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978-0-521-49672-8 - Dynamical Systems and Numerical Analysis

A. M. Stuart and A. R. Humphries

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Dynamical systems are pervasive in the modelling of naturally occurring phenomena. Most of the models arising in practice cannot be completely solved by analytic techniques; thus, numerical simulations are of fundamental importance in gaining an understanding of dynamical systems. It is therefore crucial to understand the behaviour of numerical simulations of dynamical systems in order to interpret the data obtained from such simulations and to facilitate the design of algorithms which provide correct qualitative information without being unduly expensive. These two concerns lead to the study of the convergence and stability properties of numerical methods for dynamical systems.

The first three chapters of this book contain the elements of the theory of dynamical systems and the numerical solution of initial-value problems. In the remaining chapters, numerical methods are formulated as dynamical systems, and the convergence and stability properties of the methods are examined. Topics studied include the stability of numerical methods for contractive, dissipative, gradient, and Hamiltonian systems together with the convergence properties of equilibria, phase portraits, periodic solutions, and strange attractors under numerical approximation.

This book will be an invaluable tool for graduate students and researchers in the fields of numerical analysis and dynamical systems.

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Dynamical Systems and Numerical Analysis

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Preface

Dynamical systems are pervasive in the modelling of naturally occurring phenomena. Problems as diverse as the simulation of planetary interactions, fluid flow, chemical reactions, biological pattern formation and economic markets can all be modelled as dynamical systems. The theory of dynamical systems is concerned primarily with making qualitative predictions about the behaviour of systems which evolve in time, as parameters which control the system, and the initial state of the system itself, are varied. Most of the models arising in practice cannot be completely solved by analytic techniques and thus numerical simulations are of fundamental importance in gaining understanding of dynamical systems. Hence it is crucial to understand the behaviour of numerical simulations of dynamical systems in order that we may interpret the data obtained from such simulations and in order to facilitate the design of algorithms which provide correct qualitative information without being unduly expensive. These issues are at the heart of this book.

The long-time dynamics of a system are captured in *limit sets* which are particular types of *invariant sets* – sets which are mapped into themselves under the evolution equation. Examples of invariant sets are steady state solutions, periodic solutions, quasi-periodic solutions or chaotic solutions. The basin of attraction of a limit set is the set of initial data which evolves towards the given limit set under the dynamical system. A fairly complete picture of a dynamical system may be obtained by determining all possible limit sets, determining how these limit sets change with respect to control parameters in the system, and then determining the basins of attraction of individual limit sets. This is suggestive of an overall strategy for the numerical investigation of a dynamical system:

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STEP I Perform simulations of the dynamical system for a variety of different initial conditions and a variety of different system parameters. In so doing, determine candidate limit sets.

STEP II Where possible, set up *defining equations* for the limit sets observed and solve these numerically, varying the system parameters to obtain families of limit sets. Examples of such defining equations are the equations governing the existence of steady states or the two-point boundary-value problem (in time) governing the existence of periodic solutions.

STEP III Having obtained a thorough understanding of the possible limit sets in the system, and their dependence upon parameters, perform further numerical simulations to gain a deeper understanding of the basins of attraction.

STEP IV Iterate on this process, incorporating additional information from, for example, analytic and geometric study of the equations to motivate choice of initial conditions and parameters.

Steps I, II and III comprise two distinct approaches to computations associated with the dynamical system. The first approach, employed in Steps I and III, is a straightforward integration of the initial value problem; it is termed the *indirect approach* since the limit sets are observed indirectly as a consequence of the initial-value simulation. The second approach, employed in Step II, requires the development of special techniques tailored to compute particular invariant sets such as equilibria and periodic solutions; this approach is termed the *direct approach* since the limit sets are computed directly. (To the best of our knowledge, the terminology “direct” and “indirect” was introduced in this context by W.-J. Beyn in [35].) In this book we concentrate entirely on the indirect approach. The subject of direct methods is sufficiently large to warrant a separate volume in itself; we do, however, give a number of references to direct computational techniques at the end of Chapter 6.

In the classical numerical analysis of initial-value problems two questions are of fundamental importance. These are the *convergence* and the *stability* of the numerical method. We briefly discuss these questions and, at the same time, describe suitable generalisations to the dynamical systems context which is the focus of this book. Consider an initial value problem of the form

$$\frac{du}{dt} = f(u), \quad u(0) = U,$$

where $u(t) \in \mathbb{R}^p$ for each $t \in \mathbb{R}^+$ and $f : \mathbb{R}^p \mapsto \mathbb{R}^p$. We introduce the constant time-step Δt and the points $t_j = j\Delta t$, $j = 0, 1, \dots$. The numerical approximation to $u(t_j)$ is denoted by U_j . We define the error at time t_j by

$$e_j := \|u(t_j) - U_j\|$$

for some norm $\|\bullet\|$ on $\mathbb{R}^p$. Convergence and stability are now discussed in turn.

Convergence Under reasonable smoothness and well-posedness assumptions a bound of the form

$$e_j \leq c_1 e^{c_2 T} \Delta t^r, \quad \forall j, \Delta t : 0 \leq t_j \leq T,$$

may be found for some positive constants c_1 and c_2 . Of course such a bound is very important in the numerical analysis of initial-value problems and should be regarded as a minimal requirement for any method. Note, however, that in the context of Step I outlined above such a bound is of limited value since Step I involves computing over long time-intervals until the limit sets of the equation are found. Thus for the concept of convergence to be of direct use in the simulation of dynamical systems we need ask a different convergence question. A natural generalisation is this:

Question I. Assume that the differential equation has a particular invariant set. Does the numerical method have a corresponding invariant set which converges to the true invariant set as $\Delta t \rightarrow 0$? If so, what is the rate of convergence?

For example, it is natural to ask whether the fixed points of the numerical method are close to the equilibria of the differential equation; it is natural to ask whether the numerical method has a closed invariant curve or invariant torus whenever the differential equation has a periodic solution or quasi-periodic solution; and finally it is natural to ask whether the numerical method has a strange “chaotic” attractor whenever the underlying differential equation has such an object. These and related questions will form a substantial portion of this book, especially Chapters 6 and 7. $\square$

Stability Roughly speaking, stability is concerned with controlling the effect of small perturbations on the numerical method. In particular the classical theory of numerical stability is concerned with finding methods which mimic the damping properties of certain model differential equa-

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tions under mild or no restrictions on the time-step. The first important model equation in this context is

$$\frac{du}{dt} = \lambda u, \quad u(0) = U$$

where $\operatorname{Re}(\lambda) < 0$ and $u(t) \in \mathbb{C}$ for each $t \in \mathbb{R}^+$. Clearly all solutions of this equation decay to zero as $t \rightarrow \infty$ and much of numerical stability theory is concerned with finding conditions under which numerical methods mimic this property. For most methods a restriction on Δt in terms of λ will be required to ensure this occurs; for certain special methods no such restriction on Δt is required. It is natural to seek generalisations of these ideas to nonlinear dynamical systems. Generally we can ask:

Question II. Assume that the vector field defining the differential equation has a particular structural property which confers certain properties on the dynamical behaviour of the equation. Find special numerical methods which inherit these structural properties under mild or no restrictions on the time-step or, for general numerical methods, find conditions on Δt under which these structural properties are inherited.

For example, there are classes of problems, called gradient systems, for which all limit sets are equilibria. It is natural to seek numerical methods for gradient systems with the property that, for any time-step, all limit sets are also the equilibria of the differential equation. For Hamiltonian problems the Hamiltonian is conserved by the differential equation and it is sometimes natural to seek numerical methods which automatically enforce this conservation property for all time-steps Δt . These and related questions will form a substantial portion of the book, especially Chapters 5 and 8. Alternatively it is also natural to look at arbitrary numerical methods and ask for conditions on Δt in terms of the parameters of the problem and the initial data under which certain dynamical properties are inherited. Such questions are investigated in Chapter 7. $\square$

The principal aim of the book is to address the above questions. There are now a considerable number of results concerning these questions in the literature. Our intention here is to collect these results together to form a comprehensive and cogent account of the indirect approach for the numerical analysis of dynamical systems. Thus we have endeavoured to include the majority of the basic results in this field. The account is intended to be accessible to anyone familiar with either dynamical systems or numerical analysis theory and, with a little work, to someone

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familiar with neither; we include the basic theory required from both fields in the first three chapters of the book. Nonetheless we progress to the boundaries of current research in the subject and hence knowledge of the contents (or just a fraction thereof) of this book should provide a thorough grounding for anyone wishing to pursue research in this area. Thus the book should be of use both to someone wishing to study this field for the first time, and to someone requiring a reference text for the major results in the field.

We now summarise the contents of the book. In Chapters 1 and 2 we lay the foundational theory of dynamical systems for maps and for ordinary differential equations respectively. The two chapters run parallel to one another; each section in Chapter 1 has a corresponding section in Chapter 2. The chapters start with a basic introduction to the idea of a dynamical system, including important issues such as existence, uniqueness and continuity with respect to initial data. This is followed by the definition of limit sets together with study of their properties. The concept of stability is introduced and followed by a discussion of bifurcation. Using bifurcation theory, chaos is introduced through the study of period-doubling in mappings and then, in Chapter 2, a connection is made between the theory of mappings and the theory of differential equations by using the Lorenz equations as an example. The concept of phase portraits is discussed and stable and unstable manifolds are defined and constructed by means of an abstract invariant manifold theorem. With a basic understanding of “chaotic” attractors from the study of period-doubling, the notion of a stable fixed point or periodic solution is generalised to the stability of a general invariant set and attractors are defined; the use of Lyapunov functions is extended to such attracting sets. Global properties of dynamical systems are then studied employing assumptions about the defining dynamical system such that a global attractor exists; these conditions include contractivity, dissipativity and a gradient flow assumption. In some cases, such as contractive and gradient problems, the structure of the global attractor may be completely determined and this theory is described. The last sections of the chapters are concerned with Hamiltonian differential equations and the underlying theory of symplectic mappings.

In Chapter 3 we introduce the basic numerical methods used to solve ordinary differential equations, namely Runge–Kutta and multi-step methods. We review the classical notions of order, consistency, zero-stability and convergence and follow this theory with a brief introduction to the topic of stiffness and the resulting concepts of stability.

In Chapter 4 we show how the standard numerical methods introduced in the previous chapter may be formulated as dynamical systems. Thus we study the existence, uniqueness and continuous dependence of solutions to the numerical methods. We prove two kinds of results. In the first we assume only some form of Lipschitz condition on the vector field arising in the differential equation. In the second we make stronger structural assumptions about the vector field motivated by those introduced in Sections 1.8 and 2.8. Having shown that the numerical methods have a local solution we then discuss more precisely the approximation properties of order and consistency introduced in the previous chapter. Finally we show how strictly zero-stable multistep methods behave like one-step methods after a sufficiently large number of time-steps. To be precise, we show that such multistep methods possess an attractive invariant manifold on which they behave as a one-step method. This enables us to use much of the theory of one-step methods to study multistep methods.

Chapter 5 is concerned with numerical stability: finding numerical methods which replicate the global properties introduced in Section 2.8 under mild or no restrictions on the time-step. For both Runge–Kutta methods and multistep methods we start with the classical theories of stability for linear problems and contractive nonlinear problems, building on this theory to study problems with more complicated dynamical behaviour such as dissipative and gradient problems.

Chapter 6 is concerned with the convergence of invariant sets under numerical approximation. We do not work with any particular class of numerical method but instead work with a general set of assumptions which includes all Runge–Kutta methods, together with multistep methods restricted to their one-step invariant manifold. The chapter starts with the standard convergence result for trajectories over a finite time interval and also includes a proof that the derivative of the semigroup with respect to initial data converges at the same rate. These results are then extended to the study of convergence over infinite time intervals when the true solution is asymptotic to an exponentially stable equilibrium point. The effect of numerical approximation on equilibria is then discussed and the properties of local phase portraits near equilibria studied. In particular, stable and unstable manifolds are shown to converge with the same order as the standard convergence of trajectories; furthermore, backward error analysis results are proved showing that every solution of the differential equation which remains near an equilibrium point can be approximated by a nearby solution of the numerical

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method starting with a different initial condition, independently of the time-interval under consideration. Finally, using techniques similar to those employed to show convergence of the unstable manifold, it is shown that periodic solutions of the differential equation become nearby closed invariant curves of the numerical method. For all invariant sets studied in this chapter the rate of convergence is the same and is given by the order of the numerical method.

In Chapter 7 both stability and convergence are studied. The structural assumptions of Section 2.8 are again studied but, in contrast to Chapter 5, we do not seek special methods which replicate these properties globally under mild or no restrictions on the time-step. Instead we seek conditions on the time-step Δt , depending upon initial data, which ensure that these conditions are enforced locally on a compact set. Using these conditions we deduce the existence of local attractors for the numerical method when the differential equation has a global attractor. Various methods are employed to prove these results, including a form of backward error analysis where the numerical method is shown to come from the samples of a nonautonomous perturbation of the original differential equation. Having shown the existence of numerical attractors, we turn our attention to the approximation properties of these numerical attractors, studying their convergence as $\Delta t \rightarrow 0$. It is not possible to prove convergence results as strong as those for the simpler invariant sets of Chapter 6 and this matter is investigated in some detail. The concepts of *upper and lower semicontinuity* of sets are used to formulate the results.

The final chapter, Chapter 8, is concerned with the numerical approximation of Hamiltonian and related problems. Two classes of methods are given special attention: those which preserve the symplectic two-form of the underlying differential equation and those which preserve the Hamiltonian. Arbitrary one-step symplectic methods for linear Hamiltonian problems are characterized and then symplectic Runge–Kutta and multistep methods characterized for nonlinear problems. For Hamiltonian-conserving methods a variety of different approaches is introduced. Both symplectic and Hamiltonian-conserving methods are shown to have favourable error propagation properties when applied to certain problems with periodic solutions. Finally a variety of other non-Hamiltonian problems with conservation properties is studied and a connection made between methods beneficial in this context and in the context of preservation of the symplectic two-form.

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A mathematical theory of the interaction between dynamical systems and numerical analysis has been developing steadily over the last fifteen years or so. Various conference proceedings, survey articles and reviews of the subject area which predate this book are contained in [35], [47], [48], [49], [187], [188], [244], [311], [314], [348] and [349]. We will attempt to survey the literature in detail at the end of each chapter but here in the preface it is interesting to mention a few of the names of key individuals who have developed the subject; the brief treatment given here is of course from a subjective viewpoint and we realise that many important contributions cannot be done justice in this short space. We hope the reader will bear with this. The nonlinear stability analyses of Chapter 5 stem to a large extent from the pioneering work of G. Dahlquist for multistep methods and K. Burrage and J. Butcher for Runge–Kutta methods. The attendant solvability theory for implicit methods, described in Chapter 4, was developed subsequently, and the seminal book of K. Dekker and J. Verwer is of central importance here. The work of M. Spijker and co-workers also underlies a substantial portion of the theory of Chapters 4 and 5. The convergence theory for invariant sets of numerical methods, described in Chapters 6 and 7, has been developed by several individuals but perhaps the works of W.-J. Beyn and J.K. Hale have been the most fundamental in establishing this subject area. The subject of numerical methods for Hamiltonian problems has generated a great deal of interest in recent years and again many people have contributed; of central importance in this field are the contributions of J.M. Sanz-Serna.

This book has developed from lecture courses on the theory of dynamical systems and the numerical analysis of dynamical systems given at the University of Bath and at Stanford University over the last five years. Thus, although it is primarily a research monograph, we anticipate that it can also be used as the basis for a variety of different courses. To this end we have included exercises, most of which have been tested in the classroom, at the end of each section. Chapters 1, 2 and 3 describe the basic theory of dynamical systems and of numerical methods so that the book can be used by individuals with a background in either area: those well grounded in dynamical systems need only pass briefly through Chapters 1 and 2 to familiarise themselves with notation whilst for those well grounded in the numerical analysis of ordinary differential equations the same considerations apply to Chapter 3.

Chapters 1 and 2 themselves form the basis of a single term or quarter course if studied in detail. Such a course is at the level of an advanced

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United Kingdom undergraduate student or a beginning level postgraduate student in the United States. A second follow-up course, discussing the numerical analysis of dynamical systems, can be built as desired from the remaining chapters. Those interested in stability issues would concentrate primarily on material from Chapters 3, 4, 5 and selected material from 7 and 8; those interested primarily in convergence of invariant sets would concentrate on material from Chapters 3, 4, 6, 7 and selected material from 8; those interested purely in Hamiltonian systems would concentrate on material from Chapters 3, 4 and 8. The course concerned with convergence of invariant sets is more demanding than the others and would probably be appropriate as an advanced graduate course in the United Kingdom or United States. The courses on numerical stability or on Hamiltonian problems are at the beginning graduate student level and could also be given to advanced undergraduates. Alternatively a single high-level course, lasting one term or quarter, can be given from the whole book if the material is selected carefully. At different times we have taught the material in the book in all of the different ways detailed above. Our approach in teaching this subject reflects a general principle which can be applied throughout mathematics: *computation and numerical analysis should often be taught as an integral part of courses in applied mathematics and applied analysis, and not as separate courses in their own right.*

The book is concerned primarily with ordinary differential equations and their approximation. This was a difficult choice to make, particularly as much of the material in the book appeared originally in the context of partial differential equations. However, in order to allow a very general and complete description we have decided to concentrate on finite dimensions. We nonetheless believe that the book will be of use to people working in the field of partial differential equations. To assist in this, partial differential equations are discussed briefly in some of the exercises and extensive references to the literature concerning partial differential equations are also given.

We conclude with a table briefly summarising the inter-connectivity of this book. This will be useful for those individuals who wish to teach the material or for those who wish to use the book as a reference volume. Note that Sections 1.1, 1.2, 2.1, and 2.2 are required as basic background throughout the book, and also that the first section of each chapter is required for the remainder of that chapter. Any sections not listed in the accompanying table have no other required reading.

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8.2	1.9, 2.9
8.3	1.9, 2.9, 3.2
8.4	1.9, 2.9, 3.3
8.5	1.9, 2.9
8.6	1.9, 2.9, 7.2
8.7,	1.9, 2.9, 7.2
8.8	1.9, 2.9

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