotonically increase \( \lambda \) from zero to one. However, this often fails due to the curve \( H(x, \lambda) = 0 \) “folding back”. If the curve does fold back then you might try to change the homotopy and/or start from a different \( G \). This can work sometimes, but it fails more often than it succeeds.

If you try doing continuation in \((x, \lambda)\) space and simply try to follow the curve, whether
or not it folds back, then you can do much better than using old style continuation. As long as the \( (n+1) \times n \) Jacobian matrix \( \nabla_H(x, \lambda) \) has full rank then the curve, locally, is a smooth curve and not something more complex (like a pitchfork bifurcation or something nastier). If the homotopy \( H(x, \lambda) \) is already given, such as for following a branch of solutions, then bifurcations, or other problems where \( \nabla_H(x, \lambda) \) fails to have full rank, may be unavoidable. This sort of continuation is called natural continuation.

However, if you are willing to follow a path merely to get to the other end, then we can incorporate some randomness which ensures that there is a smooth path almost every time the algorithm is run. The trick is to incorporate an extra vector of parameters into \( H \) so that the matrix \( \nabla_{(x, \lambda)} H(x, \lambda; a) \) always has full rank, except possibly at \( \lambda = 1 \). For example, we could take the linear homotopy

\[
H(x, \lambda; a) - (1 - \lambda)(x - a) + \lambda F(x),
\]

\( \lambda \rightarrow 0 \). Prove that \( x = a \) is the obvious, trivial, solution. By a generalization of the Morse-Sard lemma, for almost all \( a \), the matrix \( \nabla_{(x, \lambda)} H(x, \lambda; a) \) has full rank whenever \( H(x, \lambda; a) \neq 0 \). This kind of continuation is called artificial parameter continuation.

7.4. Applications of continuation

Tracking equilibria Equilibria for ODEs and maps are simply solutions of (nonlinear) functions given in the ODE or map. For the ODE case, they are given by \( f(x) = 0 \); in the case of maps, we should look for fixed points: \( x = g(x) = 0 \).

Most codimension 1 bifurcations in the dynamics are either not a problem for modern continuation methods (fold bifurcations) or are ignored completely (Hopf and flip bifurcations). However, at pitchfork bifurcations either \( \nabla f(x) \) or \( I - \nabla g(x) \) is singular, for the ODE and map cases respectively, which can cause problems.

Tracking periodic solutions Periodic solutions of maps, or periodically forced ODEs, can be accomplished easily within the continuation framework. In this case the period \( T \) is predetermined, and it is just a matter of solving the equations \( x = \varphi(x, T) = 0 \) where \( \varphi(\cdot, T) \) is the map or flow generated by the ODE or map at time \( T \). Tracking periodic solutions of autonomous ODEs is more complex. This is because there is an extra parameter (the period \( T \)) which needs to be computed, and there is some redundancy as there is no need to distinguish different points on the same periodic orbit. Local continuation can be done, provided we restrict perturbations to be (for example) perpendicular to the direction of the vector field. However, global properties cannot be guaranteed, at least in "probability one" form.

Tracking homoclinic and heteroclinic orbits Homoclinic orbits and heteroclinic orbits
can be tracked for varying parameters if the stable and unstable manifolds intersect transversally by setting up two point boundary value problems. If the stable and unstable manifolds do not intersect transversally then the situation is not structurally stable, and we can expect numerical methods to work.

Suppose we want to compute a connecting orbit between two hyperbolic equilibria, from $x$ to $y$. (We could have $x = y$ for the case of a homoclinic orbit.) Suppose also that the stable and unstable manifolds intersect transversally so that the intersection of $W^u(x)$ and $W^s(y)$ occurs at an angle and that $\dim W^u(x) + \dim W^s(y) > n$. Small perturbations of the manifolds will not destroy transversal intersection. Close to $x$ we can approximate $W^u(x)$ by the linear manifold $x + V^u(x)$, and similarly we can approximate $W^s(y)$ near $y$ by $y + V^s(y)$. (Taylor series approaches can improve on this, although the arithmetic is terrible.)

For a suitably large $T > 0$ we consider the boundary value problem

$$u = f(u), \quad u(0) \in x + V^u(x), \quad u(T) \in y + V^s(y)$$

or an analogous system for maps. While this is potentially an extremely ill-conditioned problem if treated as an initial value problem, it can still be very well behaved if multiple shooting type methods are used. Pick an integer $N > 0$ and we split the interval $[0, T]$ into pieces $[kT/N, (k+1)T/N], k = 0, \ldots, N-1$ so that the matrix functions $\nabla_x f(T/N)$ are always well conditioned. This can be done if the differential equation has a Lipschitz constant $K$ and we pick $N$ to make $N = O(KT)$. In practice, it would be desirable to have $N \leq o(1)$ where $o$ is the range zero to five. Then we have to solve a $(N-1)n$ system of equations

$$u_{n+1} = f(u_n, T/N) = 0$$

together with the boundary conditions $u_1 \in x + V^u(x)$ and $u_N \in y + V^s(y)$. We also need to make sure that $u_1$ is close enough to $x$, and that $u_N$ is close enough to $y$; if it isn’t we need to make $T$ larger. The value of $T$ does not have to be enormous, as the trajectories will converge to $x$ and $y$ at an exponential rate. This can be fast enough that the linear approximation to $W^u(x)$ and $W^s(y)$ is all that is needed rather than taking higher order approximations: the distance to the equilibria are exp($-O(T - T_i)$) where $T_i$ is the time to travel between reference points near to $x$ and $y$.

Provided $x$ and $y$ are hyperbolic equilibria, and the intersection is transversal, the Newton equations are well conditioned. If we have $\dim W^u(x) + \dim W^s(y) > n$ then we have an underdetermined system. This can be solved using QR factorisations which can be used to give the solution with minimal 2-norm. For hyperbolic homoclinic orbits we have $\dim W^u(x) + \dim W^s(y) = n$ so the Newton system is a square system of $Nn$ equations in $Nn$ unknowns.

### 7.5. Continuation techniques

Given a homotopy function $H(x, \lambda)$ whose zero curve we wish to follow, to actually perform continuation we need the following:

- a way to step along the path.
- a way to see that we are keeping the right direction and haven’t accidentally reversed.
- a way to correct for drifting from the path.

For the remainder of this section we use $z = (x, \lambda)$ and write $H(z)$ for $H(x, \lambda)$ and gradient $\partial H$ with respect to $z$ unless otherwise indicated.

**Stepping schemes** The simplest way to obtain a step for a homotopy method is to step along the tangent plane to the curve. We will need to work out the correct direction, but that will be dealt with next. It isn’t hard to compute the tangent plane for $H(z) = 0$. It
is just the kernel of the \( n \times (n+1) \) matrix \( \nabla H(z) \). This can be determined by computing the QR factorisation of \( \nabla H(z)^T \); the last column of the resulting \( Q \) matrix is a unit vector in the kernel.

Once the direction has been computed, we can do the simplest thing and step a fixed amount in that direction. Applied to ODEs this is just Euler's method. This is a rather dangerous strategy; it is better to check on, say, \( H(z + a\Delta z) \), and reduce the step if this is too large. Alternatively, this step control strategy could be built into the correction step which takes us back close to the true path.

If we think of \( z = (x, \lambda) = (x(s), \lambda(s)) =: z(s) \) where \( s \) is the arc length of the curve in \((x, \lambda)\) space, then \( dz/ds \) is just the unit direction vector computed for that point. This can be thought of as defining an ODE for the curve. Techniques from ODEs have been applied to get better stepping schemes, such as using Runge-Kutta or multistep methods. Also interpolation methods have been applied. One of the best seems to be extrapolation based on Hermite interpolants as they use not only position information but also derivatives at the endpoints.

**Keeping the right direction** The unit vector computed from the QR factorisation could be in the right direction or the opposite. There are two ways of determining if we are heading in a consistent direction. The simplest is just to take the inner product with the previous computed direction. If the inner product is negative then something is quite wrong. In fact, this inner product is used in some codes to detect sharp bends; there is some tolerance \( t_d \) such that if \( (z_d)^T z_{\text{new}} < 1 - t_d \), the step size would be reduced.

To start this method off, we need to know if the first direction is in the right direction. This is easy. We just want \( \lambda > 0 \). If the computed direction has \( \lambda < 0 \), then it must be reversed.

There is a more sophisticated way of ensuring that the direction stays consistent. That is to compute the sign of \( \det(\nabla H(z)^T z) \). This sign should be constant. The reference sign is computed as the sign of the path following, and thereafter used to check directions. The sign of the determinant can in fact be computed quite quickly in terms of the \( Q \) and \( R \) factors.

**Keeping to the narrow path** Provided we are not too far from the path, then Newton's method can be used to correct and bring us closer to the true path. This is a slightly unusual Newton method as it is an underdetermined system of equations:

\[
\nabla H(z) \Delta z = -H(z) \in \mathbb{R}^n, \quad z \in \mathbb{R}^{n+1}
\]

where \( z = (x, \lambda) \). As noted above, this can be dealt with by means of QR factorisations.
Since Newton’s method is only guaranteed to converge if it is started close enough to the true solution, care must be taken to prevent problems caused by taking steps that are “too large.” Careful step size control strategies should be built into the Newton method to make it robust and reliable. A standard technique is known as the Aitken line search: Compute the step $\Delta z$ from Newton’s method. While $\|H(z + \Delta z)\| > \|H(z)\|$, set $\Delta z \leftarrow \Delta z / 2$. Now set $z \leftarrow z + \Delta z$. This ensures that $\|H(z)\|$ does not increase. Scaling strategies can also be important. In addition the strategies for ensuring that the computed points don’t stray too far, should be incorporated into the stepping algorithm discussed above.

7.5. When a path meets a bifurcation...

Provided simple bifurcations occur, and the type of bifurcation can be identified, then it is not too hard to jump over the bifurcation point and continue on the other side. For example, in Fig. 15 is shown a pitchfork bifurcation, which has the property that the far branch is tangential to the near branch at the bifurcation. At the bifurcation point the equations we wish to solve become degenerate and the Jacobian matrix becomes singular. The main trick is to identify (roughly) where the bifurcation point is, and to jump far enough (but not too far) so that the predicted point lies within the domain of convergence of the Newton method. This is illustrated in Fig. 15.

8. Inertial manifold theory

The world abounds with dynamical systems that are not only chaotic, but have very large dimension. Perhaps one of the best known is the weather. It is not only now known to be chaotic, but it is described by partial differential equations. That is, the equations describing the weather (temperatures, pressures, humidities etc.) not only describe how these quantities vary over time, but also how they vary over space. To describe a single “snapshot” of the earth’s weather fields requires a vast amount of information. The number of simple scalar quantities that are needed to describe such a snapshot is indeed very large. This means that weather is a large-scale or high-dimensional dynamical system. Indeed, in most mathematical formulations of the way weather behaves, it is an infinite-dimensional system.

In spite of the fact that a detailed description of the state of the weather system requires vast numbers of simple scalar quantities, it is commonly observed that a few crucial (selected or averaged) quantities can be remarkably good at predicting the behaviour of the overall system. Perhaps the most successful example of this is the “southern oscillation” index which is used to quantify the “El Niño” effect. Of course, this is just one of a number of quantities that could be used to give a more-or-less complete
description of the weather state. This suggests that, despite the infinite number of degrees of freedom of the system, it is behaving as if it were a low-dimensional system.

The idea can be put into a mathematical form in terms of inertial manifolds. Inertial manifolds are manifolds or “surfaces” in the state space of a dynamical system which
- are finite dimensional,
- are smooth, or at least Lipschitz.

If such a manifold exists, the long-term behaviour of the large-scale system can be reduced to asking about the long-term behaviour of the system on its inertial manifold. This reduces an infinite-dimensional problem (or very large-scale problem) to a finite-dimensional, and therefore, in principle, tractable problem.

Even if existence can be proved, there are of course a number of practical issues which need to be considered, such as the difficulty of finding an inertial manifold for a large-scale system, and the dimension of the inertial manifold so constructed.

The maximum dimension of any inertial manifold a system can have is the lowest integer greater than or equal to the fractal or Hausdorff dimension of its attractor. Since any trajectory is attracted exponentially fast to an inertial manifold, the attractor(s) must lie within the inertial manifold. The dimension of the attractor must therefore be no more than that of an inertial manifold.

Proving the existence of inertial manifolds is not a trivial exercise, and involves a great deal of technical machinery. However, the basic idea is not so difficult to describe. In some form or other, there needs to be some form of dissipation in the dynamical system. Some systems do not have dissipation and do not have inertial manifolds. A simple example is the wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}. $$

(This is a wave in one space dimension. Here $c$ is the speed of the wave.) These equations describe the vibrations of a guitar string and waves of electromagnetic radiation. Wave equations have the property of being reversible. This means that if you take the film of a solution of the wave equation, and run it backwards, the resulting picture would also be a solution of the wave equation. Since the equation is reversible, there is no loss of information, and no attraction to some part of the state space. This means that there is no reduction in the number of quantities needed to accurately describe the state of the system, and since the starting conditions cannot be completely described with a finite number of quantities, there cannot be an inertial manifold.

However, if some sort of dissipation is introduced (air resistance or friction for the guitar string, or electrical resistance for the electromagnetic wave), then the situation changes radically. Such dissipation quickly removes the rapidly oscillating parts of the solution leaving the lower frequency components, which decay much more slowly.

If the system were left to itself, even the slowly decaying modes would eventually damp out, and the system would relax to a state of maximum uniformity. For example, in the case of weather, if it were not for the energy input to the atmosphere from the sun and the perturbing effect of the departure of the solid earth from a spherical ball, the system would relax to one of spherical symmetry.

However, if low frequency energy is injected into the system the lower frequency components may not decay away completely, and in fact may be generated spontaneously from bifurcations breaking the symmetry of the relaxed, background state. For example, in the case of weather the heating of the land during the day may drive large scale convective instabilities. The degrees of freedom corresponding to rapidly decaying motions
(the “slave modes”) will still be excited as an adiabatic response to slow driving by the
large scale modes (the “master modes”), but their response will be smaller the farther
the driving is from their natural frequency.

The effect of damping is to pull the solution towards some finite dimensional manifold
within the infinite dimensional state space of the fluid equations. This is the inertial
manifold, on which the coefficients of the master modes form a coordinate system. The
effect of the response of the slave modes is to distort this manifold away from its tangent
space at the origin, the tangent space being the linear vector space spanned by the
eigenmodes with very small growth or damping (the master modes) found by linearising
about the stationary background state.

A full treatment of weather should also include the turbulent boundary layer near the
surface of the earth. The treatment of turbulence requires the recognition of an interme-
diate scale, between the molecular scale and the macroscopic scale of the weather map,
on which instabilities produce small-scale eddies which modify the transport equations
describing the dynamics on the macroscopic scale. This is an example of a hierarchical
complex system in which the macroscopic elements on one scale are microscopic on an-
other. The proper derivation of turbulent transport is still an unresolved matter, and
often semi-empirical “anomalous” transport coefficients are used.

8.1. Technical ideas

The first mathematical presentation of inertial manifold theory appears to be Mañé
(Mañé, 1977). The technical basis of the existence theory of inertial manifolds can be
found in Constantin, Foias, Nicolaenko and Témam (Constantin et al., 1988; Constantin
et al., 1989).

The basic idea is to split the equation describing the dynamics of the system into a
dominant linear part and a weaker nonlinear part. The linear part has to have a strongly
dissipative character; in addition, spectral gap or spectral barrier conditions are assumed
so that there is a separation of time scales between the slow dynamics and the slaved
response.

To illustrate how the theory works, consider

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

where $A$ is a linear, positive definite, symmetric operator, and $f$ is possibly nonlinear.
An example of such systems are the reaction-diffusion equations

$$\frac{\partial u_i}{\partial t} = \nu \nabla^2 u_i + f_i(u_1, \ldots, u_m), \quad i = 1, \ldots, m.$$ 

Here

$$\nabla^2 u_i = \frac{\partial^2 u_i}{\partial x_1^2} + \cdots + \frac{\partial^2 u_i}{\partial x_n^2}$$

in $n$-dimensional space. The term $\nu \nabla^2 u_i$ is due to diffusion, and $f_i(u_1, \ldots, u_m)$ is an
ordinary function which gives the reaction rates for the concentration $u_i$. The quantity
$\nu$ is the diffusion coefficient for the system. Reaction-diffusion equations incorporate
spatial dependence with the equations for a reaction. This should be compared with
continuous stirred-tank reactors, where the components are assumed to be so thoroughly
mixed that there is no spatial dependence. In this case the equations reduce to ordinary
differential equations:

$$\frac{du_i}{dt} = f_i(u_1, \ldots, u_m), \quad i = 1, \ldots, m.$$
With spatial variation new phenomena can be observed such as travelling waves, moving spirals, and so on.

The theory developed by Constantin, Feiss, Nicolson, and Témam starts by considering the eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots$ of $A$. Provided a gap $\lambda_{k+1} - \lambda_k$ can be found in the spectrum which is larger than the Lipschitz constant of $f$, an inertial manifold exists with dimension $k$. This idea is refined in (Constantin et al., 1988; Constantin et al., 1989) and is extended to a number of different circumstances such as the Navier-Stokes equations for fluid flow in two dimensions and Kuramoto-Sivashinsky and other related equations. However, there is still a need in this theory to have gaps in the spectrum that are in some sense “large enough” to control the nonlinear parts of the equations. In a sense, this theory is a global version of the theory of hyperbolic equilibrium and periodic points. For hyperbolic equilibrium points there is to be a separation of the eigenvalues away from the stability boundary to control the local nonlinearities; here there has to be a gap in the eigenvalues to control the global behaviour of the nonlinearities.

The need for spectral gaps or barriers of some kind has limited the theory to a few number of spatial dimensions, and there have been a number of counter-examples which show that the theory cannot be extended in its current form to even reaction-diffusion equations in four or more dimensions (Mallet-Paret & Sell, 1986).

A different approach, discussed in the next section, has also been developed which does not require spectral gaps, but gives the existence only of an approximate inertial manifold.

8.2. Approximate inertial manifolds

Approximate inertial manifolds for a dynamical system are manifolds that are:

- finite dimensional;
- smooth, or at least Lipschitz;
- attract all trajectories to within a small distance at an exponential rate.

If crucial importance are the answers to the questions “How close will trajectories be attracted?”, “How small an angle will the trajectories make to the manifold?” However, this weakening means that sensible results can be obtained even where there are no large spectral gaps. All that is required is that the eigenvalues of $A$ grow without bound. With this condition the answer to the question “How close will trajectories be attracted?”, the answer is “As close as you please.” The cost, however, is the increasing dimension of the approximate inertial manifold as the “tolerance” for closeness of trajectories is reduced.

Computational methods for finding such approximate inertial manifolds have been developed by Debussche and Marion (Debussche & Marion, 1992), Gourbet (Gourbet, 1992) and Marion (Marion, 1989).

9. Finding shadows

The final numerical analysis section of this chapter is on finding shadows of numerically computed orbits. Recall that numerically we do not compute true trajectories but rather $\delta$-pseudo trajectories: \[ \|x_{k+1} - \phi(\delta x_k)\| \leq \delta \] for all $k$. As was noted in §1.5, the exponential divergence of trajectories means that errors, even those due to the precision of the floating point arithmetic, quickly grow and overwhelm the solution. Nevertheless, the overall behaviour of the system seems to be remarkably stable.

One way to resolve this paradox is through shadowing: even though we have computed something which diverges from the true trajectory, we may be close to some trajectory
with slightly different initial conditions. An $\epsilon$-shadow of $x_k$ is a true trajectory $y_k$ where $\|x_k - y_k\| < \epsilon$ for all $k$ (see Fig. 16).

When do shadows exist? When and how can we compute them? When can we compute a value of $\epsilon$ for which there is a shadow? There are both theoretical and numerical approaches to this problem. The theoretical approach is due to Anosov and Bowen (1967; 1975) and is based on hyperbolicity. The numerical approach avoids assuming hyperbolicity, but instead explicitly computes the conditioning of the matrices that hyperbolicity implies are stable.

The basic shadowing lemma is due to Anosov and Bowen.

**Theorem 6.** If a map $g$ is hyperbolic then for every $\epsilon > 0$ there is a $\delta > 0$ such that every $\delta$ pseudo orbit has an $\epsilon$-shadow.

Of course, $g$ might be hyperbolic on an attractor, even if not globally, and provided the numerically computed orbit stays on the attractor, then a shadowing lemma applies here as well.

## 9.1. Why shadowing can be done

The basic idea behind shadowing is to consider a trajectory, not as the result of an iteration, but “all at once” as a single entity satisfying a system of equations:

$$g(y_k) - y_{k+1} = 0 \in \mathbb{R}^n.$$

Let us write $y$ for the sequence $(y_k)$. Then we have $y \in l^\infty(\mathbb{Z}, \mathbb{R}^n)$ where the space $l^\infty(\mathbb{Z}, X)$ is the set of all bounded sequences $x = (x_k)_{k \in \mathbb{Z}}$ such that $x_k \in X$ and with the norm

$$\|x\|_\infty = \sup_{k \in \mathbb{Z}} \|x_k\|_X < +\infty,$$

where $\|\cdot\|_X$ is the norm on $X$. We assume $X = \mathbb{R}^n$ and use the usual 2-norm in $\mathbb{R}^n$ as this norm. As is standard, $\mathbb{Z}$ denotes the set of all integers, positive, negative and zero.
Consider the map \( G : l^\infty(\mathbb{Z}, \mathbb{R}^n) \to l^\infty(\mathbb{Z}, \mathbb{R}^n) \) defined by
\[
G(x)_k = x_{k+1} - g(x_k).
\]
That is, \( G \) generates the sequence of errors given an arbitrary sequence \( x \in l^\infty(\mathbb{Z}, \mathbb{R}^n) \).

For the shadowing true orbit, \( y \), the errors are zero, so we need to solve \( G(y) = 0 \). Our strategy will be to solve this iteratively, taking as initial guess \( x = x \) and ending up, we hope, with \( x = y \). We know already that Newton’s method is a powerful method for solving nonlinear equations, even when simple iterative methods diverge. Clearly we have a nonlinear equation, but can we use Newton’s method on it?

Well, Newton’s method is given by
\[
\nabla G(x) \delta x + G(x) = 0
\]
where
\[
(\nabla G(x) \delta x)_k = \delta x_{k+1} - \nabla g(x_k) \delta x_k.
\]
The next step is to show that this linear operator \( \nabla G(x) \) has a bounded inverse. This requires hyperbolicity.

Recall that hyperbolicity says that there are continuous families of projections \( P^t(x) \) and \( P^u(x) \) where \( P^t(x) + P^u(x) = I \), which satisfy consistency conditions
\[
\nabla g(x) \text{ range } P^t(x) = \text{ range } P^t(g(x))
\]
and similarly for \( P^u \). The other condition is that there are constants \( K > 0 \) and \( 0 < \alpha < 1 \) where
\[
\begin{align*}
\| P^t(g(x)) \nabla(g(x)) (x) P^t(x) v \| & \leq K \alpha^k \| P^t(x) v \|, \\
\| P^u(g(x)) \nabla(g(x)) (x) P^u(x) v \| & \geq (1/K \alpha^k) \| P^u(x) v \|
\end{align*}
\]
for all \( k > 0 \). Split \( \delta x = u + v \) where \( u_k \in \text{ range } P^t(z_k) \) and \( v_k \in \text{ range } P^u(z_k) \).

Put \( y_k = P^t(u_{k+1}; \nabla g(x)_k) \) and \( \xi_k = P^u(z_{k+1}; \nabla g(x)_k) \). Then the equations for the Newton’s method become
\[
\begin{align*}
u_{k+1} = & \ - \nabla g(x_k) u_k = y_k, \\
\xi_{k+1} = & \ - \nabla g(x_k) \xi_k = \xi_k.
\end{align*}
\]

Now we solve for \( u_k \) by going forward in time, and for \( \xi_k \) by going backward in time. If we write \( \nabla g(z_k) \) for \( P^t(u_{k+1}) \nabla g(z_k) P^u(z_k) \) and similarly for \( \nabla g(z_k) \) we can write
\[
\begin{align*}
u_k = & \sum_{i \leq k} \nabla g(z_i) \cdots \nabla g(z_k) y_k, \\
\xi_k = & \sum_{k \leq i} (\nabla g(z_k))^{-1} \cdots (\nabla g(z_i))^{-1} \xi_i
\end{align*}
\]
where the inverses \( (\nabla g(z_k))^{-1} \) are understood as linear maps:
\[
\text{range } P^u(z_{k+1}) \to \text{ range } P^u(z_k).
\]

Thus we get
\[
\| u_k \| \leq \sum_{k \leq i} K \alpha^{-i} \| y_i \| \leq \frac{K_0}{1 - \alpha} \| y \|_\infty
\]
\[
\| \xi_k \| \leq \sum_{k \leq i} (K \alpha^{-i})^{-1} \| \xi_i \| \leq \frac{1}{K(1 - \alpha)} \| \xi \|_\infty
\]
Thus there is a constant \( C \) such that \( \| \delta x \|_\infty \leq C \| G(x) \|_\infty \leq C \delta \) for a \( \delta \)-pseudo orbit.
To complete the proof we need to use the Newton–Kantorovich lemma which gives a lower bound on the radius of convergence of Newton’s method in terms of \(\|\nabla^2 f(x)\|_\infty\) and the Lipschitz constant of \(\nabla^2 f(x)\). To get the second quantity we need to look at
\[
(\nabla^2 f(x) - \nabla^2 f(y)) u_k = (\nabla f(y_k) - \nabla f(x_k)) y_k.
\]
Suppose that \(L\) is a Lipschitz constant for \(\nabla f\), then
\[
\|\nabla^2 f(x) - \nabla^2 f(y)\|_\infty \leq L \|x - y\|_\infty.
\]
(Actually, we just need \(L \geq \sup_k L_k\) where \(L_k\) is the sum of local Lipschitz constants for \(\nabla f\) at \(x_k\) and \(y_k\). Thus, provided we have \(x_k\) and \(y_k\) bounded and \(g\) is \(C^1\) we can get a suitable local constant for \(\nabla^2 f\).)

Given this Lipschitz constant \(L\), the Newton method will converge provided \(\delta < 1/(C^2 L)\). The value of \(\varepsilon\) is of the order of \(C\delta\).

9.2. Numerical methods for shadows

Hammel, Yorke and Grebogi (1987) is an early paper on numerical shadowing in the case of the logistic map \(x_{n+1} = g(x_n; a) = ax_n(1 - x_n)\). In this one-dimensional case they can use a version of interval arithmetic.

This works by computing a finite sequence \((x_k)\) for \(k = 0, 1, 2, \ldots, N\) which is a \(\delta\)-pseudo orbit. In practice the \(\delta\) is a modest multiple of machine epsilon. Then a sequence of intervals is constructed, starting with \(I_N = [x_N, z_N]\). Given \(I_n\), we compute \(I_{n+1}\) to be an interval containing \(x_{n+1}\) such that \(I_n \subseteq g(I_{n+1})\). This nesting condition allows the computation of a sequence of intervals whose width generally doesn’t grow as \(n\) increases. This is because the logistic map is generally expansive, and their are no stable subspaces.

Hammel, Yorke and Grebogi claim that with the initial pseudo orbit of \(10^7\) iterates calculated with \(a = 3.8\) and \(\delta = 3 	imes 10^{-14}\), there was a shadowing radius \(\varepsilon = 10^{-6}\). To get this sort of accuracy with a straightforward direct iteration would require computations with about \(10^{13}\) digits.

Multidimensional systems require a more delicate approach which separates out the stable and the unstable subspaces. A Newton method can be set up using a truncated version of \(G\) and \(\nabla G\), and in fact works well, except that the Newton equations are under-determined with \(nN\) unknowns and \(n(N-1)\) variables. A standard QR approach is not optimal here, as we want to minimise the \(\|\cdot\|_\infty\) norm of the correction, not the 2-norm as is usual. For getting a Newton correction, a stable factorisation procedure such as LU with partial pivoting or QR factorisation should be used.

9.3. Shadowing autonomous ODEs

Shadowing autonomous ODEs has some subtleties that are not present in the problem of finding shadows for maps. The main problem is that the maps generated by flows are not actually hyperbolic; there is one Lyapunov exponent which is zero corresponding the direction of the flow. This is not just an artefact, but a real effect. To see this, suppose we have a limit cycle for, say, the van der Pol equation (see §2.5) or some other equation. If we perturb one of the parameters in the van der Pol equation we would get a new limit cycle. Can we shadow an orbit in one limit cycle by an orbit in the other limit cycle? If the two limit cycles have different periods, the answer is no. No matter how small the difference is, if you wait long enough then the two cycles will go out of phase and then back in phase. Shadowing autonomous ODEs has to also involve stretching or compressing the time variable as well.

Shadowing algorithms for autonomous ODEs have been developed, and these work by “factoring out” the time aspect. The simplest and most direct way to do this is in
terms of what are effectively Poincaré cross sections. About every point in a numerically computed flow \( \tilde{z}(t_k) \), a local Poincaré cross section can be set up which is the plane passing through \( z(t_k) \) normal to \( f(\tilde{z}(t_k)) \). The shadow trajectory that is computed (or whose existence is verified) crosses this cross section at a different time \( t_k + \tau_k \) where \( |\tau_k - \tau_k^-| \) is always small. The lack of hyperbolicity shows up in the fact that we can have \( \tau_k \to \infty \) as \( k \to \infty \), at least at a linear rate.

10. Concluding remarks

Inertial manifold theory shows how dissipative infinite-dimensional dynamical systems, such as the Navier-Stokes equation, can give rise to low-dimensional dynamical systems that can be studied using the tools developed in this article. In the Appendices we pointed out that nonequilibrium statistical mechanics takes this idea a step further back, by seeking to explain the origin of the dissipation in terms of irreversibility produced by coarse-graining of the fundamental, microscopic dynamics. This is a metaphor, and perhaps an instructive paradigm for attacking other complex systems in which there is an overwhelmingly large number of microscopic elements.

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Glossary

This glossary defines, rather heuristically, basic terms assumed known in the text. For a deeper understanding of their meaning the reader is referred to appropriate text books. Words defined in this glossary are flagged by bold type when first used in a section. For concepts defined in the text, please consult the index of this book. We assume that the basic set theory symbols \( \in \) (element of), \( \subseteq \) (subset of), \( \supset \) (superset of), \( \cup \) (union) and \( \cap \) (intersection) are understood.

action-angle transformation: A transformation of a Hamiltonian system (q.e.) such that the Hamiltonian does not depend on the new coordinates (the angles) and that the new momenta (the actions) are conserved. Such a transformation does not generally exist. When it does, the system is called integrable.

autonomous: An autonomous dynamical system is one in which there is no explicit time dependence in the equations of motion. Physically this corresponds to a closed system — one not driven by external forces, but evolving purely due to the mutual interactions of its component parts.

attractor: A set of points towards which trajectories of a dissipative dynamical system evolve as time increases to infinity. Such a set is invariant under the dynamical system, the simplest attractor being a fixed point in phase space. More complicated attractors are possible, e.g. periodic orbits or limit cycles, and can even be chaotic — the strange attractors, which have structure on all scales.

ball: The interior of the sphere of a given radius (in a space with a metric, so that length is defined). See unit ball.

diffeomorphism: A \( C^\infty \)-diffeomorphism is a map that is \( n \)-times differentiable and whose inverse function exists and is also \( n \)-times differentiable. For instance, if we take a rubber sheet and deform it by stretching it in an arbitrarily non-uniform but smooth
way, without tearing it or folding it, then we are applying a diffeomorphism to the points on the sheet.

**Differentiable**: A function \( f(x) \) is \( n \)-times differentiable (\( f \) belongs to \( C^n \)) if its \( n \)th derivative is finite and continuous.

**Full rank**: An \( m \times n \) matrix is full rank for \( m \geq n \) if all of its columns are linearly independent, and full rank for \( n \geq m \) if all of its rows are linearly independent. If a matrix is full rank then the number of linearly independent rows or columns is the maximum possible.

**Inf**: The infimum, or greatest lower bound, \( a = \inf a_n \) of a sequence \( \{ a_n \} \) is the greatest number such that \( a \leq a_n \) for all \( n \).

**Irreversibility**: The phenomenon whereby closed macroscopic systems are observed always to evolve, as time increases, toward a more disordered state (a state of higher entropy). This means that dynamical systems describing macroscopic motions are typically not invariant under time-reversal (due to terms describing transport effects like diffusion or viscous dissipation).

**Hamiltonian**: As noun — A scalar function of generalised positions \( q \) and momenta \( p \) whose partial derivatives with respect to these variables give, respectively, the negative of the time rates of change of the conjugate momenta \( \{ p_i = -\partial H/\partial q_i \} \) and the time rates of change of the generalised positions \( \{ q_i = \partial H/\partial p_i \} \), thus giving a very compact way of specifying the dynamical system. As adjective — the property of possessing such a Hamiltonian function. A Hamiltonian dynamical system is non-dissipative and conserves phase-space volume, so that it cannot have attractors.

**Jordan canonical form**: Any square matrix \( A \) may be transformed to the Jordan canonical form \( B = R^{-1} AR \) (where \( R \) is some nonsingular matrix — this is known as a similarity transformation) in which only the diagonal entries and those immediately above the diagonal may be non-zero, with the entries above the diagonal being either \( 0 \) or \( 1 \) and the entries on the diagonal being the eigenvalues. A Jordan block is a submatrix of \( B \) with diagonal composed of equal eigenvalues, and with \( 1 \)s above the diagonal.

**Lebesgue measure**: In one dimension, the total length of a set of intervals; in two dimensions, the total area of a set of areas; in three dimensions the total volume of a set of volumes, and so on. The Lebesgue measure of an infinite set may or may not be non-zero (e.g. the irrational numbers on the unit interval are of measure unity, whereas the rational numbers are of zero measure).

**Lipschitz**: A function \( f(x) \) is Lipschitz at \( x \) if there exist \( M \) and \( \delta \) such that \( |f(y) - f(x)| < M|y - x| \), where \( M \) is the Lipschitz constant. Such functions are not necessarily differentiable at \( x \) since there can be an infinite number of oscillations as \( a_n \), which, though bounded below, may not have a unique limit (e.g. \( a_n \) may wander chaotically as \( n \to \infty \)). This is distinct from the limit \( \inf a_n \) because \( \lim \inf a_n \) must be approached arbitrarily closely infinitely often as \( n \to \infty \), whereas \( \inf a_n \) must take into account points visited once or a finite number of times (see \( \inf \)).

**Lim sup**: Also denoted \( \lim \sup a_n \). This is the greatest limit point of an infinite sequence \( \{ a_n \} \). See the discussion of the analogous lower limit point \( \lim \inf \) above.

**Limit cycle**: A simple periodic attractor (a closed loop in the phase plane) that occurs in two-dimensional dissipative continuous-time dynamical systems (which cannot exhibit chaos because the Poincaré-Bendixson theorem shows that fixed points and limit cycles exhaust the possibilities for attractors of two-dimensional flows).

**Manifold**: A mathematical space that can locally be described by a Cartesian coordinate system. In general the local coordinates cannot be joined smoothly to form a single
Cartesian coordinate system. (We shall assume that the manifold itself is everywhere smooth—it is a differential manifold.) The problem is a topological one—e.g., Mercator’s projection is an attempt to describe a sphere by a Cartesian coordinate system, but it becomes singular at the poles. A manifold can always be regarded as a surface embedded in a higher dimensional space, though it is not always natural to do this—e.g., what space is the curved space-time of general relativity embedded in?

map: A map (also called a mapping or function) $f$ from a space $A$ to a space $B$ (abbreviated $f : A \to B$) is a rule for associating one or more elements of $B$ with any element of $A$. If the map is one-to-one and onto (i.e., each element of $B$ is associated uniquely with an element in $A$) then the inverse function $f^{-1} : B \to A$ exists and $f$ is called a bijection. If, further, $f$ and $f^{-1}$ are continuous, then $f$ is called a homeomorphism, while if they are smooth in some sense then it is called a diffeomorphism.

$\mathbb{R}$: The set of real numbers or the real line. $\mathbb{R}^n$ is an $n$-dimensional space describable globally by a Cartesian coordinate system.

renormalization group: A non-perturbative method, originally developed in elementary particle physics and equilibrium statistical mechanics, for calculating properties of a system at a critical point where there is structure on all scales that is selfsimilar when appropriate scaling factors are applied.

sup: The supremum, or least upper bound, $a = \sup a_n$ of a sequence $\{a_n\}$ is the least number such that $a \geq a_n$ for all $n$.

torus: An $n$-torus is an $n$-dimensional manifold such that $n$ topologically distinct (i.e., not deformable into one another) closed curves can be drawn on it. A 1-torus is a (topological) circle, and a 2-torus has the topology of the familiar doughnut or anchor ring shape which gives rise to the generic name. A coordinate system on an $n$-torus consists of $n$ angle-like variables. Plural tori.

unit ball $B_1$: A ball of unit radius. Used in conjunction with the notion of addition of sets in a vector space: $A + rB_1$, to imply the “padding out” of the set $A$ by taking the union of all balls of radius $r$ centred on the points comprising $A$.

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