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Bernd Krauskopf · Hinke M. Osinga · Jorge Galán-Vioque (Eds.)

Numerical Continuation Methods for Dynamical Systems

Path following and boundary value problems

With 200 Figures

Dedicated to Eusebius J. Doedel for his 60th birthday

Springer

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A Continuing Influence in Dynamics

A well-established method for studying a given dynamical system is to identify the compact invariant objects, such as equilibria, periodic orbits and invariant tori, and to consider the local behavior around them. This local information then needs to be assembled in a consistent way, frequently with the help of geometric and topological arguments, to obtain a unified global picture of the system. The aim is to find qualitative (and often also quantitative) representations of the different types of behavior that the system may exhibit in dependence of key parameters. The main result of such an effort is a bifurcation diagram, that is, information on the division of parameter space into regions of topologically different behavior together with representative phase portraits. The list of theoretical tools one may employ is long, well developed and dates back at least to the 19th century. However, even when one considers seemingly simple systems, theoretical tools need to be supplemented with numerical calculations.

Mainly for technological reasons, numerical methods have a shorter history than theoretical tools. The first and commonly used tool is numerical time integration, which allows one to explore the dynamics by solving a (possibly large) number of initial value problems. This approach is very practical for the representation of chaotic attractors, and especially their 'fingerprints' in a suitable Poincaré section. However, when it comes to the study of how the behavior changes as a function of parameters the tool of choice is numerical continuation — one also speaks of path following or homotopy methods. The basic idea is to compute an implicitly defined curve of a suitable system of equations that defines the dynamical object under consideration. In its basic form, numerical continuation implements the stability and bifurcation theory of equilibria of differential equations. More global objects, such as periodic and homoclinic orbits, and their bifurcations can be computed by setting up defining equations in the form of boundary value problems.

Path following in combination with boundary value problem solvers has emerged as a continuing and strong influence in the development of dynamical systems theory and its application in many diverse fields of science. It is widely acknowledged that the software package AUTO — developed by Eusebius J. Doedel about thirty years ago and further expanded and developed ever since — plays a central role in the brief history of numerical continuation. When we were thinking how best to present the origin and development of AUTO, a copy of the first edition of the AUTO86 manual, with its authentic ochre Caltech cover, came in very handy. We quote from the preface, dated May 1986:

> *The* AUTO *package was first written in 1979. It was based on a related program written in 1976 while the author was working with H.B Keller at the California Institute of Technology. A first publication referring to the package by its current name appeared in [22].*
>
> *Applications often revealed some inadequacy in the algorithms and resulted in changes. The applications also pointed to additional capabilities that would be useful to have integrated in the package, and effort was spent on making it easy to use. This explains the delay in publication of an extensive account of the algorithm implemented. Indeed, the difference in effort between a theoretical analysis of a new method and its implementation and integration appears to be considerable. We are confident, however, that the methods and software presented here will be of some use in the numerical exploration of nonlinear phenomena in ordinary differential equations.*

This quote not only highlights the intricate interplay at the very earliest stage between the development of the software and applications, but it also contains a major understatement: AUTO has not just been "of some use", but it has been used by many hundreds of researchers from all around the world! To give a rough idea of its impact in the general scientific community, ISI Web of Knowledge reveals that the different versions of the AUTO manual, which was never published other than as a Caltech preprint, has more than 700 citations. Similarly, the seminal reference [22] in the quote, the paper E.J. Doedel, AUTO: A program for the automatic bifurcation analysis of autonomous systems, *Cong. Num.* 30 (Proc. 10th Manitoba Conf. Num. Math. and Comp.), 1981, 265–284, has more than 400 citations.

This book has been compiled on the occasion of Sebius Doedel's 60th birthday with the aim to illustrate the power and versatility of numerical continuation techniques. As is demonstrated in the chapters of this book, many recent developments build on the ideas of Sebius Doedel as implemented in the package AUTO, whose core of path following routine and collocation boundary value problem solver is essentially still the same as when it was released in 1986. It lies in the nature of the subject and the versatility of Sebius Doedel's work that we had to make a choice about which topics to include. The emphasis of this book is on continuation methods for different types of systems and dynamical objects, and on examples of how numerical bifurcation analysis can be used in concrete applications. While recognizing that there are other topics that could have been included, we believe that this choice is in the spirit of the original motivation for the development of AUTO as expressed in the above quote. In this way, we hope to give an impression of the continuing influence and future potential of these powerful numerical methods for the bifurcation analysis of different types of dynamical systems.

The book opens with an extended foreword by Herb Keller, who is widely recognized as the founding father of numerical continuation. Chapter 1 is an edited part of lecture notes that Sebius Doedel has been using in his own courses. It introduces the basic concepts of numerical bifurcation analysis and forms a basis for the remainder of the book. The other eleven chapters by leading experts focus on selected topics that have been influenced strongly by Sebius Doedel's work. In fact, at least half of the chapters discuss research in which he has been involved as a co-author. Chapter 2 by Willy Govaerts and Yuri Kuznetsov surveys recent developments of interactive continuation tools. Chapter 3 by Mike Henderson is concerned with higher-dimensional continuation, and Chap. 4 by Bernd Krauskopf and Hinke Osinga discusses the computation of invariant manifolds with a continuation approach. The next three chapters are devoted to applications. In Chap. 5 Don Aronson and Hans Othmer consider the dynamics of a SQUID consisting of two Josephson junctions. Chapter 6 by Sebastian Wieczorek discusses global bifurcations in laser systems, and Chap. 7 by Emilio Freire and Alejandro Rodríguez-Luis demonstrates the use of numerical bifurcation analysis for the study of electronic circuits. The remaining chapters deal with continuation for special types of dynamical systems. Chapter 8 by John Guckenheimer and Drew LaMar is concerned with slow-fast systems, and Chap. 9 by Jorge Galán-Vioque and André Vanderbauwhede with symmetric Hamiltonian systems. Spatially extended systems are the topic of Chap. 10 by Wolf-Jürgen Beyn and Vera Thümmler and of Chap. 11 by Alan Champneys and Björn Sandstede. Finally, in Chap. 12 Dirk Roose and Róbert Szalai survey numerical continuation techniques for systems with delay.

We are very grateful for the enthusiastic support from all who were involved in this book project. First of all, we thank all authors for their contributions and for making every effort to stay within the limits of a tight production schedule. We also thank Tom Spicer of Canopus Publishing Ltd for his support of this project from its conception to the final production of the book. Last, but not least, we would like to thank Sebius Doedel for his support over many years of collaboration, and for agreeing to the publication of Chap. 1 without knowing exactly what we were up to. Happy birthday, Sebius!

Bernd Krauskopf, Hinke Osinga and Jorge Galán-Vioque
Bristol and Sevilla, March 2007.

Foreword

Herbert B Keller

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Sebius (diminutive for Eusebius) Doedel obtained his Ph.D. in Applied Mathematics from the University of British Columbia in 1976. His advisor was my friend and ex-colleague Jim Varah. As a consequence, I was able to employ Sebius as a Research Fellow in Applied Mathematics at Caltech in 1975. Over the next 26 years, he spent 13 of them at Caltech. However, he was also much appreciated at Concordia University, where he was employed in 1979 and rapidly rose to Professor of Computer Science, winning many awards which fortunately included several years on leave with pay!

We cycled together occasionally, even in Holland, where Sebius was born. I remember one ride in particular, when on a rather warm day we went east from Pasadena to Claremont, about 28 miles each way. Somewhere along the way, I became quite thirsty and so we stopped to get a cool drink. We sat outside, relaxed and, I thought, enjoyed our drinks. I started to wax poetic about how nice it was enjoying the outdoors and lovely California weather when Sebius said: "Herb, do you know where we are?" I said: "sure, near Claremont." He replied: "This is Pomona, the drive-by shooting capital of the world — I can't wait to get out of here." I have never again enjoyed going past that part of our ride.

Early during his first appointment at Caltech, Sebius became interested in bifurcation phenomena, two-point boundary value problems and numerical path-following or continuation methods, perhaps as a result of sitting in on my course in these areas. In 1976, I was writing the paper [17] in which pseudoarclength continuation was introduced and Sebius was willing to do some calculations to illustrate how these methods worked. Of course, he did a wonderful job producing all of the results in §7 of that paper, but more importantly, as a result, he essentially started working on AUTO at that time. The first publication on AUTO appeared in 1981 [7]. It has evolved dramatically since then, culminating in AUTO2000 [22], a fully parallel code in C++ with great graphics (available for free via `http://sourceforge.net/projects/auto2000/`) that was produced mainly by Randy Paffenroth, working at Caltech under Sebius's direction.

AUTO is without a doubt the most powerful and efficient tool for determining the bifurcation structure of nonlinear parameter-dependent systems of algebraic and ordinary differential equations. Influenced by his colleagues at the University of British Columbia, who developed COLSYS [5], Sebius has employed orthogonal collocation approximations and mesh refinement to obtain extremely high accuracy. The code is able to determine heteroclinic, homoclinic and periodic orbits, both stable and unstable, by means of a two-point boundary value problem formulation. Using a brilliant elimination procedure, the relatively sparse Jacobian is reduced to a low-dimensional dense matrix from which the Floquet multipliers are computed. The bifurcation structure at singular points is readily determined in this way.

The development of AUTO is but one of the main projects that Sebius has undertaken. In the course of this work powerful theoretical results have been produced, many with colleagues and his students, in the general areas of bifurcation theory, dynamical systems, periodic orbits, delay differential equations, collocation methods for nonlinear elliptic PDEs, coupled oscillator theory, control of bifurcation phenomena, continuation theory of manifolds, and numerous additional topics. However, there is no doubt that the AUTO software has had a tremendous impact on many applied mathematics areas and is, indeed, one of the leading tools in scientific computing. The code has been incorporated into many other large software systems that solve nonlinear problems involving continuation and bifurcation phenomena.

Essentially, all of the authors contributing to this volume have been coauthors with Sebius on papers related to the work presented here. However, I would like to point out a few of my favorite contributions made through these collaborations, not all of which have been fully appreciated yet. A brilliant contribution is contained in a paper by Wolf-Jürgen Beyn and Sebius Doedel [6], in which it is shown that a continuous nonlinear boundary value problem and the corresponding discretized problem have the same number of solutions for all sufficiently fine meshes.

Sebius introduced a very powerful technique to keep computed families of periodic solutions of autonomous differential equations in phase. The idea is simply to minimize the 'distance' between neighboring solutions with respect to a change in phase. That is, if $\mathbf{u}(t, \lambda)$ is the solution over the normalized period $0 \leq t \leq 1$ at parameter value λ, then the neighboring solution $\mathbf{u}(t, \lambda+\delta)$ with phase shift θ lies at distance

$$D^2(\theta) = \int_0^1 \| \mathbf{u}(t+\theta, \lambda+\delta) - \mathbf{u}(t, \lambda) \|^2 \; dt.$$

We seek to minimize this distance with respect to the phase shift θ. Standard calculus of variations near zero leads to the integral condition

$$\int_0^1 \dot{\mathbf{u}}^*(t, \lambda+\delta) \, \mathbf{u}(t, \lambda) \; dt = 0.$$

This is a generalization of the standard Poincaré phase or transversality condition that is applied only at one point on the orbit. However, the above global condition is much more robust in calculations, as has been shown in many examples [9, 10, 12] (the Poincaré condition remains preferable for analytical proofs). I am not sure when this global condition first appeared in the literature, but we have referred to it in [16] as having been introduced by Sebius in 1981 [7], which also happens to be his first publication on AUTO.

Many of Sebius's publications have to do with periodic solutions of dynamical systems. These arise in a great variety of applications starting with chemical reactors [23], then on to systems of oscillators [2, 21], heteroclinic orbits [9] in which the above phase condition is crucial, resonances in excitable systems [1] such as forced Fitzhugh-Nagumo systems, current biased and coupled Josephson junctions [3, 4], delay differential equations [11, 13, 14], modified Van der Pol oscillators [8], conservative and Hamiltonian systems [20], cardiac pacemakers [19], the circular restricted three-body problem and the figure-eight orbit of Chenciner and Montgomery [12, 15], and many more. A large number of these contributions are in the bio-physics area and, thus, it turns out that Sebius may be a closet biologist.

More recently, Sebius has returned with others to the important problem of computing higher-dimensional manifolds, either stable or unstable [18].

This brief account of some of Sebius's publications and obvious collaborations does not do justice to the impact he has had in the field of scientific computation. He has had numerous students, extremely well trained, and now making their own contributions. Furthermore, he has worked with many outstanding scientists and has invariably enhanced their ability to do significant scientific computations so much that it would be difficult to measure his tremendous influence in our field. Hopefully, he will continue as he reaches maturity.

H. B. Keller
Caltech / UCSD
November, 2006

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1

Lecture Notes on Numerical Analysis of Nonlinear Equations

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Numerical integrators can provide valuable insight into the transient behavior of a dynamical system. However, when the interest is in stationary and periodic solutions, their stability, and their transition to more complex behavior, then numerical continuation and bifurcation techniques are very powerful and efficient.

The objective of these notes is to make the reader familiar with the ideas behind some basic numerical continuation and bifurcation techniques. This will be useful, and is at times necessary, for the effective use of the software AUTO and other packages, such as XPPAUT [17], CONTENT [24], MATCONT [21], and DDE-BIFTOOL [16], which incorporate the same or closely related algorithms.

These lecture notes are an edited subset of material from graduate courses given by the author at the universities of Utah and Minnesota [9] and at Concordia University, and from short courses given at various institutions, including the Université Pierre et Marie Curie (Paris VI), the Centre de Recherches Mathématiques of the Université de Montréal, the Technische Universität Hamburg-Harburg, and the Benemérita Universidad Autónoma de Puebla.

1.1 The Implicit Function Theorem

Before starting our discussion of numerical continuation of solutions to nonlinear equations, it is important first to discuss under what conditions a solution will actually persist when problem parameters are changed. Therefore, we begin with an overview of the basic theory. The Implicit Function Theorem (IFT) is central to our analysis and we discuss some examples. The discussion in this section follows the viewpoint of Keller in graduate lectures at the California Institute of Technology, a subset of which was published in [23].

1.1.1 Basic Theory

Let $\mathcal{B}$ denote a Banach space, that is, a complete, normed vector space. In the presentation below it will be implicitly assumed that $\mathcal{B}$ is $\mathbb{R}^n$, although the results apply more generally. For $\mathbf{x}_0 \in \mathcal{B}$, we denote by $S_\rho(\mathbf{x}_0)$ the closed ball of radius ρ centered at $\mathbf{x}_0$, that is,

$$S_\rho(\mathbf{x}_0) = \{\mathbf{x} \in \mathcal{B} \mid \ \| \mathbf{x} - \mathbf{x}_0 \| \leq \rho\}.$$

Existence and uniqueness of solutions is obtained by using two theorems.

Theorem 1 (Contraction Theorem). *Consider a continuous function* $F : \mathcal{B} \to \mathcal{B}$ *on a Banach space* $\mathcal{B}$ *and suppose that for some* $\mathbf{x}_0 \in \mathcal{B}$, $\rho > 0$, *and some* K_0 *with* $0 \leq K_0 < 1$, *we have*

$$\begin{aligned} \| F(\mathbf{u}) - F(\mathbf{v}) \| &\leq K_0 \ \| \mathbf{u} - \mathbf{v} \|, \ \textit{for all } \mathbf{u}, \mathbf{v} \in S_\rho(\mathbf{x}_0), \\ \| F(\mathbf{x}_0) - \mathbf{x}_0 \| &\leq (1 - K_0)\, \rho. \end{aligned}$$

Then the equation

$$\mathbf{x} = F(\mathbf{x}), \qquad \mathbf{x} \in \mathcal{B},$$

has one and only one solution $\mathbf{x}_* \in S_\rho(\mathbf{x}_0)$, *and* $\mathbf{x}_*$ *is the limit of the sequence*

$$\mathbf{x}_{k+1} = F(\mathbf{x}_k), \qquad k = 0, 1, 2, \ldots .$$

Proof. Let $\mathbf{x}_1 = F(\mathbf{x}_0)$. Then

$$\| \mathbf{x}_1 - \mathbf{x}_0 \| = \| F(\mathbf{x}_0) - \mathbf{x}_0 \| \leq (1 - K_0)\, \rho \leq \rho.$$

Thus, $\mathbf{x}_1 \in S_\rho(\mathbf{x}_0)$. Now assume inductively that $\mathbf{x}_0, \mathbf{x}_1, \cdots, \mathbf{x}_n \in S_\rho(\mathbf{x}_0)$. Then for $k \leq n$ we have

$$\begin{aligned} \| \mathbf{x}_{k+1} - \mathbf{x}_k \| &= \| F(\mathbf{x}_k) - F(\mathbf{x}_{k-1}) \| \leq K_0 \ \| \mathbf{x}_k - \mathbf{x}_{k-1} \| \\ &= \qquad \cdots \qquad \leq K_0^k \ \| \mathbf{x}_1 - \mathbf{x}_0 \| \\ &\leq \quad K_0^k\, (1 - K_0)\, \rho. \end{aligned}$$

Thus,

$$\begin{aligned} \| \mathbf{x}_{n+1} - \mathbf{x}_0 \| &\leq \| \mathbf{x}_{n+1} - \mathbf{x}_n \| + \| \mathbf{x}_n - \mathbf{x}_{n-1} \| + \cdots + \| \mathbf{x}_1 - \mathbf{x}_0 \| \\ &\leq (K_0^n + K_0^{n-1} + \cdots + 1)\, (1 - K_0)\, \rho \\ &= (1 - K_0^{n+1})\, \rho \\ &\leq \rho. \end{aligned}$$

Hence $\mathbf{x}_{n+1} \in S_\rho(\mathbf{x}_0)$, and by induction $\mathbf{x}_k \in S_\rho(\mathbf{x}_0)$ for all k. We now show that $\{\mathbf{x}_k\}$ is a Cauchy sequence:

$$\begin{aligned}\|\mathbf{x}_{k+n}-\mathbf{x}_k\| &\le \|\mathbf{x}_{k+n}-\mathbf{x}_{k+n-1}\|+\cdots+\|\mathbf{x}_{k+1}-\mathbf{x}_k\|\\ &\le (K_0^{n-1}+K_0^{n-2}+\cdots+1)\,K_0^k\,(1-K_0)\,\rho\\ &= (1-K_0^n)\,K_0^k\,\rho\\ &\le K_0^k\,\rho.\end{aligned}$$

For given $\varepsilon > 0$, choose k such that $K_0^k\,\rho < \frac{1}{2}\,\varepsilon$. Then

$$\|\mathbf{x}_{k+\ell}-\mathbf{x}_{k+m}\|\le\|\mathbf{x}_{k+\ell}-\mathbf{x}_k\|+\|\mathbf{x}_{k+m}-\mathbf{x}_k\|\le 2K_0^k\,\rho<\varepsilon,$$

independently of ℓ and m. Hence, $\{\mathbf{x}_k\}$ is a Cauchy sequence and, therefore, converges to a unique limit $\lim \mathbf{x}_k = \mathbf{x}_*$, where $\mathbf{x}_* \in S_\rho(\mathbf{x}_0)$. Since we assumed that F is continuous, we have

$$\mathbf{x}_* = \lim \mathbf{x}_k = \lim F(\mathbf{x}_{k-1}) = F(\lim \mathbf{x}_{k-1}) = F(\lim \mathbf{x}_k) = F(\mathbf{x}_*).$$

This proves the existence of $\mathbf{x}_*$. We get uniqueness as follows. Suppose there are two solutions, say, $\mathbf{x},\mathbf{y} \in S_\rho(\mathbf{x}_0)$ with $\mathbf{x} = F(\mathbf{x})$ and $\mathbf{y} = F(\mathbf{y})$. Then

$$\|\mathbf{x}-\mathbf{y}\|=\|F(\mathbf{x})-F(\mathbf{y})\|\le K_0\ \|\mathbf{x}-\mathbf{y}\|\ .$$

Since $K_0 < 1$, this is a contradiction. □

The second theorem ensures the parameter-dependent existence of a solution.

Theorem 2 (Implicit Function Theorem). *Let* $\mathbf{G} : \mathcal{B} \times \mathbb{R}^m \to \mathcal{B}$ *satisfy:*

- $\mathbf{G}(\mathbf{u}_0, \boldsymbol{\lambda}_0) = \mathbf{0}$ *for* $\mathbf{u}_0 \in \mathcal{B}$ *and* $\boldsymbol{\lambda}_0 \in \mathbb{R}^m$*;*
- $\mathbf{G}_\mathbf{u}(\mathbf{u}_0, \boldsymbol{\lambda}_0)$ *is nonsingular with bounded inverse,*

  $$\|\mathbf{G}_\mathbf{u}(\mathbf{u}_0,\boldsymbol{\lambda}_0)^{-1}\|\le M$$

  for some $M > 0$*;*
- $\mathbf{G}$ *and* $\mathbf{G}_\mathbf{u}$ *are Lipschitz continuous, that is, for all* $\mathbf{u},\mathbf{v} \in S_\rho(\mathbf{u}_0)$*, and for all* $\boldsymbol{\lambda},\boldsymbol{\mu} \in S_\rho(\boldsymbol{\lambda}_0)$ *the following inequalities hold for some* $K_L > 0$*:*

  $$\begin{aligned}\|\mathbf{G}(\mathbf{u},\boldsymbol{\lambda})-\mathbf{G}(\mathbf{v},\boldsymbol{\mu})\| &\le K_L\,(\|\mathbf{u}-\mathbf{v}\|+\|\boldsymbol{\lambda}-\boldsymbol{\mu}\|),\\ \|\mathbf{G}_\mathbf{u}(\mathbf{u},\boldsymbol{\lambda})-\mathbf{G}_\mathbf{u}(\mathbf{v},\boldsymbol{\mu})\| &\le K_L\,(\|\mathbf{u}-\mathbf{v}\|+\|\boldsymbol{\lambda}-\boldsymbol{\mu}\|).\end{aligned}$$

Then there exists δ*, with* $0 < \delta \le \rho$*, and a unique function* $\mathbf{u}(\boldsymbol{\lambda})$ *that is continuous on* $S_\delta(\boldsymbol{\lambda}_0)$*, with* $\mathbf{u}(\boldsymbol{\lambda}_0) = \mathbf{u}_0$*, such that*

$$\mathbf{G}(\mathbf{u}(\boldsymbol{\lambda}),\boldsymbol{\lambda}) = \mathbf{0},\ \textit{for all}\ \boldsymbol{\lambda} \in S_\delta(\boldsymbol{\lambda}_0).$$

If $\mathbf{G}(\mathbf{u},\boldsymbol{\lambda}_0) = \mathbf{0}$ and if $\mathbf{G}_\mathbf{u}(\mathbf{u}_0,\boldsymbol{\lambda}_0)$ is invertible with bounded inverse, then $\mathbf{u}_0$ is called an *isolated solution* of $\mathbf{G}(\mathbf{u},\boldsymbol{\lambda}_0) = \mathbf{0}$. Hence, the IFT states that isolation (plus Lipschitz continuity assumptions) implies the existence of a locally unique *solution family* (or *solution branch*) $\mathbf{u} = \mathbf{u}(\boldsymbol{\lambda})$, with $\mathbf{u}(\boldsymbol{\lambda}_0) = \mathbf{u}_0$.