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NUMERICAL ANALYSIS AND CONTROL OF BIFURCATION PROBLEMS (I) BIFURCATION IN FINITE DIMENSIONS

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A number of basic algorithms for the numerical analysis and control of bifurcation phenomena are described. The emphasis is on algorithms based on pseudoarclength continuation for algebraic equations. Several illustrative examples computed with the AUTO software package are included. Part II of this paper deals with ordinary differential equations and will appear in the next issue.

1. Introduction and Examples

1.1. *Introduction*

This paper covers the contents of a one-semester graduate course given by Doedel at the University of Utah, at the University of Minnesota, and at Concordia University during the period 1987-1990. It is aimed at scientists and engineers who have a need for numerical techniques in the analysis of bifurcation problems that arise in their work.

The material mainly addresses numerical continuation and bifurcation techniques for nonlinear equations in the form of algebraic systems and ordinary differential equations. For the latter we consider only the boundary-value problem. However, as will be shown, this includes phenomena of interest in initial-value problems, for example, periodic solutions and homoclinic and heteroclinic orbits. Throughout, the fundamental tool is pseudo-arclength continuation which was introduced by Keller in 1977. For a closely related introductory account we refer to the Tata Institute Lecture Notes of Keller [1987], from which much of Sec. 2 of this paper was derived.

A considerable amount of original material is contained in this paper, especially in the sections on optimization and control of bifurcation problems. This material is the result of cooperation of Doedel and Kernévez on using Keller's continuation techniques in optimization and control problems. The presentation here mainly addresses optimization, but the techniques are ultimately aimed at controlling bifurcation phenomena. Work on the latter is in progress.

Most projects carried out by participants in the course on which this paper is based made use of the software package AUTO. The numerical examples in this paper were also computed using this package. However, this paper does not specifically deal with the software, which is fully described in Doedel & Kernévez, [1986]. The emphasis here is on stable and efficient implementation of basic numerical continuation and bifurcation techniques, whereas in AUTO, efficiency has in some cases been sacrificed for the sake of generality

and ease of programming. Furthermore, several algorithms described here have not been fully integrated in the software, although they can be defined by the user. This applies, in particular, to the optimization and control algorithms, and to the method for computing general heteroclinic connections. These shortcomings should be addressed at some time, and this paper describes some of the ground work for such a more efficient, robust and powerful package.

The software package AUTO was developed by Doedel in 1979 [Doedel, 1981]. The current version, AUTO86 [Doedel & Kernévez, 1986], is available from the Applied Mathematics Department at the California Institute of Technology and from the Computer Science Department at Concordia University. The package has been useful in several areas of research, and in some cases it has been integrated into a larger collection of software tools for investigating bifurcation phenomena. Also, many improvements have been suggested and sometimes these have been fully implemented elsewhere. In particular, Taylor and Kevrekidis (Chemical Engineering, Cornell University) have developed an interactive version for the Silicon Graphics Iris [Taylor & Kevrekidis, 1990], and Fairgrieve and Jepson (Computer Science, University of Toronto) have developed a significantly improved algorithm for computing the Floquet multipliers for periodic solutions [Fairgrieve *et al.*, *to appear*].

It is not our purpose here to provide a review of the literature on numerical continuation and bifurcation techniques, and our reference list is admittedly limited and one-sided. Texts in which these techniques play an important role include the books of Rheinboldt [1986], Kubiček and Marek [1983], and Seydel [1988]. See also the review paper on numerical methods for dynamical systems by Beyn [1990] for related references. An introduction to continuation methods can be found in the tutorial paper by Seydel [1991].

1.2. *A Two-compartment enzyme model*

In this and the following subsection we discuss in some detail a numerical analysis of two simple equations that arise in modeling biochemical reactions. The objectives are (i) to introduce and illustrate some bifurcation phenomena, (ii) to demonstrate the use of numerical techniques in the analysis of bifurcation problems, (iii) to mention some specific continuation methods to be covered in more detail later, and (iv) to mention some control objectives.

The equations describing both models are of the form

$$u'(t) = f(u,\lambda),\ u(\cdot), f(\cdot,\cdot) \in \mathrm{R}^n,\ \lambda \in \mathrm{R},\ t \geqslant 0 \quad . \quad (1.1)$$

First consider a one-substrate, enzyme-catalyzed reaction that takes place inside each of two identical compartments. These compartments are separated from each other by a membrane across which the substrate can diffuse. The compartments can also communicate through similar membranes with an outside reservoir. The enzyme (E) is present only inside the compartments, so that the reaction only takes place there. Schematically this system can be represented as indicated below.

$$s_0 \ \Big\| \ s_1,\ E \ \Big\| \ s_2,\ E \ \Big\| \ s_0 + \mu$$

Here s_1 and s_2 are the concentrations of the substrate S inside compartment 1 and 2 respectively, s_0 is the constant concentration of S external to compartment 1. The concentration of S external to compartment 2 is $s_0 + \mu$, where μ can be thought of as a perturbation.

A simple mathematical model of this situation is given by the following equations [Kernévez, 1980]

$$\begin{aligned} s_1' &= (s_0 - s_1) + (s_2 - s_1) - \rho R(s_1), \\ s_2' &= (s_0 + \mu - s_2) + (s_1 - s_2) - \rho R(s_2) \quad . \end{aligned} \quad (1.2)$$

We assume that the reaction rate is inhibited by an excess of substrate. More precisely, we take the reaction term to be

$$R(s) = \frac{s}{1 + s + \kappa s^2} \quad .$$

The parameter ρ in (1.2) is proportional to the characteristic diffusion time of S across the membrane and the compartment volume. It is inversely proportional to the volume of the membrane and the Michaelis constant.

Stationary behavior

We will determine the stationary solutions of (1.2), i.e., the solution structure of the algebraic system

$$\begin{aligned} (s_0 - s_1) + (s_2 - s_1) - \rho R(s_1) &= 0, \\ (s_0 + \mu - s_2) + (s_1 - s_2) - \rho R(s_2) &= 0 \quad . \end{aligned} \quad (1.3)$$

In (1.3) we take $\rho = 100$ and $\kappa = 1$. Thus there are two *control parameters* left, viz., s_0 and μ. First consider the unperturbed case where $\mu = 0$. A *bifurcation diagram* (or *response diagram*) for this case with s_0 as bifurcation parameter is given in Fig. 1.1. As vertical axis we have chosen s_2. The curves in the diagram then represent *branches* (or *one-dimensional continua*) of solutions to (1.3). Solid and dashed curves represent stable and unstable stationary solutions respectively.

Recall that a solution u_0 of (1.1) at $\lambda = \lambda_0$ is called (*asymptotically*) *stable* if all eigenvalues of $f_u(u_0, \lambda_0)$ lie in the negative half plane, and *unstable* if there is an eigenvalue with positive real part. Stable solutions are locally attracting.

Note that there are multiple stable solutions for certain ranges of the control parameter s_0 . The upper and lower part of the primary S-shaped branch consist of stable solutions. Solutions along this primary branch are *symmetric*, i.e., $s_1 = s_2 \equiv s$ along this branch. Thus these steady states are simply solutions of

$$(s_0 + s) - \rho R(s) = 0 \quad .$$

The secondary branch, which intersects the primary branch at two bifurcation points, consists of *asymmetric* solutions, i.e., $s_1 \neq s_2$, except at the bifurcation points. Note that the secondary branch has two portions that consist of stable solutions. Thus here we have four different coexisting stable solutions: Two different symmetric states and two asymmetric states. The two asymmetric states are related. Indeed, if (s_1, s_2) is a solution couple of (1.3) with $\mu = 0$ then so is (s_2, s_1). This also enables us to read both the steady-state values of s_1 and of s_2 from Fig. 1.1.

Singular points

Two types of singular points appear in Fig. 1.1, namely *folds* (or *limit points*) where a branch turns back, and *bifurcation points*, where two distinct branches intersect.

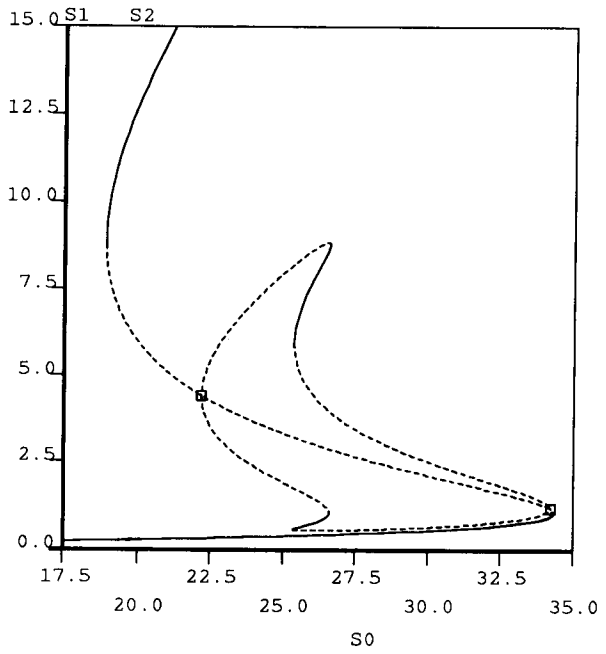


Fig. 1.1. Bifurcation diagram for Eq. (1.3) with $\mu = 0$, $\rho = 100$, $\kappa = 1$.

The two bifurcation points have been marked by open square symbols. Bifurcation points are in a sense exceptional (not '*generic*'), in that they do not 'normally' appear in a one-parameter analysis. But our problem is itself exceptional because of the symmetry noted above. Indeed, we will see below that these bifurcations do not persist when the symmetry is broken by letting μ be nonzero.

Perturbation

We now determine how the perfect diagram Fig. 1.1 changes when we introduce a nonzero perturbation μ in (1.3). This can be answered by numerically tracing out folds in the two parameters s_0 and μ. In Fig. 1.1 there are two folds on the primary branch that can be continued, and another four on the secondary branch. Moreover the two bifurcations also give rise to folds when μ becomes nonzero. The resulting curves of folds are shown in Fig. 1.2. Note the presence of the cusp near $\mu = 3.6$, $s_0 = 25$. This cusp is obtained by continuation of the folds that border the stable asymmetric solutions on the secondary branch in Fig. 1.1. Actually there are two such stable regions and correspondingly there are two cusps. The second cusp is not indicated in Fig. 1.2.

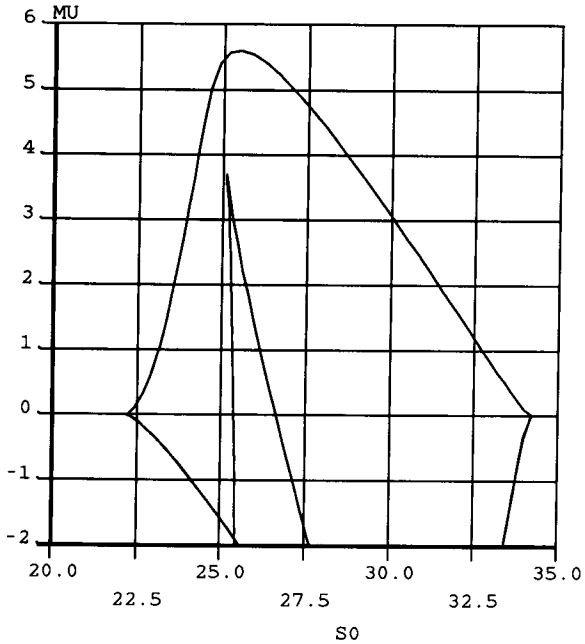


Fig. 1.2. Curves of folds for Eq. (1.3) with $\rho = 100$, $\kappa = 1$.

The information contained in Fig. 1.2 can be best illustrated by taking a few more horizontal cross sections in this diagram. The unperturbed diagram of Fig. 1.1 corresponds to the cross section at $\mu = 0$ in Fig. 1.2. Some perturbed diagrams are shown in Figs. 1.3 to 1.6.

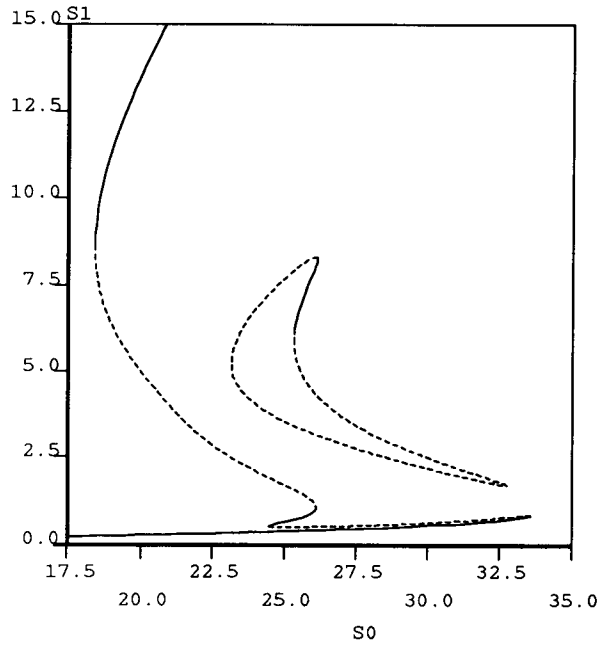


Fig. 1.3. Concentration in compartment 1 versus bifurcation parameter s_0 for Eq. (1.3) with $\mu = 1.0$, $\rho = 100$, $\kappa = 1$.

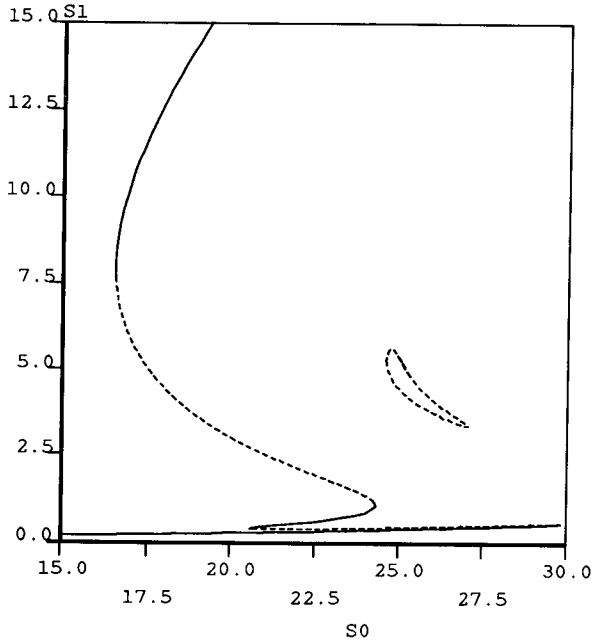


Fig. 1.5. Concentration in compartment 1 versus bifurcation parameter s_0 for Eq. (1.3) with $\mu = 5.0$, $\rho = 100$, $\kappa = 1$.

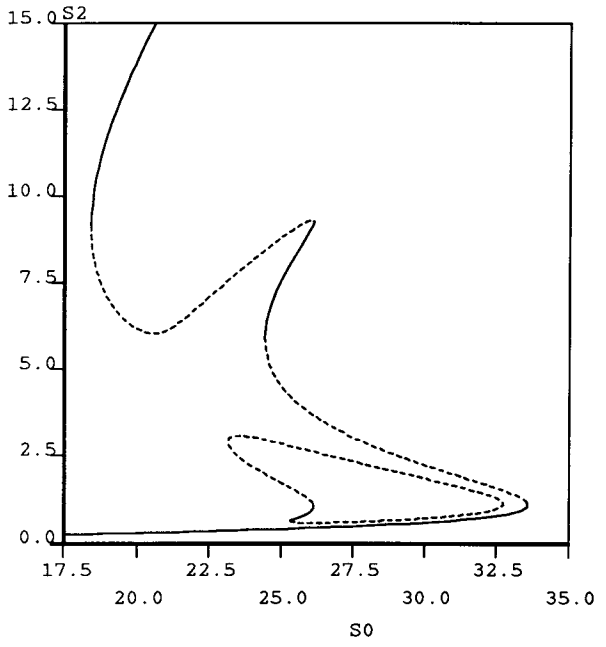


Fig. 1.4. Concentration in compartment 2 versus bifurcation parameter s_0 for Eq. (1.3) with $\mu = 1.0$, $\rho = 100$, $\kappa = 1$.

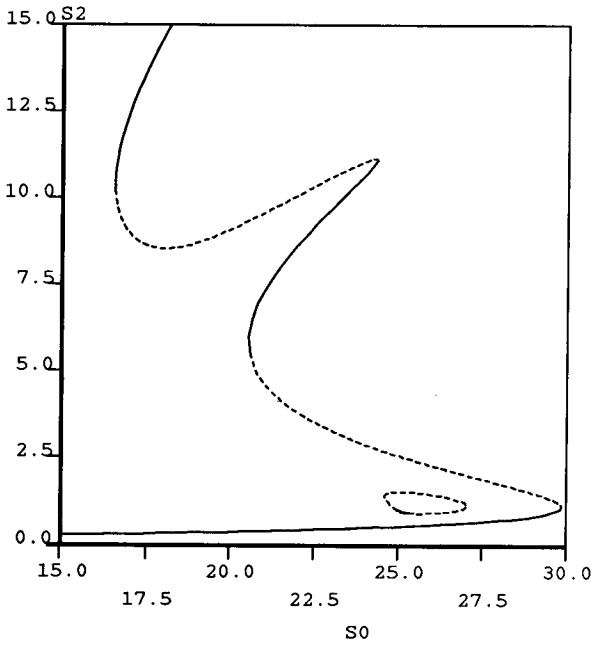


Fig. 1.6. Concentration in compartment 2 versus bifurcation parameter s_0 for Eq. (1.3) with $\mu = 5.0$, $\rho = 100$, $\kappa = 1$.

Numerical aspects

The main numerical algorithms used in the analysis of the two-compartment model above are (i) the continuation of solutions, including continuation past folds, (ii) the detection of folds and bifurcation points, (iii) branch switching at bifurcation points, and (iv) the continuation of folds in two parameters. These numerical techniques are described in some detail in this paper.

We shall also consider certain algorithms for optimization and control based on numerical continuation. These are useful when one wants to optimize a functional in a system possessing multiple solutions, as is the case in the example above. Other possible applications of practical importance include the control of folds and the control of stability regions.

1.3 *A One-Compartment Activator-Inhibitor Model*

A simple one-compartment activator-inhibitor model is given by the following system of ordinary differential equations [Kernévez, 1980]:

$$\begin{aligned} \frac{ds}{dt} &= (s_0 - s) - \rho R(s, a) \quad , \\ \frac{da}{dt} &= \alpha(a_0 - a) - \rho R(s, a) \quad , \end{aligned} \tag{1.4}$$

where s and a denote the concentrations of the two chemical species S and A inside the compartment. Here S stands for *substrate* and A for *activator*, though both are substrates in a reaction where they are consumed. This reaction is catalyzed by an enzyme with reaction rate proportional to

$$R(s, a) = \frac{sa}{1 + s + \kappa s^2} \quad \kappa > 0 \quad . \tag{1.5}$$

It is evident from the form of $R(s, a)$ in (1.5) that S inhibits the reaction when its concentration is high. The parameter ρ is a ratio of characteristic times, $\rho = \theta_T/\theta_R$ where θ_T is the characteristic time of diffusion of S from the outside reservoir into the compartment, and θ_R is the characteristic time of the enzyme reaction. The terms $(s_0 - s)$ and $\alpha(a_0 - a)$ describe the transport from the outside reservoir where the concentrations are held at a constant s_0 and a_0. The parameter α represents the ratio of diffusion coefficients between the reservoir and the compartment. The parameters s_0, a_0, ρ, α, and κ are all dimensionless and positive, as are the state variables s and a. We take $s_0 = 100$, $a_0 = 500$, $\alpha = 0.2$, and $\kappa = 0.1$. Schematically we have the following situation:

$$s_0, a_0 \;\|\; s, a, E \;\|\; s_0, a_0$$

The bifurcation behavior as ρ varies is shown schematically in the bifurcation diagram of Fig. 1.7. There are now also periodic solutions. The horizontal axis is the bifurcation parameter ρ, and the vertical axis is the maximum of s. That is, for stationary solutions we plot s, and for periodic solutions we plot $\max_{[0,T]} s(t)$, where T denotes period.

There are two *Hopf bifurcations* indicated by solid squares. If we increase the bifurcation parameter ρ then at the left Hopf bifurcation two complex eigenvalues of f_u (evaluated at the stationary solution) move into the right half of the complex plane. Thus solutions along the stationary branch become unstable at this point. At the right Hopf bifurcation the eigenvalues move back into the left half-plane and solutions along the branch of stationary solutions regain stability. According to the well-known Hopf bifurcation theorem a branch of periodic solutions of locally small amplitude emanates from these bifurcation points.

Figure 1.7 also shows the large-amplitude periodic solutions. The solid dots denote stable periodic solutions, and the open circles represent unstable periodic solutions. In particular, we see that the branches that bifurcate from the two Hopf bifurcation points actually connect. From Fig. 1.7 we can deduce the dynamical behavior of (1.4) as ρ is slowly varied. When ρ is increased past the

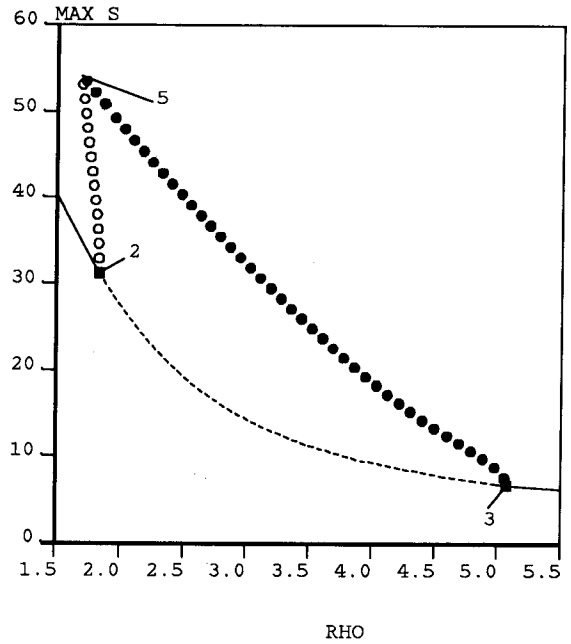


Fig. 1.7. Bifurcation diagram for the one-compartment model (1.4), (1.5) with $s_0 = 100$, $a_0 = 500$, $\alpha = 0.2$, $\kappa = 0.1$

first Hopf bifurcation the system will jump to a large-amplitude oscillation. Oscillatory behavior will persist until the second Hopf bifurcation point is passed, after which the system will assume a steady state. Now decreasing ρ will produce similar behavior in reverse, except that the jump from oscillatory behavior back to stationary behavior will take place at a lower ρ-value because of the fold on the branch of periodic solutions. The orbit at the fold, labeled 5 in Fig. 1.7, is shown in Fig. 1.8. The period of the oscillations along the branch of periodic solutions is given in Fig. 1.9.

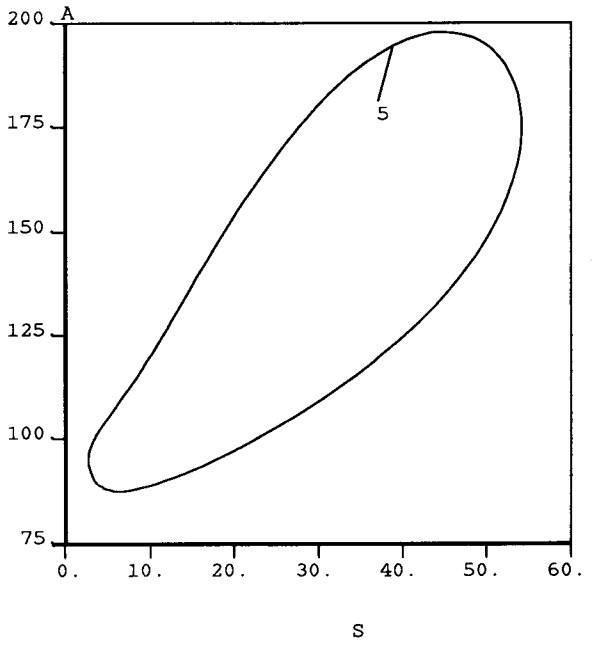


Fig. 1.8. The orbit at the fold (label 5) in Fig. 1.7.

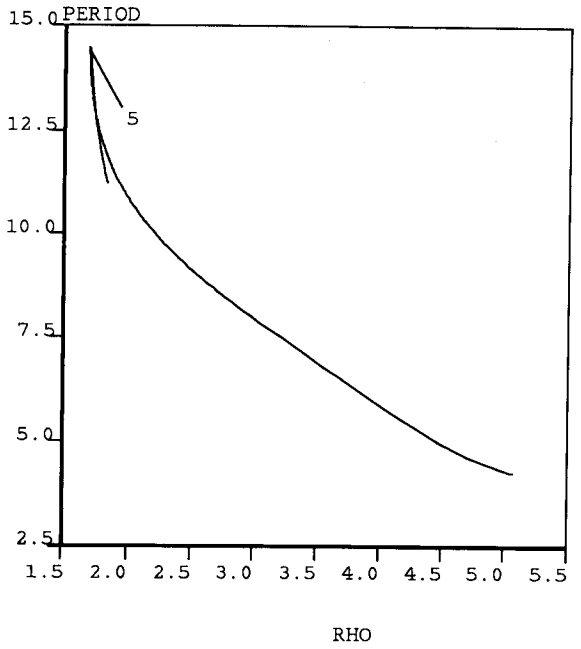


Fig. 1.9. Period versus ρ for the branch of periodic solutions in Fig. 1.7.

Perturbation

We now determine how the bifurcation diagram changes as a second parameter is varied. Here we choose s_0 as this second parameter. In particular we want to determine what happens to the Hopf bifurcation points and to the folds on the branch of periodic solutions as s_0 is varied. Both of these phenomena are structurally stable, i.e., they persist under general small perturbations, and thus one expects to find curves of these points in the ρ–s_0 plane. The results are shown in Fig. 1.10. For example, the location of the Hopf bifurcation point and the fold in Fig. 1.7 can be found in Fig. 1.10 by drawing a horizontal line at $s_0 = 100$.

From Fig. 1.10 we can draw the following conclusions: Increasing s_0 above 107.0 gives rise to a second fold on the branch of periodic solutions. Further increase of s_0 beyond approximately 110.5 results in the coalescence

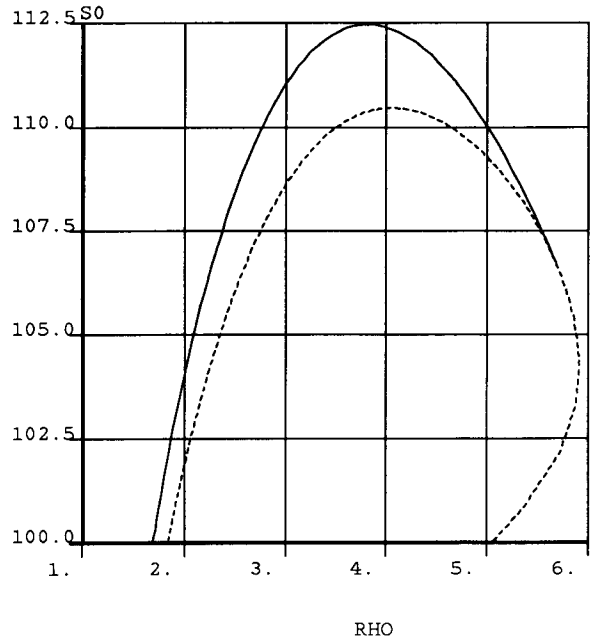


Fig. 1.10 A two-parameter diagram of Hopf bifurcation points (dashed) and folds for the one-compartment model (1.4), (1.5) with $a_0 = 500$, $\alpha = 0.2$, $\kappa = 0.1$.

and subsequent disappearance of the Hopf bifurcation points. However the two folds are still present above $s_0 = 110.5$. In the absence of other phenomena, the only possible conclusion is that an *isola* of periodic solutions

has been formed. Further increase in s_0 to about 112.50 results in the coalescence and disappearance of the folds as the isola shrinks to a point. The conclusions from Fig. 1.10 agree with one-parameter bifurcation diagrams computed in the region of interest, i.e., by taking horizontal cross sections at appropriate s_0-values in the ρ-s_0 diagram. Two such bifurcation diagrams are given in Fig. 1.11 and Fig. 1.12 for s_0-values of 110.0 and 111.0. These figures show clearly the emergence of the isola. Observe the multiple hysteresis behavior in Fig. 1.11. In Fig. 1.12 note the stability of all stationary solutions, which for ρ between 3.0 and 4.7 coexist with a stable and an unstable orbit. Obviously the existence of the isola and its associated stable periodic behavior cannot be detected in the continuation of the stationary branch since there are no Hopf bifurcations. Indeed, as illustrated, the detection of such phenomena will generally require use of two parameters. Sometimes, time integration using 'random' initial data may be useful for generating a starting point on an as yet undiscovered solution branch.

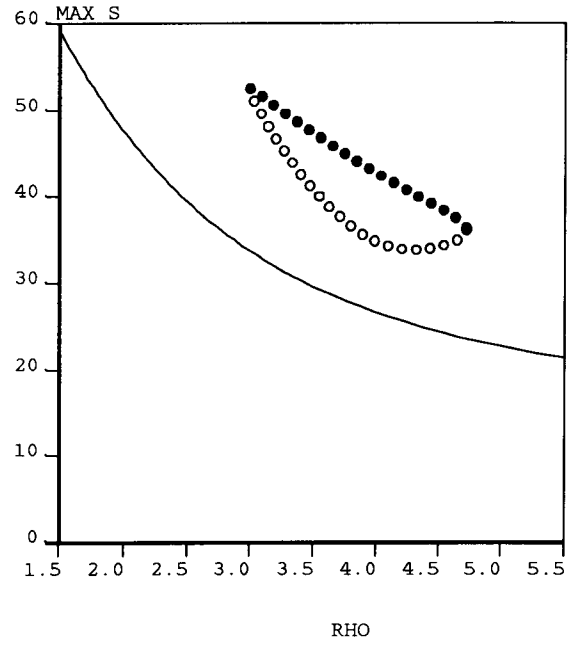


Fig. 1.12. Bifurcation diagram for the one-compartment model (1.4), (1.5) with $s_0 = 111$, $a_0 = 500$, $\alpha = 0.2$, $\kappa = 0.1$.

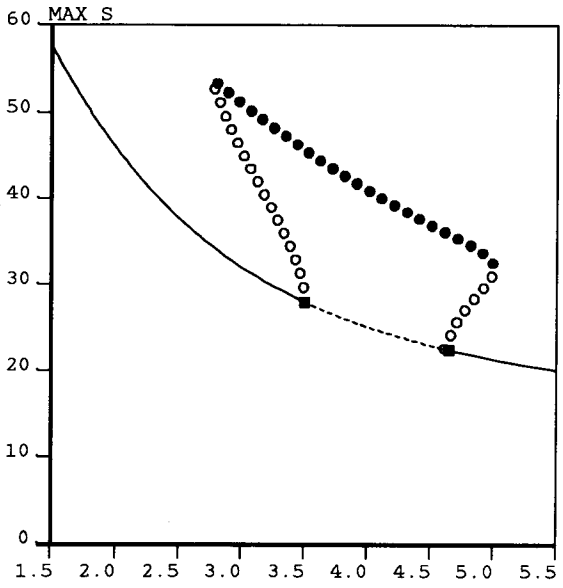


Fig. 1.11. Bifurcation diagram for the one-compartment model (1.4), (1.5) with $s_0 = 110$, $a_0 = 500$, $\alpha = 0.2$, $\kappa = 0.1$.

Numerical aspects

The main numerical algorithms used in the analysis of the one-compartment model above are (i) the detection of Hopf bifurcations, (ii) the computation of stable and unstable periodic solutions, (iii) the determination of the stability of the periodic solutions, (iv) the continuation of Hopf bifurcation points in two parameters, and (v) the continuation of folds on branches of periodic solutions in two parameters. A description of such algorithms is included in this paper. We shall also briefly consider the discretization of bifurcation problems in ordinary differential equations and discuss its effect on the solution structure.

In practical applications there is a variety of optimization aspects that arises in connection with problems of the type illustrated above. We treat such optimization problems in the basic framework of numerical continuation. Specific optimization problems suggested by the example above include the optimization of periodic solutions (e.g., their amplitude or their stability), the control of Hopf bifurcation points, and the control of folds on branches of periodic solutions.

2. Finite Dimensional Bifurcation Problems

2.1 *Continuation of Solutions*

A first step in the bifurcation analysis of (1.1) consists of determining the stationary solution *branches* (or solution *paths*). These are solutions $[u(s), \lambda(s)]$ of the nonlinear system of equations

$$f(u, \lambda) = 0, \quad u, f \in \mathrm{R}^n, \quad \lambda \in \mathrm{R}, \qquad (2.1)$$

where s denotes some parametrization. Throughout we assume that f is sufficiently smooth. Let $x = (u, \lambda)$. Then we can write (2.1) as

$$f(x) = 0, \quad f: \mathrm{R}^{n+1} \to \mathrm{R}^n \quad . \tag{2.2}$$

In the formulation (2.2) we do not distinguish between parameter and state. A solution path to (2.2) is denoted as $x(s)$. The computation of curves of folds and curves of Hopf bifurcation points also leads to systems of the form (2.2) and such computations will be considered later. Much of the material below is from the work of Keller (e.g., [Keller, 1977, 1987]).

Regular solution paths

A solution $x_0 \equiv x(s_0)$ is called *regular* if $f_x^0 \equiv f_x(x_0)$ has rank n. A segment of a solution path is regular if $x(s)$ is regular along the segment. In the parameter formulation (2.1) we have Rank $[f_x^0]$ = Rank $[f_u^0 | f_\lambda^0] = n$ iff either (i) f_u^0 is nonsingular, or (ii) dim $N(f_u^0) = 1$ and $f_\lambda^0 \notin R(f_u^0)$. If a solution x_0 is regular then the path $x(s)$ will also be regular near x_0.

Remark. If Rank $[f_u^0 | f_\lambda^0] = n$ then either f_u^0 is nonsingular and by the Implicit Function Theorem we have $u = u(\lambda)$ near $x_0 \equiv (u_0, \lambda_0)$, or else we can interchange colums in f_x^0 to see that the solution can be locally parametrized by one of the components of u. More precisely, in the latter case let $\hat{u} \equiv (u^1, u^2, \ldots, u^{i-1}, \lambda, u^{i+1}, \ldots, u^n)$ where i is chosen such that $f_{\hat{u}}^0$ is nonsingular. Then it follows from the Implicit Function Theorem that we can parametrize the solution locally in terms of the component u^i, i.e., $\hat{u} = \hat{u}(u^i)$ near (u_0, λ_0).

Thus we see that a unique branch of solutions passes through a regular solution. Throughout we assume that f is sufficiently smooth so that the Implicit Function Theorem indeed holds and so that the resulting solution branch is smooth.

Folds

A solution (u_0, λ_0) is called a *simple fold* (or *simple limit point*) if

$$\dim N(f_u^0) = 1 \quad \text{and} \quad f_\lambda^0 \notin R(f_u^0) \quad .$$

From differentiating $f[u(s), \lambda(s)] = 0$ we have

$$f_u \dot{u}(s) + f_\lambda \dot{\lambda}(s) = 0 \quad . \tag{2.3}$$

We can choose the parametrization such that

$$\left\| \dot{u} \right\|^2 + \dot{\lambda}^2 = 1 \quad (\textit{arclength parametrization}),$$

where $\left\| u \right\| \equiv \left\| u \right\|_2 \equiv \sqrt{u * u}$. From (2.3) we have $\dot{\lambda}_0 = 0$ at a fold point (u_0, λ_0) because $f_\lambda^0 \notin R(f_u^0)$. Thus $f_u^0 \dot{u} = 0$, and since dim $N(f_u^0) = 1$ we have $N(f_u^0) = \text{Span}\{\dot{u}_0\}$.

From differentiating (2.3) we have

$$f_u^0 \ddot{u}_0 + f_\lambda^0 \ddot{\lambda}_0 + f_{uu}^0 \dot{u}_0 \dot{u}_0 + 2 f_{u\lambda}^0 \dot{u}_0 \dot{\lambda}_0 + f_{\lambda\lambda}^0 \dot{\lambda}_0 \dot{\lambda}_0 = 0 \quad . \tag{2.4}$$

At a simple fold (u_0, λ_0) let

$$N(f_u^0) = \text{Span}\{\phi\}, \quad N[(f_u^0)^*] = \text{Span}\{\psi\} \quad .$$

If ϕ is suitably normalized then $\phi = \dot{u}_0$. Multiply (2.4) on the left by ψ^* and use $\dot{\lambda}_0 = 0$ and $\psi \perp R(f_u^0)$ to find

$$\psi^* f_\lambda^0 \ddot{\lambda}_0 + \psi^* f_{uu}^0 \phi\phi = 0 \quad .$$

Now $\psi^* f_\lambda^0 \neq 0$ since $f_\lambda^0 \notin R(f_u^0)$. Thus

$$\ddot{\lambda}_0 = \frac{-\psi^* f_{uu}^0 \phi\phi}{\psi^* f_\lambda^0} \quad .$$

If the *curvature* $\ddot{\lambda}_0 \neq 0$ then (u_0, λ_0) is called a *simple quadratic fold.*

Natural parameter continuation

Here the continuation parameter is taken to be λ. Suppose we have a solution (u_0, λ_0) of (2.1) as well as the direction vector $\dot{u}_0$. (Here $\dot{u} \equiv \frac{du}{d\lambda}$.) To find the solution u_1 at a fixed, nearby value of λ, say, $\lambda = \lambda_1 \equiv \lambda_0 + \Delta\lambda$, we can use Newton's method

$$f_u(u_1^{(\nu)}, \lambda_1)\, \Delta u_1^{(\nu)} = -f(u_1^{(\nu)}, \lambda_1) \qquad \nu = 0, 1, 2, \ldots$$
$$u_1^{(\nu+1)} = u_1^{(\nu)} + \Delta u_1^{(\nu)} \quad .$$

As initial approximation we can take $u_1^{(0)} = u_0 + \Delta\lambda\, \dot{u}_0$. If $f_u(u_1, \lambda_1)$ is nonsingular and $\Delta\lambda$ sufficiently small then the convergence theory for Newton's method assures us that the iteration will converge. After convergence of the Newton iterations the new direction $\dot{u}_1$ can be obtained with only one extra backsubstitution because from differentiating $f(u(\lambda), \lambda) = 0$ with respect to λ we have the equation

$$f_u(u_1, \lambda_1)\, \dot{u}_1 = -f_\lambda^1 \quad .$$

It is clear that natural parameter continuation fails at a simple quadratic fold.

Example. Consider *Bratu's Problem*

$$u''(x) + \lambda e^{u(x)} = 0 \text{ for } x \in [0,1], \; u(0) = 0, \; u(1) = 0$$

When $\lambda = 0$ this boundary-value problem has $u(x) \equiv 0$ as solution. This solution can be continued and the resulting solution branch is represented below.

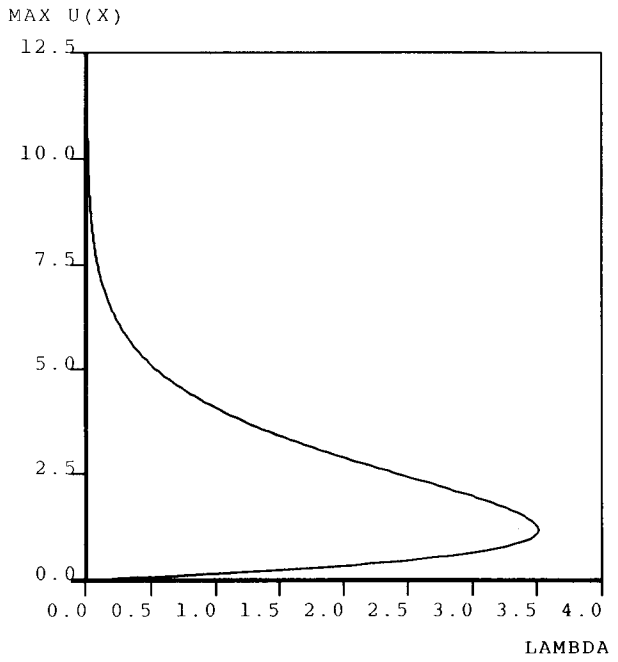


Fig. 2.1. The solution branch of Bratu's problem.

We discretize Bratu's equation by introducing a mesh

$$\{0 = x_0 < x_1 < \ldots < x_N = 1\}$$
$$x_j - x_{j-1} = h, \quad (1 \leqslant j \leqslant N), \quad h = 1/N \ ,$$

and by using a second-order centered approximation to the second derivative. This gives the discrete equations

$$\frac{u^{j+1} - 2u^j + u^{j-1}}{h^2} + \lambda e^{u^j} = 0, \ j = 1, \ldots, N-1,$$
$$u^0 = u^N = 0 \ .$$

If we let $U \equiv (u_1, u_2, \ldots, u^{N-1})$ then these discrete equations can be written as

$$F(U, \lambda) = 0, \quad F: R^n \times R \to R^n, \quad n \equiv N - 1 \ .$$

Natural parameter continuation with λ as parameter now proceeds as follows. Suppose we have λ_0, U_0, and $\dot{U}_0$ where $\dot{U} \equiv \frac{dU}{d\lambda}$. Set $\lambda_1 = \lambda_0 + \Delta\lambda$. Solve for U_1 using the Newton iteration

$$F_U(U_1^{(\nu)}, \lambda_1)\, \Delta U_1^{(\nu)} = -F(U_1^{(\nu)}, \lambda_1) \qquad \nu = 0, 1, 2, \ldots$$
$$U_1^{(\nu+1)} = U_1^{(\nu)} + \Delta U_1^{(\nu)}$$

As an initial guess use $U_1^{(0)} = U_0 + \Delta\lambda\dot{U}_0$. After convergence find $\dot{U}_1$ from

$$F_U(U_1, \lambda_1)\dot{U}_1 = -F_\lambda(U_1, \lambda_1) \ .$$

Now repeat the above procedure to find U_2, etc. Above

$$F_U(U,\lambda) = \begin{pmatrix} -\frac{2}{h^2} + \lambda e^{u^1} & \frac{1}{h^2} & & \\ \frac{1}{h^2} & -\frac{2}{h^2} + \lambda e^{u^2} & \frac{1}{h^2} & \\ & \cdot & \cdot & \cdot \\ & & \frac{1}{h^2} & -\frac{2}{h^2} + \lambda e^{u^{N-1}} \end{pmatrix}.$$

Thus we must solve a tridiagonal system at each Newton iteration and also when computing the direction $\dot{U}$.

It is clear from Fig. 2.1 that the natural parameter continuation method will fail when the fold on the solution branch is passed.

Norm continuation

To allow the computation to proceed past a fold one can choose some other continuation parameter, e.g., $s = \|u\|_2 = \sqrt{u * u}$:

$$f(u(s), \lambda(s)) = 0,$$
$$u(s) * u(s) - s^2 = 0 \ .$$

If we are given a solution (u_0, λ_0) and the direction vector $(\dot{u}_0, \dot{\lambda}_0)$, where $\cdot \equiv \frac{d}{ds}$, then Newton's method for taking a step along the solution path consists of solving

$$\begin{pmatrix} (f_u^1)^{(\nu)} & (f_\lambda^1)^{(\nu)} \\ 2(u_1^{(\nu)})^* & 0 \end{pmatrix} \begin{pmatrix} \Delta u_1^{(\nu)} \\ \Delta\lambda_1^{(\nu)} \end{pmatrix}$$
$$= -\begin{pmatrix} f(u_1^{(\nu)}, \lambda_1^{(\nu)}) \\ (u_1^{(\nu)})^* u_1^{(\nu)} - s^2 \end{pmatrix}, \quad \nu = 0, 1, 2, \ldots$$

followed by setting $u_1^{(\nu+1)} = u_1^{(\nu)} + \Delta u_1^{(\nu)}$ and $\lambda_1^{(\nu+1)} = \lambda_1^{(\nu)} + \Delta\lambda_1^{(\nu)}$. As an initial approximation we can use

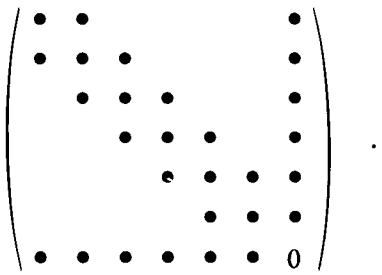
$$u_1^{(0)} = u_0 + \Delta s\, \dot{u}_0, \quad \lambda_1^{(0)} = \lambda_0 + \Delta s\, \dot{\lambda}_0 \ .$$

Again one extra backsubstitution finds the next direction vector:

$$\begin{pmatrix} f_u^1 & f_\lambda^1 \\ 2u_1^* & 0 \end{pmatrix} \begin{pmatrix} \dot{u}_1 \\ \dot{\lambda}_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 2s \end{pmatrix} .$$

This last equation is obtained by differentiating $f(u(s), \lambda(s)) = 0$ and $u(s)^* u(s) - s^2 = 0$ with respect to s.

Example. In Bratu's problem the matrix in the above linear systems has a *bordered tridiagonal form*, i.e., f_u is tridiagonal and the extra column f_λ and row $2u^*$ generally consist of nonzero elements. Schematically the form of the matrix is as follows.



We shall show later how to solve such linear systems efficiently by the bordering algorithm.

The Bordering Lemma

For the norm-continuation method to work at a fold (u_0, λ_0) we need to check that the matrix

$$\hat{A}_{\text{norm}} \equiv \begin{pmatrix} f_u & f_\lambda \\ 2u^* & 0 \end{pmatrix}$$

is nonsingular at (u_0, λ_0).

Lemma. [Keller, 1977] *Let* $\hat{A} = \begin{pmatrix} A & c \\ b^* & d \end{pmatrix}$. *Then the following hold:*

(a) *A nonsingular $\Rightarrow$ ($\hat{A}$ nonsingular if $d \neq b^* A^{-1} c$),*
(b) $(\dim N(A) = \dim N(A^*) = 1) \Rightarrow$ *($\hat{A}$ nonsingular iff $(c \notin R(A)$ and $b \notin R(A^*))$),*
(c) *If* $\dim N(A) \geqslant 2$ *then $\hat{A}$ is singular.*

Proof.

(a) In this case $\hat{A} = \begin{pmatrix} A & 0 \\ b^* & 1 \end{pmatrix} \begin{pmatrix} I & A^{-1}c \\ 0^* & e \end{pmatrix}$, where $e = d - b^* A^{-1} c$. Clearly $\hat{A}$ is nonsingular iff $e \neq 0$.
(b) Suppose $\hat{A}$ is singular:

$$Ax + \xi c = 0,$$
$$b^* x + \xi d = 0.$$

If $\xi \neq 0$ then $c \in R(A)$ which contradicts the assumptions. If $\xi = 0$ and $x \neq 0$ then $N(A) = \text{Span}\{x\}$ and $b \in N(A)^\perp = R(A^*)$, which also contradicts the assumptions.
(c) is obvious. ■

Thus applying the Lemma to $\hat{A}_{\text{norm}}$ we see that norm continuation works at a fold (u_0, λ_0) provided $f_\lambda^0 \notin R(f_u^0)$, which always holds at a quadratic fold, and provided $u_0 \notin R(f_u^0)^*$. This last condition need not always be satisfied, e.g., it fails to hold at the fold $u = 0, \lambda = 0$ of $f(u, \lambda) = u^2 - \lambda = 0$.

Pseudoarclength continuation

This is the most popular continuation method. It is due to Keller [1977]. Note that arclength continuation can be formulated as

$$f(u(s), \lambda(s)) = 0, \quad \left\| \dot{u}(s) \right\|^2 + \dot{\lambda}(s)^2 = 1 .$$

This is mainly a theoretical tool. It becomes useful for computations if we use the approximate formulation

$$f(u_1, \lambda_1) = 0, \quad (u_1 - u_0)^* \dot{u}_0 + (\lambda_1 - \lambda_0) \dot{\lambda}_0 - \Delta s = 0,$$

known as *pseudoarclength* continuation. Geometrically interpreted, this method finds a solution (u_1, λ_1) to $f(u, \lambda) = 0$ in a hyperplane that is at distance Δs from (u_0, λ_0) and that is perpendicular to the direction vector $(\dot{u}_0, \dot{\lambda}_0)$.

Newton's method for solving these equations is now

$$\begin{pmatrix} (f_u^1)^{(\nu)} & (f_\lambda^1)^{(\nu)} \\ \dot{u}_0^* & \dot{\lambda}_0 \end{pmatrix} \begin{pmatrix} \Delta u_1^{(\nu)} \\ \Delta \lambda_1^{(\nu)} \end{pmatrix} = - \begin{pmatrix} f(u_1^{(\nu)}, \lambda_1^{(\nu)}) \\ (u_1^{(\nu)} - u_0)^* \dot{u}_0 + (\lambda_1^{(\nu)} - \lambda_0) \dot{\lambda}_0 - \Delta s \end{pmatrix} .$$

The next direction vector $(\dot{u}_1, \dot{\lambda}_1)$ can be defined by the equations

$$f_u^1 \dot{u}_1 + f_\lambda^1 \dot{\lambda} = 0, \quad (\dot{u}_0)^* \dot{u}_1 + \dot{\lambda}_0 \dot{\lambda}_1 = 1 \quad \text{(normalization)}.$$

Again $(\dot{u}_1, \dot{\lambda}_1)$ can then be found by one extra backsubstitution at the end of the Newton iterations. Also the orientation of the branch is preserved if Δs is sufficiently small. It is necessary to rescale the direction vector so that indeed $\left\| \dot{u}_1 \right\|^2 + \dot{\lambda}_1^2 = 1$.

Theorem. *The pseudo-arclength method works whenever (u_0, λ_0) is a regular solution point and Δs is suf-*

ficiently small. In particular the method works at a quadratic fold.

Proof. We can prove this using the Lemma. But the proof becomes even simpler if we use the uniform formulation (2.2). Then the pseudoarclength algorithm can be written as

$$f(x_1) = 0, \quad (x_1 - x_0)^* \dot{x}_0 - \Delta s = 0, \quad (\|\dot{x}_0\| = 1) \ .$$

The matrix in Newton's method is $\begin{pmatrix} f_x^1 \\ \dot{x}_0^* \end{pmatrix}$. It suffices to show that $\begin{pmatrix} f_x^0 \\ \dot{x}_0^* \end{pmatrix}$ is nonsingular at a regular solution. If on the contrary $\begin{pmatrix} f_x^0 \\ \dot{x}_0^* \end{pmatrix}$ is singular then $f_x^0 z = 0$ and $x_0^* z = 0$ for some vector z with $\|z\| = 1$. Also $f_x^0 \dot{x}_0 = 0$ by definition of $\dot{x}_0$. But by assumption of regularity, f_x^0 has rank n. Thus z must be the same as $\dot{x}_0$ except possibly for sign. But then $\dot{x}_0^* z = \dot{x}_0^* \dot{x}_0 = \|\dot{x}_0\|^2 = 1$ which is a contradiction. ■

Example. Consider the discretized Bratu problem. The matrix in Newton's method applied to the pseudoarclength equations then again has a bordered tridiagonal form. We shall now show to solve such linear systems efficiently.

The bordering algorithm

The linear systems that arise when Newton's method is applied to the pseudoarclength algorithm are of thc form

$$\begin{pmatrix} A & c \\ b^* & d \end{pmatrix} \begin{pmatrix} x \\ z \end{pmatrix} = \begin{pmatrix} f \\ h \end{pmatrix} \ . \tag{2.5}$$

If A is a sparse matrix whose LU decomposition can be found relatively cheaply (e.g., if A is tridiagonal), then the following *bordered LU decomposition* will be efficient:

$$\begin{pmatrix} A & c \\ b^* & d \end{pmatrix} = \begin{pmatrix} L & 0 \\ \beta^* & 1 \end{pmatrix} \begin{pmatrix} U & \gamma \\ 0^* & \delta \end{pmatrix} \ .$$

After finding the decomposition $A = LU$ (which may require pivoting) we compute γ, β and δ from

$$L\gamma = c, \quad U^*\beta = b, \quad \delta = d - \beta^*\gamma \ .$$

The linear system can then be written as

$$\begin{pmatrix} L & 0 \\ \beta^* & 1 \end{pmatrix} \begin{pmatrix} U & \gamma \\ 0^* & \delta \end{pmatrix} \begin{pmatrix} x \\ z \end{pmatrix} = \begin{pmatrix} f \\ h \end{pmatrix} \ .$$

Defining

$$\begin{pmatrix} \hat{f} \\ \hat{h} \end{pmatrix} \equiv \begin{pmatrix} U & \gamma \\ 0^* & \delta \end{pmatrix} \begin{pmatrix} x \\ z \end{pmatrix} \ ,$$

we obtain the solution (x, z) by the following steps:

$$L\hat{f} = f, \quad \hat{h} = h - \beta^*\hat{f}, \quad z = \hat{h}/\delta, \quad Ux = \hat{f} - z\gamma,$$

in the given order. This algorithm will work if both A and the full matrix

$$\hat{A} \equiv \begin{pmatrix} A & c \\ b^* & d \end{pmatrix}$$

are nonsingular. To see this, note that we must have $\delta \neq 0$. But from the above

$$\begin{aligned} \delta &= d - \beta^*\gamma = d - (U^{*-1}b)^*(L^{-1}c) \\ &= d - b^*U^{-1}L^{-1}c = d - b^*(LU)^{-1}c = d - b^*A^{-1}c \end{aligned}$$

which is nonzero by Conclusion (a) of the Bordering Lemma.

The case of singular A [Keller, 1987]

Now consider the special case where A is singular but where the full matrix $\hat{A}$ is nonsingular in (2.5). Thus we must have $N(A) = \text{Span}\{\phi\}$, $N(A^*) = \text{Span}\{\psi\}$, $c \notin R(A)$, and $b \notin R(A^*)$. The right null vector ϕ and the left null vector ψ can be computed efficiently as will be shown below. From (2.5) we have $Ax + zc = f$, so that $(f - zc) \in R(A)$, i.e., $\psi^*(f - zc) = 0$. Since $\psi^* c \neq 0$ we have

$$z = \frac{\psi^* f}{\psi^* c} \ .$$

Therefore x is a solution of $Ax = f - \frac{\psi^* f}{\psi^* c} c$. Now $x = x_p + \alpha\phi$, where x_p is a particular solution which is easily computed as shown below. Also from (2.5) we have $b^*(x_p + \alpha\phi) + dz = h$. Since $b^*\phi \neq 0$ we find

$$\alpha = \frac{h - d\,\frac{\psi^* f}{\psi^* c} - b^* x_p}{b^*\phi} \ .$$

Computation of the right null vector

The left and right nullvectors ϕ and ψ can be computed very efficiently. To find ϕ we assume that A has been decomposed by Gauss elimination with row and column interchanges into $A = P\hat{L}\hat{U}Q$, where P and Q are permutation matrices and

$$\hat{L} = \begin{pmatrix} L & 0 \\ l^* & 1 \end{pmatrix}, \quad \hat{U} = \begin{pmatrix} U & u \\ 0^* & 0 \end{pmatrix} \ ,$$

where L is lower triangular with 1's along the main diagonal and U is upper triangular with nonzero entries along the main diagonal. Thus ϕ is a solution of $P\hat{L}\hat{U}Q\phi = 0$, or equivalently, since P and $\hat{L}$ are nonsingular, of

$$\begin{pmatrix} U & u \\ 0^* & 0 \end{pmatrix} \begin{pmatrix} v \\ \mu \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} ,$$

where $\begin{pmatrix} v \\ \mu \end{pmatrix} \equiv Q\phi$. Choose $\mu = -1$. Then find v from backsubstitution in $Uv = u$. Since Q is a permutation matrix we have $\phi = Q^* \begin{pmatrix} v \\ \mu \end{pmatrix}$. Note that if A has already been decomposed then only one additional backsolve is needed for computing ϕ.

Computation of the left null vector

Similarly we can find ψ by just one backsolve as follows: From $A^*\psi = 0$ we have $Q^*\hat{U}^*\hat{L}^*P^*\psi = 0$, or equivalently, since Q is nonsingular

$$\begin{pmatrix} U^* & 0 \\ u^* & 0 \end{pmatrix} \begin{pmatrix} L^* & l \\ 0^* & 1 \end{pmatrix} \begin{pmatrix} w \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} ,$$

where $\begin{pmatrix} w \\ v \end{pmatrix} \equiv P^*\psi$. Since U is nonsingular we must have

$$\begin{pmatrix} L^* & l \\ 0^* & 1 \end{pmatrix} \begin{pmatrix} w \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ \nu \end{pmatrix} ,$$

where $\nu \neq 0$ is arbitrary, e.g., $\nu = -1$. Then w *is found from* $L^*w = l$. *Finally* $\psi = P\begin{pmatrix} w \\ -1 \end{pmatrix}$.

Computation of a particular solution

To compute a particular solution x_p of $Ax_p = \tilde{f}$, when $N(A) = \text{Span}\{\phi\}$, $\tilde{f} \in R(A)$, we have the LU decomposed form

$$P \begin{pmatrix} L & 0 \\ l^* & 1 \end{pmatrix} \begin{pmatrix} U & u \\ 0^* & 0 \end{pmatrix} Qx_p = \tilde{f} .$$

First solve

$$\begin{pmatrix} L & 0 \\ l^* & 1 \end{pmatrix} \begin{pmatrix} \hat{f} \\ \hat{h} \end{pmatrix} = P^*\tilde{f} ,$$

followed by

$$\begin{pmatrix} U & u \\ 0^* & 0 \end{pmatrix} Qx_p = \begin{pmatrix} \hat{f} \\ \hat{h} \end{pmatrix},$$

where $\hat{h} = 0$ because $\tilde{f} \in R(A)$ (the system must be solvable). Write $\begin{pmatrix} y_p \\ z_p \end{pmatrix} \equiv Qx_p$. Then we see that z_p can have any value, e.g., $z_p = 0$. Now find y_p from $Uy_p = \hat{f}$. Finally $x_p = Q^* \begin{pmatrix} y_p \\ z_p \end{pmatrix}$ (permutation).

Implementation in AUTO

In AUTO it is assumed that a regular solution (u_0, λ_0) is known for some particular value λ_0. In most applications such a (u_0, λ_0) is easily found. If not, then it is usually possible to introduce a homotopy parameter in order to reach a suitable starting point. From the preceding discussion we have seen that the direction $(\dot{u}_0, \dot{\lambda}_0)$ of the branch at a regular starting point coincides with the normalized null vector of the n by $n+1$ dimensional matrix $(f_u(u_0, \lambda_0) \mid f_\lambda(u_0, \lambda_0))$. (A bifurcation point should not be used as starting point, since there the nullspace is at least two-dimensional.) The null vector can be computed efficiently by applying the procedure discussed earlier to the matrix $\begin{pmatrix} f_u^0 & f_\lambda^0 \\ 0^* & 0 \end{pmatrix}$. We scale $(\dot{u}_0, \dot{\lambda}_0)$ so that $\theta_u^2 \dot{u}_0^* \dot{u}_0 + \theta_\lambda^2 \dot{\lambda}_0^2 = 1$, where θ_u and θ_λ are preassigned constants that may be used to reflect a difference in scale between u and λ. By default $\theta_u = \theta_\lambda = 1$. More generally, we equip the space $\mathrm{R}^n \times \mathrm{R}$ with the inner product

$$\langle (u_1, \lambda_1), (u_2, \lambda_2) \rangle \equiv \theta_u^2 u_1^* u_2 + \theta_\lambda^2 \lambda_1 \lambda_2 .$$

From the starting point the branch is traced out in a stepwise manner using pseudoarclength continuation. Assuming (u_{j-1}, λ_{j-1}) and $(\dot{u}_{j-1}, \dot{\lambda}_{j-1})$ have been computed, the next solution (u_j, λ_j) is determined from the equations

$$f(u_j, \lambda_j) = 0, \tag{2.6a}$$

$$\theta_u^2 (u_j - u_{j-1})^* \dot{u}_{j-1} + \theta_\lambda^2 (\lambda_j - \lambda_{j-1}) \dot{\lambda}_{j-1} - \Delta s = 0, \tag{2.6b}$$

where Δs is the step size along the branch. The direction vector $(\dot{u}_{j-1}, \dot{\lambda}_{j-1})$ can be computed as previously discussed or it can be computed approximately, viz., $\dot{u}_{j-1} \approx \frac{1}{\Delta s}(u_{j-1} - u_{j-2})$ and similarly for $\dot{\lambda}_{j-1}$. It is then necessary to rescale so that indeed $\theta_u^2 \dot{u}_{j-1}^* \dot{u}_{j-1} + \theta_\lambda^2 \dot{\lambda}_{j-1}^2 = 1$, for otherwise instabilities in the continuation procedure can arise. The advantage of using the inflated system (2.6) is its capability to compute past folds on a branch. Similar to what has already been shown, the Jacobian of (2.6) $\begin{pmatrix} f_u(u, \lambda) & f_\lambda(u, \lambda) \\ \theta_u^2 \dot{u}^* & \theta_\lambda^2 \dot{\lambda} \end{pmatrix}$, with $\theta_u \neq 0$ and $\theta_\lambda \neq 0$, is nonsingular at regular solution points, which includes simple folds.

One can choose the step size Δs to be fixed or to be adaptive. The following simple adaption scheme is used: If Newton's method converges rapidly, then the step size is increased. If the Newton iteration converges slowly or if it fails to converge at all, then the step size is halved. If a selected maximum step size is reached, then Δs

will not exceed that value; if a selected minimum step size is reached, then the program will signal non-convergence. Convergence criteria can also be selected: Convergence is said to have occurred if the Newton increments satisfy

$$\frac{|\Delta\lambda|}{1+|\lambda|} < \epsilon_\lambda \text{ and } \frac{\|\Delta u\|_\infty}{1+\|u\|_\infty} < \epsilon_u,$$

where ϵ_λ and ϵ_u can be selected.

2.2. *Bifurcation and branch switching*

Simple singular points

A solution $x_0 \equiv x(s_0)$ along a solution branch $x(s)$ of (2.2) is called a *simple singular point* if $f_x^0 \equiv f_x(x_0)$ has rank $n-1$. In terms of the parameter formulation (2.1) (u_0, λ_0) is a simple singular point iff either one of the following holds:

(i) $\dim N(f_u^0) = 1, \quad f_\lambda^0 \in R(f_u^0)$,

(ii) $\dim N(f_u^0) = 2, \quad f_u^0 \notin R(f_u^0)$.

An example of case (*i*) is

$$f(u, \lambda) = u(u-\lambda) \text{ at } (u_0, \lambda_0) = (0, 0),$$

where $f_u^0 = 0$ and $f_\lambda^0 = 0$. As an example of case (*ii*) consider

$$f(u, \lambda) = \begin{pmatrix} \lambda - u_1^2 - u_2^2 \\ u_1 u_2 \end{pmatrix} \text{ at } u_0 = \begin{pmatrix} u_1^0 \\ u_2^0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} .$$

Here $f_u^0 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ and $f_\lambda^0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

The Algebraic Bifurcation Equation

Suppose we have a smooth solution branch $x(s)$ of $f(x) = 0$. By differentiation we have $f_x(x(s))\,\dot{x}(s) = 0$ at any point along the branch. Here $\dot{x}(s)$ is the tangent to the branch. We may assume that $\|\dot{x}(s)\| = 1$. Let $x_0 \equiv x(s_0)$ be a simple singular point with $N(f_x^0) = \text{Span}\{\phi_1, \phi_2\}$ and $N((f_x^0)^*) = \text{Span}\{\psi\}$. The direction vector $\dot{x}_0$ lies in $N(f_x^0)$ because the equation $f_x((x(s))\,\dot{x}(s) = 0$ holds in particular at x_0, *i.e.*, $f_x^0 \dot{x}_0 = 0$. Thus $\dot{x}_0$ has the form $\dot{x}_0 = \alpha\phi_1 + \beta\phi_2$ for some $\alpha = \alpha_1$, $\beta = \beta_1$. We want to investigate when there is another branch that passes through x_0 with direction, say, $\alpha_2\phi_1 + \beta_2\phi_2$ with $(\alpha_2, \beta_2) \neq (\alpha_1, \beta_1)$.

From differentiating $f(x(s)) = 0$ twice and evaluating at x_0 we also have

$$f_u^0 \ddot{x}_0 + f_{xx}^0 \dot{x}_0 \dot{x}_0 = 0 \ .$$

Multiply this relation on the left by ψ^* to get $\psi^* f_{xx}^0 \dot{x}_0 \dot{x}_0 = 0$. Now substitute $\dot{x}_0 = \alpha\phi_1 + \beta\phi_2$ to obtain

$$\psi^* f_{xx}^0 (\alpha\phi_1 + \beta\phi_2)(\alpha\phi_1 + \beta\phi_2) = 0,$$

which can also be written as the following quadratic equation in α and β:

$$c_{11}\alpha^2 + 2c_{12}\alpha\beta + c_{22}\beta^2 = 0, \quad c_{ij} \equiv \psi^* f_{xx}^0 \phi_i \phi_j, \quad i,j = 1,2. \tag{2.7}$$

This equation is called the *Algebraic Bifurcation Equation* (ABE) [Keller, 1977].

We want solution pairs (α, β) of the ABE with not both α and β equal to zero. If for example $\alpha \neq 0$ then we can rewrite the ABE as

$$c_{11} + 2c_{12}\frac{\beta}{\alpha} + c_{22}\left(\frac{\beta}{\alpha}\right)^2 = 0 \ .$$

Thus we see that if the discriminant $\Delta_0 \equiv c^2{}_{12} - c_{11}c_{22}$ is positive then (2.7) has two distinct real nontrivial solution pairs (α_1, β_1) and (α_2, β_2) which are unique up to scaling. The discriminant Δ_0 cannot be negative, since we already have one real root (α_1, β_1) corresponding to the direction vector $\dot{x}_0$. If $\Delta_0 > 0$ then we have two distinct 'direction vectors,' $\alpha_1\phi_1 + \beta_1\phi_1$ and $\alpha_2\phi_1 + \beta_2\phi_2$, and we expect a bifurcation, i.e., we expect a second branch to pass through x_0.

Practical computation of the bifurcation direction

From the discussion above we can take one of the two null vectors, say ϕ_1, to be the direction of the 'given' branch at the bifurcation point, i.e., $\phi_1 = \dot{x}_0$. Then $(\alpha_1, \beta_1) = (1,0)$ is a root of (2.7) and $c_{11} = 0$. Under the assumption that $\Delta_0 > 0$ we also have $c_{12} \neq 0$. Then from (2.7) we find that the second root satisfies $\alpha_2/\beta_2 = -c_{22}/2c_{12}$.

Evaluation of c_{12} and c_{22} requires computation of the null vectors ϕ_1, ϕ_2 and ψ. We have already chosen $\phi_1 = \dot{x}_0$. Choose $\phi_2 \perp \phi_1$. Then ϕ_2 is a null vector of $F_x^0 = \begin{pmatrix} f_x^0 \\ \dot{x}_0^* \end{pmatrix}$. In fact, the null space of F_x^0 is only one-dimensional as will be shown later. It is also not difficult to see that $\begin{pmatrix} \psi \\ 0 \end{pmatrix}$ is a simple null vector of $(F_x^0)^* = ((f_x^0)^*\,\dot{x}_0)$. We have already shown how to compute null vectors efficiently. After determining the coefficients α_2 and β_2 the direction $x_0' \equiv \alpha_2\phi_1 + \beta_2\phi_2$ of the bifurcating branch is normalized so that $\|x_0'\| = 1$.

Practical branch switching

After the computation of the direction x_0' of the bifurcating branch, the first solution x_1 on the bifurcating branch away from the bifurcation point x_0 can be computed by the regular pseudoarclength continuation method:

$$\begin{aligned} f(x_1) &= 0, \\ (x_1 - x_0)^* x_0' - \Delta s &= 0, \end{aligned} \tag{2.8}$$

with initial approximation $x_1^{(0)} = x_0 + \Delta s\, x_0'$.

As we have seen above, the computation of the bifurcation direction requires evaluation of the second derivative f_{xx}^0. This is avoided by the *orthogonal direction method* which uses the vector ϕ_2 rather than the actual direction x_0' in (2.8). Recall that we have chosen $\phi_2 \perp \phi_1$ with $\phi_1 = \dot{x}_0$. The branch switching procedure then simply consists of computing the null vector ϕ_2, followed by the first pseudoarclength continuation step

$$\begin{aligned} f(x_1) &= 0, \\ (x_1 - x_0)^* \phi_2 - \Delta s &= 0, \end{aligned}$$

This method need not always be successful. But it works well in most practical applications.

Detection of bifurcation points

Let $F(x; s) \equiv \begin{pmatrix} f(x) \\ (x - x_0)^* \dot{x}_0 - s \end{pmatrix}$ and let x_0 be a simple singular point. Then $F_x^0 \equiv F_x(x_0; s_0) = F_x(x_0) = \begin{pmatrix} f_x^0 \\ \dot{x}_0^* \end{pmatrix}$. As above, make the specific choice $\phi_0 = \dot{x}_0$ for the first null vector of f_x^0, and choose the second null vector ϕ_2 such that $\phi_2^* \phi_1 = 0$. Thus $F_x^0 = \begin{pmatrix} f_x^0 \\ \phi_1^* \end{pmatrix}$. We see that ϕ_2 is also a null vector of F_x^0 but that ϕ_1 is not. Therefore F_x^0 has a one-dimensional nullspace. Also, the null vector of $(F_x^0)^*$ is given by $\Psi \equiv \begin{pmatrix} \psi \\ 0 \end{pmatrix}$, where ψ is the null vector of $(f_x^0)^*$.

Theorem. [Keller, 1987] *Let $x_0 = x(s_0)$ be a simple singular point on a smooth solution branch $x(s)$ of $f(x) = 0$. Assume that the discriminant Δ_0 is positive and that 0 is an algebraically simple eigenvalue of F_x^0. Then $\det F_x$ changes sign at x_0.*

Proof. Consider the parametrized eigenvalue problem

$$F_x(x(s))\phi(s) = \kappa(s)\phi(s),$$

where $\kappa(s)$ and $\phi(s)$ are smooth near s_0, with $\kappa(s_0) = 0$ and $\phi(0) = \phi_2$. This can be done because we have assumed that 0 is an algebraically simple eigenvalue. Differentiation of the above equation and evaluation at s_0 gives

$$F_{xx}^0 \dot{x}_0 \phi_2 + F_x^0 \dot{\phi}(s_0) = \dot{\kappa}_0 \phi_2,$$

and upon multiplying this on the left by Ψ^* we find

$$\dot{\kappa}_0 = \frac{\Psi^* F_{xx}^0 \phi_1 \phi_2}{\Psi^* \phi_2} = \frac{\psi^* f_{xx}^0 \phi_1 \phi_2}{\Psi^* \phi_2} = \frac{c_{12}}{\Psi^* \phi_2}$$

where $\Psi^* \phi_2 \neq 0$ and where c_{12} is one of the coefficients in (2.7). By assumption $\Delta_0 \neq 0$. As before this implies that $c_{12} \neq 0$ and hence $\kappa_0 \neq 0$. ■

Remark. The following theorem states that there must be a bifurcation at x_0. This result can be proven by degree theory [Keller, 1978; 1987].

Theorem. *Let $x(s)$ be a smooth solution branch of $F(x; s) = 0$, where $F: R^{n+1} \times R \to R^{n+1}$ is C^1, and assume that $\det F_x(x(s); s)$ changes sign at $s = s_0$. Then $x(s_0)$ is a bifurcation point, i.e., every open neigborhood of x_0 contains a solution of $F(x; s) = 0$ that does not lie on $x(s)$.*

Implementation in AUTO

The determinant of the Jacobian F_x is monitored along the solution branch $x(s) = (u(s), \lambda(s))$. Points where the determinant changes sign are located by a secant iteration scheme. More specifically, let $q(s)$ denote the scalar function of which a zero is sought. In the current application $q(s)$ is the determinant of the Jacobian F_x along the solution branch $x(s)$, but there will be other applications later. If a change of sign of $q(s)$ is noticed along the branch then the zero is approximated by the secant iteration

$$s^{\nu+1} = s^\nu - \frac{s^\nu - s^{\nu-1}}{q(s^\nu) - q(s^{\nu-1})}\, q(s^\nu), \tag{2.9}$$

where ν is the iteration index.

Solution points where the determinant of the Jacobian F_x changes sign are potential bifurcation points by the earlier discussion. Also we know that the determinant is nonzero at simple folds. After the computation of a given branch has been completed, each potential bifurcation point found on it is considered in turn and branch switching is attempted. To switch from one solution branch to another the orthogonal direction method outlined above is used. It performs well in most appli-

cations, although difficulties can occur if the branches intersect at a very small angle.

In the implementation the computation of the basic branch and of any bifurcating branch is discontinued if either λ or $\| u \|$ reaches preset limits, if a user-specified maximum number of steps have been taken, or if the procedure fails to converge. The number of successively detected bifurcations at which branch switching is to be done can be selected. One can choose to trace out only one leg, which is useful, for example, in case of symmetric bifurcations where the solutions on each leg are equivalent.

Example. Here we give a simple example to illustrate use of the algebraic bifurcation equations. Consider the predator-prey model [Doedel & Kernévez, 1986]

$$u_1' = p_2 u_1(1 - u_1) - u_1 u_2 - p_1(1 - e^{-p_3 u_1}),$$
$$u_2' = -u_2 + p_4 u_1 u_2 \ .$$

The term $p_1(1 - e^{-p_3 u_1})$ can be thought of as modeling the 'harvesting' of u_1. The exponential term reflects the increased difficulty of harvesting when u_1 is small. We fix $p_2 = p_4 = 3$ and $p_3 = 5$ and we consider the bifurcation behavior when p_1 is varied. Let $x \equiv (u_1, u_2, p_1)$. Note that $x = (0, 0, p_1)$ is a solution branch with $\dot{x} = (0, 0, 1)$. The Jacobian f_x is

$$f_x(u_1, u_2, p_1) = \begin{pmatrix} p_2(1 - 2u_1) - u_2 - p_1 p_3 e^{-p_3 u_1} & -u_1 & -(1 - e^{-p_3 u_1}) \\ p_4 u_2 & -1 + p_4 u_1 & 0 \end{pmatrix} .$$

Along $x = (0, 0, p_1)$ we have

$$f_x(0, 0, p_1) = \begin{pmatrix} p_2 - p_1 p_3 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix},$$

and a simple singular point is at $x = (0, 0, p_1^0)$, where $p_1^0 = p_2/p_3 = 3/5$. The Jacobian at the singular point is

$$f_x(0, 0, p_1^0) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix},$$

with right and left null vectors $\psi = (1, 0)^*$, $\phi_1 = \dot{x}_0 = (0, 0, 1)^*$ and $\phi_2 = (1, 0, 0)^*$, $\phi_2 \perp \phi_1$. Also $F_x = \begin{pmatrix} f_x \\ \dot{x}_0^* \end{pmatrix}$ with $\dot{x}^* = (0, 0, 1)$, so that the determinant of

$$F_x^0 = \begin{pmatrix} p_2 - p_1 p_3 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

changes sign at p_1^0, and zero is a simple eigenvalue. The second derivative is

$$f_{xx} = \begin{pmatrix} (-2p_2 + p_1 p_3^2 e^{-p_3 u_1}, -1, -p_3 e^{-p_3 u_1}) & (-1, 0, 0) & (-p_3 e^{-p_3 u_1}, 0, 0) \\ (0, p_4, 0) & (p_4, 0, 0) & (0, 0, 0) \end{pmatrix}$$

and at the singular point

$$f_{xx}^0 = \begin{pmatrix} (-2p_2 + p_1^0 p_3^2, -1, -p_3) & (-1, 0, 0) & (-p_3, 0, 0) \\ (0, p_4, 0) & (p_4, 0, 0) & (0, 0, 0) \end{pmatrix} .$$

The algebraic bifurcation equation is

$$c_{11}\alpha^2 + 2c_{12}\alpha\beta + c_{22}\beta^2 = 0,$$

where

$$c_{11} = \psi^* f_{xx}^0 \phi_1 \phi_1 = (1, 0) f_{xx}^0 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = (1, 0) \begin{pmatrix} -p_3 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0,$$

$$c_{12} = \psi^* f_{xx}^0 \phi_1 \phi_2 = (1, 0) f_{xx}^0 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = (1, 0) \begin{pmatrix} -p_3 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = -p_3 = -5,$$

$$c_{22} = \psi^* f_{xx}^0 \phi_2 \phi_2 = (1, 0) f_{xx}^0 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = (1, 0) \begin{pmatrix} -2p_2 + p_1^0 p_3^2 & -1 & -p_3 \\ 0 & p_4 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$
$$= -2p_2 + p_1^0 p_3^2 = 9 \ .$$

Thus the quadratic equation is

$$9\beta^2 - 10\alpha\beta = 0,$$

and up to a scaling factor its roots are

$$(\alpha_1, \beta_1) = (1,0) \quad \text{and} \quad (\alpha_2, \beta_2) = (9, 10) \ .$$

The direction of the given branch corresponds to the root $(\alpha_1, \beta_1) = (1, 0)$, i.e.,

$$\dot{x}_0 = \alpha_1\phi_1 + \beta_1\phi_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \ .$$

The direction of the bifurcating branch is

$$x_0' = \alpha_2\phi_1 + \beta_2\phi_2 = \begin{pmatrix} 10 \\ 0 \\ 9 \end{pmatrix} \ ,$$

before normalization.

In particular the u_2-component of the direction of the bifurcating branch is zero. In fact the bifurcating branch lies entirely in the $u_2 = 0$ plane as can be seen in Fig. 2.2. Also shown is a third branch of stationary solutions from which a family of periodic solutions bifurcates through a Hopf bifurcation. The branch of periodic solutions terminates in a heteroclinic orbit as indicated. The stable behavior is as follows: When we increase p_1 starting at $p_1 = 0$ the branch of stationary solutions along which both u_1 and u_2 are nonzero will be followed until the Hopf bifurcation point is reached. Along this stationary branch the harvested species u_1 is constant, but the predator u_2 decreases in level! Between the Hopf bifurcation and the heteroclinic orbit the system will be in an oscillatory mode. After the heteroclinic orbit the system will go to the stable stationary state with both u_1 and u_2 zero.

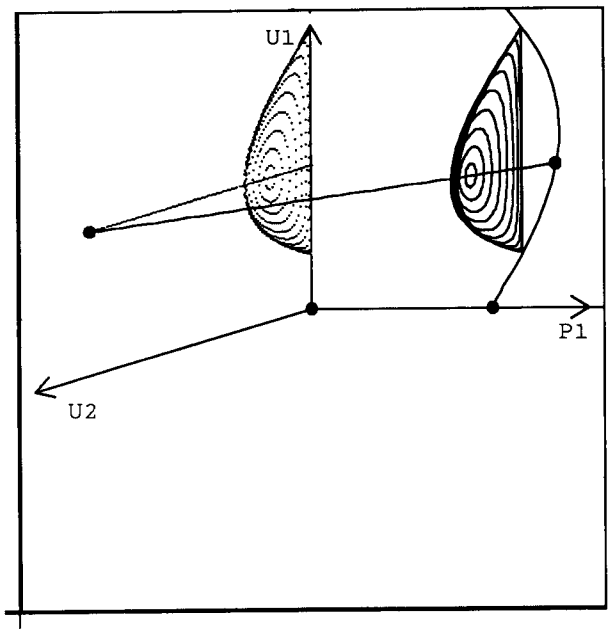


Fig. 2.2. Bifurcation behavior of the two-species predator prey model.

2.3. *Folds and their continuation*

Recall that a simple fold on a solution branch $(u(s), \lambda(s))$ of $f(u, \lambda) = 0$ is a point (u_0, λ_0) satisfying

$$N(f_u^0) = \text{Span}\{\phi_0\}, \quad f_\lambda^0 \notin R(f_u^0),$$

We have $\dot{\lambda}_0 = 0$ and $\phi_0 = \dot{u}_0$.

Change of stability

Now assume in addition that zero is an algebraically simple eigenvalue of f_u^0. Then there is a smooth parametrization of the eigenvalue-eigenvector relation near s_0:

$$f_u(u(s), \lambda(s))\phi(s) = \kappa(s)\phi(s), \quad \kappa(s_0) = 0, \quad \phi(s_0) = \phi_0 \ .$$

Differentiate this equation with respect to s and evaluate at s_0 to get

$$f_{uu}^0\phi_0\phi_0 + f_u^0\dot{\phi}_0 = \dot{\kappa}_0\phi_0 \ .$$

Let $N((f_u^0)^*) = \text{Span}\{\psi_0\}$ and multiply the above equation on the left by ψ_0^* to find

$$\dot{\kappa}_0 = \frac{\psi_0^* f_{uu}^0 \phi_0\phi_0}{\psi_0^*\phi_0} \ , \quad \psi_0^*\phi_0 \neq 0 \ .$$

Previously we found

$$\ddot{\lambda}_0 = \frac{\psi_0^* f_{uu}^0 \phi_0\phi_0}{\psi_0^* f_\lambda^0} \ , \quad (\psi_0^* f_\lambda^0 \neq 0 \text{ at a simple fold}),$$

and (u_0, λ_0) is called a quadratic fold if $\ddot{\lambda}_0 \neq 0$. Thus we see that if (u_0, λ_0) is a simple quadratic fold and if 0 is an algebraically simple eigenvalue of f_u^0 then $\kappa(s)$ changes sign at (u_0, λ_0). Hence if the branch consists of stable solutions 'before' the fold then the solutions will be unstable past the fold, i.e., a change of stability takes place.

The extended system

To continue a fold in two parameters ('fold following') we make use of an *extended system* [Fier, 1985; Griewank & Reddien, 1984; Jepson & Spence, 1985; Rheinboldt, 1982]

$$\begin{aligned} f(u, \lambda, \mu) &= 0, \\ f_u(u, \lambda, \mu)\phi &= 0, \\ \phi^*\phi_0 - 1 &= 0 \ . \end{aligned} \tag{2.10a}$$

Here $\mu \in \mathbf{R}$ is a second parameter in the equations. Up to now μ was considered fixed. The vector ϕ_0 belongs to a 'reference solution' $(u_0, \phi_0, \lambda_0, \mu_0)$ which in practical continuation is the latest computed solution point on the branch. At a fold the Eqs. (2.10a) can clearly be satisfied. This above system has the form

$$F(U, \mu) = 0, \quad U \equiv (u, \phi, \lambda), \quad F{:}R^{2n+1} \times R \to R^{2n+1},$$

or, using the uniform formulation,

$$F(X) = 0, \quad X \equiv (U, \mu), \quad F{:}R^{2n+2} \to R^{2n+1} \quad .$$

Parameter continuation

First we consider continuing a solution (u_0, ϕ_0, λ_0) of (2.10a) at $\mu = \mu_0$ by varying μ, i.e., we treat μ as the continuation parameter. This can be viewed as natural parameter continuation. By the implicit function theorem there exists a smooth solution branch $U(\mu) = (u(\mu), \phi(\mu), \lambda(\mu))$ to (2.10a) provided the Jacobian

$$F_U^0 \equiv \frac{dF}{dU}(U_0) = \begin{pmatrix} f_u^0 & O & f_\lambda^0 \\ f_{uu}^0 \phi_0 & f_u^0 & f_{u\lambda}^0 \phi_0 \\ 0^* & \phi_0^* & 0 \end{pmatrix}$$

is nonsingular. We have the following elementary continuation result:

Theorem. *A simple quadratic fold with respect to λ can be continued locally using the second parameter μ as continuation parameter.*

Proof. Suppose F_U^0 is singular. Then

(i) $f_u^0 x + z f_\lambda^0 = 0$,
(ii) $f_{uu}^0 \phi_0 x + f_u^0 y + z f_{u\lambda}^0 \phi_0 = 0$,
(iii) $\phi_0^* y = 0$,

for some $x, y \in R^n$, $z \in R$. Since $f_\lambda^0 \notin R(f_u^0)$ we have from (i) that $z = 0$ and hence $x = c_1 \phi_0$ for some $c_1 \in R$. Multiply (ii) on the left by ψ_0^* to get

$$c_1 \psi_0^* f_{uu}^0 \phi_0 \phi_0 = 0 \quad .$$

Thus $c_1 = 0$ because by assumption $\psi_0^* f_{uu}^0 \phi_0 \phi_0 \neq 0$. So $x = 0$, and from (ii) we now have $f_u^0 y = 0$, i.e., $y = c_2 \phi_0$. But then by (iii) $c_2 = 0$. Thus $x = y = 0$ and $z = 0$ and hence F_U^0 must be nonsingular. ■

Note that the theorem does not require zero to be an algebraically simple eigenvalue of f_u^*. Thus, for example, f_u^0 may have the form $\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, provided the fold remains simple and quadratic.

Pseudoarclength continuation

Natural parameter continuation in μ is too restrictive, since it would fail at folds with respect to μ. These could correspond to cusp points, bifurcation points, or isola formation points [Dellwo *et al.*, 1982; Seoane *et al.*, 1991]. Therefore we apply the pseudoarclength continuation method to compute a solution branch

$$(u(s), \phi(s), \lambda(s), \mu(s))$$

That is, we treat μ as one of the unknowns in (2.10a) and we add the equation

$$(u-u_0)^* \dot{u}_0 + (\phi-\phi_0)^* \dot{\phi}_0 + (\lambda-\lambda_0)\dot{\lambda}_0 + (\mu-\mu_0)\dot{\mu}_0 - \Delta s = 0. \tag{2.10b}$$

As before, $(\dot{u}_0, \dot{\phi}_0, \dot{\lambda}_0, \dot{\mu}_0)$ is the direction of the branch at the current solution point $(u_0, \phi_0, \lambda_0, \mu_0)$. The Jacobian of (2.10a) with respect to u, ϕ, λ *and* μ at $X_0 = (u_0, \phi_0, \lambda_0, \mu_0)$ is now

$$F_X^0 \equiv \frac{dF}{dX}(X_0)$$

$$\equiv \begin{pmatrix} f_u^0 & O & f_\lambda^0 & f_\mu^0 \\ f_{uu}^0 \phi_0 & f_u^0 & f_{u\lambda}^0 \phi_0 & f_{u\mu}^0 \phi_0 \\ 0^* & \phi_0^* & 0 & 0 \end{pmatrix} . \tag{2.11}$$

For pseudoarclength continuation to work we need only check that F_X^0 has full rank. For a simple quadratic fold with respect to λ this follows from the above theorem. If $\psi_0^* f_{uu}^0 \phi_0 \phi_0 \neq 0$, and $f_\lambda^0 \in R(f_u^0)$, but if $f_\mu^0 \notin R(f_u^0)$, i.e., if we have a simple quadratic fold with respect to μ, then we can apply the theorem to F_X^0 with the second last column struck out to see that F_X^0 still has full rank.

Efficient implementation

As we have seen, if $\psi_0^* f_{uu}^0 \phi_0 \phi_0 \neq 0$, and if either $f_\lambda^0 \notin R(f_u^0)$ or $f_\mu^0 \notin R(f_u^0)$, then after interchanging the last two columns, if necessary, we can put the Jacobian $\begin{pmatrix} F_X^0 \\ X_0 \end{pmatrix}$ of (2.10a, b), in the form $\begin{pmatrix} A & c \\ b^* & d \end{pmatrix}$, where A is nonsingular. The linear systems in Newton's method then have the form

$$\begin{pmatrix} A & c \\ b^* & d \end{pmatrix} \begin{pmatrix} x \\ z \end{pmatrix} = \begin{pmatrix} f \\ h \end{pmatrix},$$

$$\text{or} \quad \begin{pmatrix} A & 0 \\ b^* & e \end{pmatrix} \begin{pmatrix} I & A^{-1}c \\ O & 1 \end{pmatrix} \begin{pmatrix} x \\ z \end{pmatrix} = \begin{pmatrix} f \\ h \end{pmatrix}, \tag{2.12}$$

where $e = d - b^*A^{-1}c$. Omitting explicit bordered LU-decomposition here, we can still solve (2.12) efficiently through the following steps:

$$A\hat{c} = c,$$
$$e = d - b^*\hat{c} \quad (\neq 0),$$
$$A\hat{f} = f,$$
$$z = (h - b^*\hat{f})/e,$$
$$x = \hat{f} - z\hat{c} \ .$$

Next we show how to solve the linear systems above that have A as coefficient matrix. From (2.11) we see that such systems have the form

$$\begin{pmatrix} \tilde{A} & O & c_1 \\ B & \tilde{A} & c_2 \\ 0^* & \phi^* & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} f \\ g \\ h \end{pmatrix} , \tag{2.13}$$

where $N(\tilde{A}) = \text{Span}\{\phi_0\}$ and $N(\tilde{A}^*) = \text{Span}\{\psi\}$, with $\tilde{A} = f_u^0$, $B = f_{uu}^0\phi_0$, and $c_1 = f_\lambda^0$, $c_2 = f_{u\lambda}^0\phi_0$, or $c_1 = f_\mu^0$, $c_2 = f_{u\mu}^0\phi_0$ in case $f_\lambda^0 \in R(f_u^0)$ but $f_\mu^0 \notin R(f_u^0)$.

We have from the first of the equations in (2.13) that $\tilde{A}x = f - zc_1$. Thus we need $(f - zc_1) \in R(\tilde{A})$, i.e., $\psi^*(f - zc_1) = 0$, or

$$z = z_0 \equiv \frac{\psi^* f}{\psi^* c_1}, \quad (\psi^* c_1 \neq 0 \text{ by assumption}) \ .$$

Then

$$x = x_p + \alpha\phi_0 \ .$$

A particular solution x_p is easily found by solving

$$\tilde{A}x_p = f - z_0c_1$$

using row and column pivoting as has been shown earlier.

From the second of the equations in (2.13) we have $\tilde{A}y = g - Bx - z_0c_2$, and thus we need $\psi^*(g - Bx - z_0c_2) = 0$, i.e., $\psi^*g - \psi^*B(x_p + \alpha\phi_0) - z_0\psi^*c_2 = 0$, from which

$$\alpha = \alpha_0 \equiv \frac{\psi^*g - z_0\psi^*c_2 - \psi^*Bx_p}{\psi^*B\phi_0} ,$$

where $\psi^*B\phi_0 = \psi^* f_{uu}^0 \phi_0\phi_0 \neq 0$ by assumption. Now y also has the form

$$y = y_p + \beta\phi_0,$$

and as before a particular solution can be computed from

$$\tilde{A}y_p = g - B(x_p + \alpha_0\phi_0) - z_0c_2 \ .$$

But by the third equation in (2.13) we have $\phi_0^* y = h$, i.e., $\phi_0^*(y_p + \beta\phi_0) = h$, so that

$$\beta = \frac{h - \phi_0^* y_p}{\phi_0^*\phi_0} \ .$$

Implementation in AUTO

The direction $(\dot{u}, \dot{\lambda})$ of a solution branch of (2.1) at a regular solution point (u, λ) can be obtained by solving

$$\begin{pmatrix} f_u(u, \lambda) & f_\lambda(u, \lambda) \\ \dot{u}_0 & \dot{\lambda}_0 \end{pmatrix} \begin{pmatrix} \dot{u} \\ \dot{\lambda} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} ,$$

followed by normalization. Here $(\dot{u}_0, \dot{\lambda}_0)$ denotes the direction of the branch at the preceding solution point (u_0, λ_0). It is assumed that (u_0, λ_0) is sufficiently close to (u, λ). Simple quadratic folds along branches of solutions $(u(s), \lambda(s))$ of (2.1) correspond to simple zeroes of the function $q(s) = \dot{\lambda}(s)$ and these are located accurately using the secant iteration (2.9).

Once a simple quadratic fold has been detected it can be continued in the two parameters λ and μ using (2.10a, b). This algebraic continuation problem is treated numerically as any other system of nonlinear equations. In the implementation the inflated system is generated automatically and the bifurcation analysis is done by the same program segment used for general algebraic systems. This is done, in fact, for all continuation problems that take the form of algebraic systems. The procedure for starting a two-parameter continuation at a previously located fold is very simple in the implementation.

2.4. *Hopf Bifurcation points and their continuation*

According to the Hopf bifurcation theorem, a bifurcation of a branch of periodic solutions to $u' = f(u, \lambda)$ from a stationary solution branch $(u(\lambda), \lambda)$ takes place if a complex conjugate pair of eigenvalues $\alpha(s) \pm i\beta(s)$ of the Jacobian $f_u(u(\lambda), \lambda)$ crosses the imaginary axis at nonzero 'speed,' i.e., if for some λ_0 we have $\alpha(\lambda_0) = 0$, $\beta(\lambda_0) \neq 0$, and $\dot{\alpha}(\lambda_0) \neq 0$. We also assume that f_u^0 is nonsingular, so that the stationary solution branch can be parametrized locally in λ. The computation of the branch of periodic solutions will be treated later. Here we consider the algebraic continuation problem of tracking a branch of Hopf bifurcation points in two parameters [Doedel *et al.*, 1984; Griewank & Reddien, 1983].

If the eigenvalue $i\beta(\lambda_0)$ is algebraically simple then we have locally a smooth solution branch to the parametrized right and left eigenvalue-eigenvector problems:

$$f_u(u(\lambda), \lambda)\phi(\lambda) = \kappa(\lambda)\phi(\lambda), \tag{2.14a}$$
$$\psi^*(\lambda)f_u(u(\lambda), \lambda) = \kappa(\lambda)\psi^*(\lambda), \tag{2.14b}$$
$$\psi^*(\lambda)\phi(\lambda) = 1, \quad (\text{and also } \phi^*(\lambda)\phi(\lambda) = 1), \tag{2.14c}$$

with $\kappa(\lambda_0) = i\beta(\lambda_0)$. Above * denotes conjugate transpose. Differentiation gives

$$f_{uu}\,\dot{u}\phi + f_{u\lambda}\phi + f_u\dot{\phi} = \dot{\kappa}\phi + \kappa\dot{\phi}, \tag{2.15a}$$

$$\psi^* f_{uu}\,\dot{u} + \psi^* f_{u\lambda} + \dot{\psi}^* f_u = \dot{\kappa}\psi^* + \kappa\dot{\psi}^*, \tag{2.15b}$$

$$\dot{\psi}^*\phi + \psi^*\dot{\phi} = 0 \ . \tag{2.15c}$$

Multiply (2.15a) on the left by ψ^* and (2.15b) on the right by ϕ to get

$$\psi^* f_{uu}\,\dot{u}\phi + \psi^* f_{u\lambda}\phi + \psi^* f_u\dot{\phi} = \dot{\kappa}\psi^*\phi + \kappa\psi^*\dot{\phi}, \tag{2.16a}$$

$$\psi^* f_{uu}\,\dot{u}\phi + \psi^* f_{u\lambda}\phi + \dot{\psi}^* f_u\phi = \dot{\kappa}\psi^*\phi + \kappa\dot{\psi}^*\phi \ . \tag{2.16b}$$

Adding (2.16a) and (2.16b), using (2.14c) and (2.15c), and

$$\psi^* f_u\dot{\phi} + \dot{\psi}^* f_u\phi = \kappa(\psi^*\dot{\phi} + \dot{\psi}^*\phi) = 0,$$

we find

$$\dot{\kappa} = \psi^*[f_{uu}\,\dot{u} + f_{u\lambda}]\phi \ .$$

From differentiating $f(u(\lambda), \lambda) = 0$ with respect to λ we have

$$\dot{u} = -(f_u)^{-1} f_\lambda,$$

so that

$$\dot{\kappa} = \psi^*[-f_{uu}(f_u)^{-1} f_\lambda + f_{u\lambda}]\phi \ .$$

Thus the crossing is transversal, i.e., $\dot{\alpha}(s_0) = \mathrm{Re}(\dot{\kappa}_0) \neq 0$, provided

$$\mathrm{Re}(\psi_0^*[f_{uu}^0 (f_u^0)^{-1} f_\lambda^0 - f_{u\lambda}^0]\phi_0) \neq 0 \ . \tag{2.17}$$

This condition is also required for the nonsingularity of the extended system given below and for the numerical stability of the solution algorithm.

The extended system: Complex formulation

The *extended system* for computing a branch of Hopf bifurcation points consists of the necessary conditions

$$\begin{aligned} &f(u, \lambda, \mu) = 0, \\ &f_u(u, \lambda, \mu)\phi - i\beta\phi = 0, \\ &\phi^*\phi_0 - 1 = 0, \end{aligned} \tag{2.18}$$

to which we want to compute a solution branch $(u, \phi, \beta, \lambda, \mu)$, with $u \in \mathrm{R}^n$, $\phi \in \mathrm{C}^n$, $\beta, \lambda, \mu \in \mathrm{R}$. In (2.18) ϕ_0 belongs to a 'reference solution' $(u_0, \phi_0, \beta_0, \lambda_0, \mu_0)$ which in practical continuation is the latest computed solution point on a branch. First we consider parametrizing this branch using the second problem parameter μ as continuation parameter, i.e., we seek a solution branch $(u(\mu), \phi(\mu), \beta(\mu), \lambda(\mu))$. However, in practice we use pseudoarclength continuation.

Equation (2.18) defines a mapping

$$F: \mathrm{R}^n \times \mathrm{C}^n \times \mathrm{R}^2 \to \mathrm{R}^n \times \mathrm{C}^n \times \mathrm{C} \ .$$

The derivative with respect to $(u, \phi, \beta, \lambda)$ at the solution point $(u_0, \phi_0, \beta_0, \lambda_0, \mu_0)$ is

$$\begin{pmatrix} f_u^0 & O & 0 & f_\lambda^0 \\ f_{uu}^0\phi_0 & f_u^0 - i\beta_0 I & -i\phi_0 & f_{u\lambda}^0\phi_0 \\ 0^* & \phi_0^* & 0 & 0 \end{pmatrix},$$

which is of the form

$$\begin{pmatrix} A & O & 0 & c_1 \\ C & D & -i\phi_0 & c_2 \\ 0^* & \phi_0^* & 0 & 0 \end{pmatrix} \ .$$

Here $A = f_u^0$ is assumed nonsingular, $C = f_{uu}^0\,\phi_0$, $c_1 = f_\lambda^0$, $c_2 = f_{u\lambda}^0\,\phi_0$, and $D = f_u^0 - i\beta_0 I$, with $N(D) = \mathrm{Span}\{\phi_0\}$, $N(D^*) = \mathrm{Span}\{\psi_0\}$, $\psi_0^*\phi_0 = 1$, and $\phi_0^*\phi_0 = 1$.

We shall now show that the above matrix is nonsingular if the eigenvalue crossing is transversal, i.e., if (2.17) holds. We do this by constructing a solution $x \in \mathrm{R}^n$, $y \in \mathrm{C}^n$, z_1, $z_2 \in \mathrm{R}$, to

$$\begin{pmatrix} A & O & 0 & c_1 \\ C & D & -i\phi_0 & c_2 \\ 0^* & \phi_0^* & 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} f \\ g \\ h \end{pmatrix},$$

$$f \in R^n, \quad g \in C^n, \quad h \in C \ . \tag{2.19}$$

The first of the three equations in (2.19) is $Ax + z_2c_1 = f$, where by assumption A is nonsingular. Thus we can write $x = A^{-1}f - z_2A^{-1}c_1$. The second equation can then be written

$$CA^{-1}f - z_2CA^{-1}c_1 + Dy - z_1 i\phi_0 + z_2c_2 = g,$$

and upon multiplying this on the left by ψ_0^* we have

$$\psi_0^* CA^{-1}f - z_2\psi_0^* CA^{-1}c_1 - z_1 i\psi_0^*\phi_0 + z_2\psi_0^* c_2 = \psi_0^* g$$

We have chosen ψ_0 such that $\psi_0^* \phi_0 = 1$. For notational convenience define

$$\tilde{f} \equiv CA^{-1}f, \quad \tilde{c}_1 \equiv CA^{-1}c_1 \ .$$

Computationally $\tilde{f}$ and $\tilde{c}_1$ are obtained from

$$A\hat{f} = f, \quad \tilde{f} = C\hat{f}, \quad A\hat{c}_1 = c_1, \quad \tilde{c}_1 = C\hat{c}_1 \ . \qquad (2.20)$$

Then the above equation can be written as

$$iz_1 + \psi_0^*(\tilde{c}_1 - c_2)z_2 = \psi_0^*(\tilde{f} - g) \ .$$

Separate the real and imaginary part of this equation and use the fact that z_1 and z_2 are real to get

$$\mathrm{Re}(\psi_0^*[\tilde{c}_1 - c_2])z_2 = \mathrm{Re}(\psi_0^*[\tilde{f} - g]) \ ,$$
$$z_1 + \mathrm{Im}(\psi_0^*[\tilde{c}_1 - c_2])z_2 = \mathrm{Im}(\psi_0^*[\tilde{f} - g]),$$

from which

$$z_2 = \frac{\mathrm{Re}(\psi_0^*[\tilde{f} - g])}{\mathrm{Re}(\psi_0^*[\tilde{c}_1 - c_2])} \ ,$$

$$z_1 = -z_2\mathrm{Im}(\psi_0^*[\tilde{c}_1 - c_2]) + \mathrm{Im}(\psi_0^*[\tilde{f} - g]) \ .$$

Now solve for x in

$$Ax = f - z_2 c_1, \qquad (2.21)$$

and compute a particular solution y_p to

$$Dy = g - Cx + iz_1\phi_0 - z_2 c_2 \ . \qquad (2.22)$$

Then

$$y = y_p + \alpha\phi_0, \quad \alpha \in \mathbb{C} \ . \qquad (2.23)$$

The third equation in (2.19) reads $\phi_0^* y = \phi_0^* y_p + \alpha\phi_0^*\phi_0 = h$, from which

$$\alpha = \frac{h - \phi_0^* y_p}{\phi_0^*\phi_0} = h - \phi_0^* y_p \ . \qquad (2.24)$$

The above construction can be carried out if $\mathrm{Re}(\psi_0^*[\tilde{c}_1 - c_2]) \neq 0$. But, using the definition of $\tilde{c}_1$ and c_2, we have

$$\begin{aligned}\mathrm{Re}(\psi_0^*[\tilde{c}_1 - c_2]) &= \mathrm{Re}(\psi_0^*[CA^{-1}c_1 - c_2]) \\ &= \mathrm{Re}(\psi_0^*[f_{uu}^0\phi_0(f_u^0)^{-1}f_\lambda^0 - f_{u\lambda}^0\phi_0]) \\ &= \mathrm{Re}(\psi_0^*[f_{uu}^0(f_u^0)^{-1}f_\lambda^0 - f_{u\lambda}^0]\phi_0) \\ &= \mathrm{Re}(\dot{\kappa}_0),\end{aligned}$$

which we assume to be nonzero (See (2.17)). Thus the matrix in (2.19) is nonsingular and there exists locally a branch $(u(\mu), \phi(\mu), \beta(\mu), \lambda(\mu))$ of solutions to (2.18), i.e., the Hopf bifurcation persists under small perturbation of the second problem parameter μ.

Algorithm

The above construction can be used in the algorithm for solving (2.18) by Newton or Chord iteration. First one computes the left and right null vectors ψ_0 and ϕ_0 of the complex matrix D. Then the steps (2.20)–(2.24) are carried out in the order of appearance.

Further efficiency can be gained by making use of the fact that certain calculations in the construction are real or involve real variables. For a more efficient real formulation see Griewank & Reddien [1983]. For large n most of the computational effort is spent on LU decomposing A and D. Here A is real and assumed nonsingular. D is complex with a one-dimensional nullspace. The decomposition of D requires row and column pivoting. The null vector ϕ of D and the null vector ψ of D^* can be computed efficiently as already shown in Sec. 2.1 except that now we have to use complex arithmetic.

Pseudoarclength continuation

In practical computation one does not want to use the second problem parameter μ as continuation parameter in the extended system (2.18) because a solution branch may contain folds with respect to μ. Thus, as before, we treat μ as an additional unknown and we add the pseudoarclength relation

$$(u - u_0)^*\dot{u}_0 + (\phi - \phi_0)^*\dot{\phi}_0 + (\beta - \beta_0)\dot{\beta}_0 + (\lambda - \lambda_0)\dot{\lambda}_0 + (\mu - \mu_0)\dot{\mu}_0 - \Delta s = 0 \ .$$

Newton's method applied to the enlarged system then leads to linear systems with matrices of the form $\begin{pmatrix} A & c \\ b^* & d \end{pmatrix}$ where A represents the matrix in (2.19). The solution algorithm for such systems has already been given in Sec. 2.3 [See Eq. (2.12)]. It involves solving subsystems with A as matrix as already discussed.

Implementation in AUTO

In the software a standard eigenvalue solver is used to compute the eigenvalues of $f_u(u(s), \lambda(s))$ along the stationary solution branches. By monitoring the number of eigenvalues in the left half-plane together with the real part of the eigenvalue closest to the imaginary axis, the software package is capable of detecting Hopf bifurcation

points. The precise location is determined by secant iteration (2.9) on the real part of the critical conjugate pair of eigenvalues. Success of this procedure depends of course on the step size Δs being sufficiently small and on the Hopf bifurcations being nondegenerate.

The two parameter continuation of Hopf bifurcation points is done using the pseudoarclength continuation scheme applied to the equivalent real formulation of (2.18). Then this equation represents a nonlinear system of $3n + 2$ equations in $3n + 3$ unknowns. Generally one will have branches of solutions with possible bifurcation points. In the implementation the expanded system for two parameter continuation of Hopf bifurcation points is generated automatically and the computation is channeled through the basic routines for general algebraic systems. The complete starting data are also generated automatically using data from a previous run in which the Hopf bifurcation point was detected. No advantage is taken of the special structure of the Jacobian of the enlarged system.

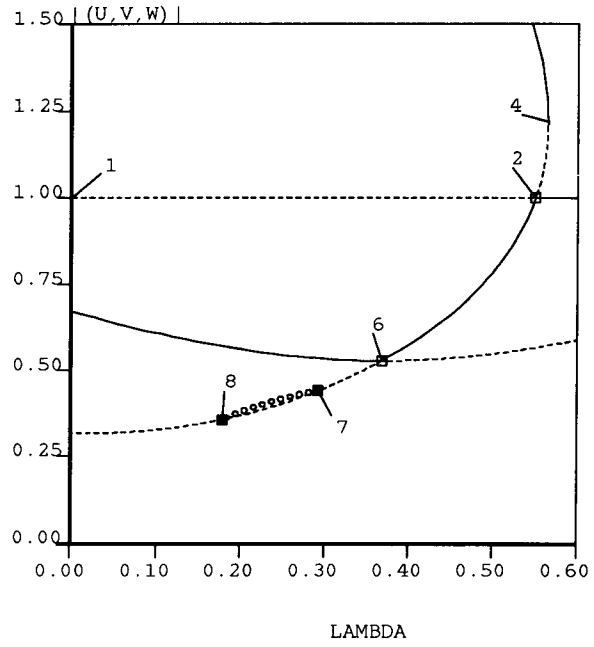


Fig. 2.3. Bifurcation diagram when $c_{uv} = 3$.

Example. Consider the equations

$$u'(t) = u(1 - u) - c_{uv}uv,$$

$$v'(t) = -c_v v + c_{uv}uv - c_{vw}vw - \lambda(1 - e^{-c_e v}),$$

$$w'(t) = -c_w w + c_{vw}vw \ .$$

This can be thought of as a simple predator-prey model where, say, u, v and w represent plankton, fish, and sharks, respectively [Doedel, 1984]. The term $\lambda(1 - e^{-c_e v})$ represents fishing, the parameter λ being the fishing quota. The factor $(1 - e^{-c_e v})$ models the fact that the quota cannot be met if the fish population is small. The other parameters are fixed: $c_v = 1/4$, $c_w = 1/2$, $c_{uv} = 3$, $c_{vw} = 3$, and $c_e = 5$.

The bifurcation behavior with λ as parameter is shown in Fig. 2.3. The vertical axis is the L_2-norm of (u, v, w). There are two Hopf bifurcation points. The stable behavior as λ increases in Fig. 2.3 is as follows: For small λ one follows the branch of stable stationary solutions (solid curve) that starts at the left of the diagram. Along this branch the values of u and v are constant, but w decreases. At the stationary bifurcation point (label 6) the value of w is zero, and one switches to the bifurcating stationary branch along which $w = 0$ everywhere. This second branch is followed until the top right bifurcation point (label 2) where v is also zero. Thereafter one follows the third (horizontal) branch along which both v and w are zero and $u = 1$.

The results of the two-parameter continuation of the Hopf bifurcation points in Fig. 2.3 is shown in Fig. 2.4. As second parameter we use c_{uv}. The curve of Hopf bifurcations contains two bifurcation points (*meta* bifurcations!). Clearly, in a certain range of values of c_{uv} *the* λ*-bifurcation diagram has four Hopf bifurcation points. The one-parameter bifurcation diagram that corresponds to the cross section of Fig. 2.4 at* $c_{uv} = 4$ is given in Fig. 2.5.

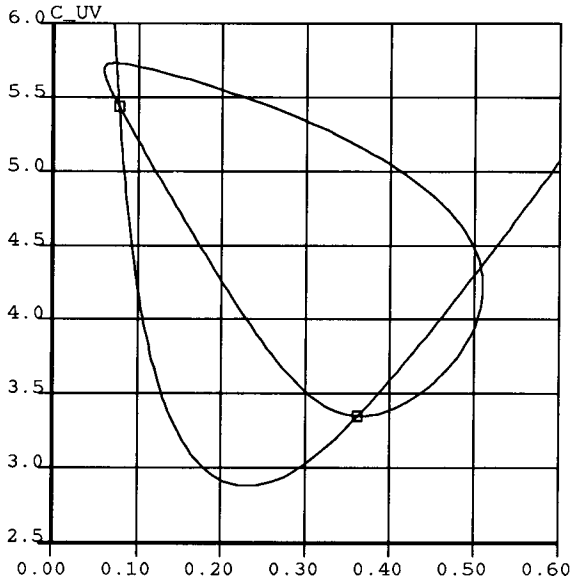


Fig. 2.4. Loci of Hopf bifurcation points.

The stable behavior as λ varies in Fig. 2.5 is as follows: For small λ one follows the branch of stationary solutions that starts in the top left of the diagram. Along this branch the values of u and v are constant, but w decreases for increasing λ. At the Hopf bifurcation the behavior becomes time periodic in (u, v, w). The two branches of periodic solutions intersect in a transcritical bifurcation near $\lambda = 3$. Here one switches to the second branch of periodic solutions along which w is identically zero. This second branch is followed until the top right Hopf bifurcation where the solutions become stationary, still with w equal to zero. Further increase in λ leads to decreasing and ultimately vanishing v much like in Fig. 2.3.

Some orbits are shown in Fig. 2.6. We see a family of orbits in (u, v, w) in which the w-component becomes smaller and ultimately negative. One of these orbits has w equal to zero and thus lies in the u, v-plane. This orbit connects to the second family of which all orbits lie in the u, v-plane. The orbit where the two families meet corresponds to the secondary periodic bifurcation in Fig. 2.5.

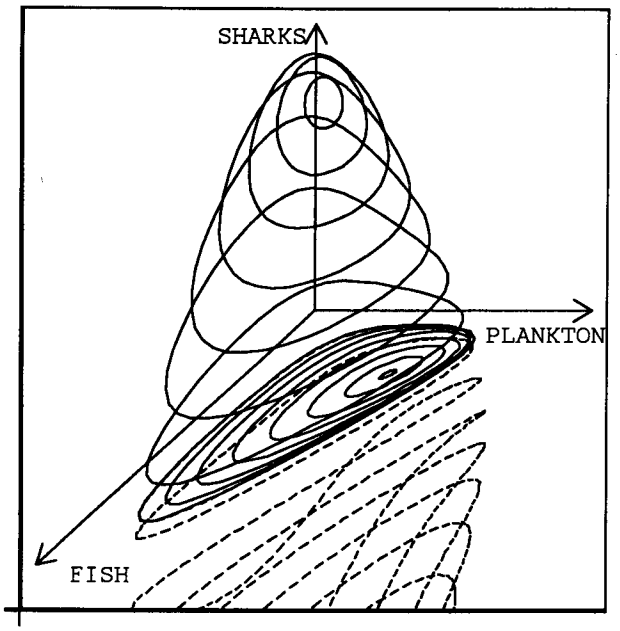


Fig. 2.6. The two families of periodic solutions. One family lies entirely in the u, v-plane. Of the other family only one orbit is in the u, v-plane. This orbit is common to both families and corresponds to the secondary periodic bifurcation near $\lambda = 3$ in Fig. 2.5.

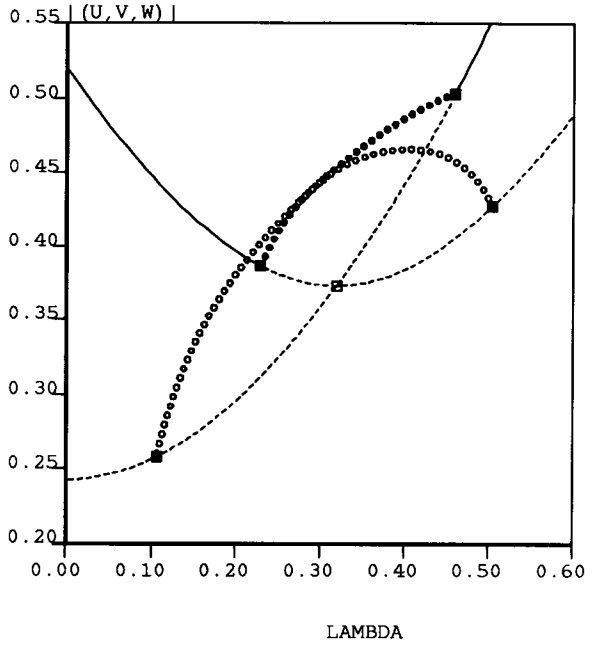


Fig. 2.5. Bifurcation diagram when $c_{uv} = 4$.

2.5. *Fixed points, folds, and Hopf bifurcation for maps*

The continuation schemes presented so far have analogues for discrete maps. Consider a fixed-point iteration

$$u_{k+1} = g(u_k, \lambda), \quad k = 0, 1, 2, \ldots,$$

where k is the iteration index and λ a free parameter. Such iterations can give very complicated dynamical behavior. The concept of steady state, or *fixed point* arises here, as does the concept of Hopf bifurcation. The fixed point analysis consists of studying the solution structure of

$$f(u, \lambda) \equiv g(u, \lambda) - u = 0,$$

which is a special case of (2.1). The treatment of bifurcation points and the detection of folds with their subsequent continuation in two parameters is then identical to the procedures described in Secs. 2.1-2.3.

Hopf bifurcation for a map corresponds to the crossing of the unit circle of a conjugate pair of eigenvalues of the Jacobian matrix $g_u(u, \lambda)$. This gives rise to the bifurcation of an invariant curve from the fixed-point branch. The detection of these Hopf bifurcations proceeds in much the same way as the detection of such points for differential equations. Let $e_k(f_u)$ denotes the kth eigenvalue of $f_u(u, \lambda)$. We have $e_k(f_u) = e_k(g_u) - 1$, so that Hopf bifurcation corresponds to the crossing of the imaginary axis of one of the quantities $\log[1 + e_k(f_u)]$.

Given a Hopf bifurcation point for a map from a one-parameter numerical analysis, one can continue such points in two parameters by using the following modification of the extended system (2.18)

$$g(u, \lambda, \mu) - u = 0,$$
$$g_u(u, \lambda, \mu)\phi - e^{i\beta}\phi = 0,$$
$$\phi^*\phi_0 - 1 = 0,$$

where β is the angle of the conjugate pair on the unit circle.

The computation of the branch of invariant circles that bifurcates from a branch of fixed points of a map at a Hopf bifurcation point is not included in AUTO. For some methods for this purpose see [Chan, 1983; Kevrekidis *et al.*, 1985, and van Veldhuizen, 1987]. One difficulty in such computations is the possible loss of differentiability of such invariant curves [Aronson *et al.*, 1982].

3. CONTROL OF BIFURCATION PROBLEMS IN FINITE DIMENSIONS

Here we consider the problem of minimizing an objective functional

$$\omega = g(u, \lambda),$$

when the control and state variables λ and u are related by the *state equation*

$$f(u, \lambda) = 0 \quad . \tag{3.1}$$

Here $g: \mathrm{R}^n \times \mathrm{R}^{n_\lambda} \to \mathrm{R}$ and $f: \mathrm{R}^n \times \mathrm{R}^{n_\lambda} \to \mathrm{R}^n$ are C^1. We let $X \equiv \mathrm{R}^n \times \mathrm{R}^{n_\lambda}$, with element $x = (u, \lambda)$. The specific objectives are:

(i) Optimization in systems where the state equation has a 'complicated' solution structure. For example, we may want to locate a solution with certain desired features.

(ii) Control of bifurcation phenomena. For example, we may want to control the location of a fold or a Hopf bifurcation point. A more complicated case is the control of the distance between two folds (e.g., elimination of hysteresis, or elimination of unwanted solutions).

In the presentation below we give special attention to numerically stable and efficient implementation. For earlier work see Doedel & Kernévez [1987a, b].

In addition to the equality constraint (3.1) we may have inequality constraints

$$h_i(u, \lambda) \leqslant 0, \quad i = 1, \ldots, n_h,$$

where each $h_i: X \to R$ is C^1. Inequality constraints are often needed for existence of an optimal solution $x_0 = (u_0, \lambda_0)$ since they introduce boundedness. Only those that are active, i.e., those that satisfy

$$h_i(u_0, \lambda_0) = 0, \quad i \in I_a, \quad \mathrm{card}(I_a) \equiv n_a,$$

have to be taken into account in the optimality system and they can be considered as included in $f(u, \lambda) = 0$.

3.1. *The optimality equations*

Necessary conditions for a solution x_0 of $f(x) = 0$ to locally minimize $g(x)$ are stated below:

Theorem. *Let x_0 minimize $g(x)$ over all x close to x_0 with $f(x) = 0$. Assume that $f_x^0 \equiv f_x(x_0)$ has full rank. Then there exist $p \in \mathrm{R}^n$, $q \in \mathrm{R}$ such that*

$$(f_x^0)^*p + (g_x^0)^*q = 0, \tag{3.2}$$
$$p^*p + q^2 = 1 \quad .$$

Proof. Since f_x^0 has full rank we can permute the components of $x \in \mathrm{R}^{n+n_\lambda}$ and write $x = (y, z)$ where $y \in \mathrm{R}^n$, and $z \in \mathrm{R}^{n_\lambda}$, so that

$$f_x^0 = (f_y^0 \; f_z^0), \quad \text{where } f_y^0 \text{ is nonsingular.}$$

By the implicit function theorem we can locally parametrize the solution to $f(y, z) = 0$ as $y = w(z)$. Then $g(x) = g(y, z) = g(w(z), z)$. A necessary condition for g to have a minimum at (y_0, z_0) is that

$$g_y^0 w_z^0 + g_z^0 = 0$$

Also, from differentiating $f(w(z), z) = 0$ with respect to z we have

$$f_y^0 w_z^0 + f_z^0 = 0.$$

Thus

$$\begin{pmatrix} f_y^0 \\ g_y^0 \end{pmatrix} w_z^0 = - \begin{pmatrix} f_z^0 \\ g_z^0 \end{pmatrix},$$

and therefore the $n + 1$ by $(n + n_\lambda)$-dimensional matrix

$$A_0 \equiv \begin{pmatrix} f_y^0 & f_z^0 \\ g_y^0 & g_z^0 \end{pmatrix}$$

has rank $\leqslant n$. In fact, A_0 has rank n because by assumption the n by n submatrix f_y^0 is nonsingular. The $n + n_\lambda$ by $n + 1$ dimensional transpose matrix A_0^* therefore also has rank n and consequently it has a one-dimensional null space, i.e.,

$$\begin{pmatrix} (f_y^0)^* & (g_y^0)^* \\ (f_z^0)^* & (g_z^0)^* \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad p^*q + q^2 = 1,$$

for some $p \in \mathrm{R}^n$, $q \in \mathrm{R}$. This final equation is equivalent to (3.2). ■

Remarks.

(1) Since $x = (u, \lambda)$, Eq. (3.2) splits into

$$(f_u^0)^*p + (g_u^0)^*q = 0,$$
$$(f_{\lambda_i}^0)^*p + g_{\lambda_i}^0 q = 0, \quad i = 1, \ldots, n_\lambda, \tag{3.3}$$
$$p^*p + q^2 = 1.$$

(2) If we distinguish the active constraints $h_i(u, \lambda) = 0$, $i \in I_a$, from the state equation $f(u, \lambda) = 0$ then we have the optimality system

$$
\begin{aligned}
&f(u, \lambda) = 0,\\
&h_i(u, \lambda) = 0, \quad i \in I_a,\\
&(f_u^0)^* p + (g_u^0)^* q + (h_u^0)^* r = 0,\\
&(f_{\lambda_i}^0)^* p + g_{\lambda_i}^0 q + (h_{\lambda_i}^0)^* r = 0, \quad i = 1, \ldots, n_\lambda\ .\\
&p^* p + q^2 + r^* r = 1,
\end{aligned}
$$

where $p \in \mathrm{R}^n$, $q \in \mathrm{R}$, and $r \in \mathrm{R}^{n_a}$.

(3) One needs two parameters (in a 'generic' system) in order to have bifurcations. Finding a bifurcation in a one parameter bifurcation diagram is 'exceptional' for such a system. For an objective functional to reach its minimum at a simple bifurcation point, while using only one control parameter, is even more exceptional. Thus we expect to encounter this situation only when there are at least two control parameters. Now $f_x \equiv (f_u\ f_{\lambda_1}\ f_{\lambda_2})$ will have full rank ($= n$) at such a bifurcation point. For example, if the bifurcation point is a simple bifurcation with respect to λ_1 then $f_{\lambda_1} \in R(f_u)$ but typically $f_{\lambda_2} \notin R(f_u)$. Similarly we can expect the full-rank condition of the theorem to hold at a cusp, at an isola formation point, and similarly at higher-order singularities, when the system is generic. Of course, many systems are not generic and exceptional points can arise.

Example. Assume that we have a solution curve containing a fold $\mathcal{F}$ to

$$f(u, \lambda, \mu) = 0, \tag{3.4}$$

for fixed control parameters λ and varying scalar parameter μ. The aim is to find $(u, \lambda, \mu) \in \mathrm{R}^n \times \mathrm{R}^{n_\lambda} \times \mathrm{R}$ so that the fold $\mathcal{F}$ is as far to the right as possible. There are several applications where such control is of interest, for example in certain ignition problems. We can consider the parameter μ as a component of the state variable. Define the objective functional as

$$g(u, \lambda, \mu) = \mu,$$

and begin by optimizing with respect to μ. Starting from a point (u_0, μ_0) on the manifold $f(u, \mu) = 0$ we continue a branch $[u(s), \mu(s)]$ and find the fold. At this point the optimality conditions (3.3) are

$$
\begin{aligned}
&f_u^* p = 0,\\
&f_\mu^* p + q = 0,\\
&p^* p + q^2 = 1
\end{aligned}
\tag{3.5}
$$

The successive continuation algorithm given below can lead to a solution that also satisfies the other optimality relations:

$$f_u^* \mathrm{p} = 0, \quad i = 1, \ldots, n_\lambda. \tag{3.6}$$

Remark. As already stated, in case some constraints $h_i(u, \lambda, \mu) \leqslant 0$ are active, we need to augment (3.4) with the corresponding equations $h_i(u, \lambda, \mu) = 0$, augment the adjoint state p with Lagrange multipliers r_i, and replace (3.5), (3.6) by

$$
\begin{aligned}
&f_u^* p + \sum_{j \in I_a} (h_j)_u^* r_j = 0,\\
&f_{\lambda_i}^* p + \sum_{j \in I_a} (h_j)_{\lambda_i}^* r_j = 0, \quad i = 1, \ldots, n_\lambda,\\
&f_\mu^* p + \sum_{j \in I_a} (h_j)_\mu^* r_j + q = 0,\\
&p^* p + q^2 + \sum_{j \in I_a} r_j^2 = 1\ .
\end{aligned}
$$

3.2. *Successive Continuation*

The necessary conditions (3.3) give rise to the system

$$
\begin{aligned}
&f(u, \lambda) = 0,\\
&g(u, \lambda) - \omega = 0,\\
&f_u^* p + g_u^* q = 0,\\
&f_{\lambda_i}^* p + g_{\lambda_i}^* q = \tau_i, \quad i = 1, \ldots, n_\lambda,\\
&p^* p + q^2 = 1,
\end{aligned}
\tag{3.7}
$$

where we have introduced new parameters $\tau_1, \ldots, \tau_{n_\lambda}$. The algorithm then consists of the following successive continuation strategy applied to (3.7):

(1) INITIALIZATION: Find a solution (u, λ) to $f(u, \lambda) = 0$ and evaluate $\omega = g(u, \lambda)$.

(2) STARTING PROCEDURE: Continue a branch of solutions to

$$f(u, \lambda) = 0, \quad g(u, \lambda) - \omega = 0,$$

with all control parameters λ_i fixed, except one, say λ_k. For notational simplicity we may take $k = 1$. Each point on the branch then consists of (λ_1, u, ω). Locate a quadratic extremum of ω. Such a point can also be thought of as a fold with respect to ω on the branch.

(3) GENERATION OF STARTING POINT: At each extremum from Step (2) we can find p and q, not both zero, and $\{\tau_i\}_{i=1}^{n_\lambda}$ with $\tau_1 = 0$, satisfying the last three equations in (3.7).

(4) MAIN ALGORITHM: Free another control parameter, say, λ_2, and compute an entire branch of solutions $(\lambda_1, \lambda_2, u, p, q, \tau_2, \ldots, \tau_{n_\lambda}, \omega)$ to (3.7). Locate zero intercepts of the remaining τ_i using, say, the secant iteration (2.9). Restart the continuation procedure at each of these zeroes, fixing the corresponding τ_i at zero and freeing one of the remaining λ_i. Continue doing this as long as further zero intercepts are found and while there are still unused control parameters left.

Remarks.

(1) Continuation of solution branches to (3.7) is done using pseudoarclength continuation with branch switching at eventual bifurcation points.

(2) If there are also inequality constraints $h_i(u, \lambda) \leqslant 0$, then monitor the values of $h_i(u, \lambda)$ along solution branches and locate zero intercepts. From these points the algorithm can be repeated with the corresponding active inequality constraint included in the state equation $f(u, \lambda) = 0$.

Efficient implementation

Rewrite the Eq. (3.7) in the successive continuation algorithm as

$$\begin{aligned} &f(x) = 0, \\ &g(x) - \omega = 0, \\ &f_x^* p + g_x^* q = 0, \\ &f_\mu^* p + g_\mu^* q - \tau = 0, \\ &p^* p + q^2 - 1 = 0, \end{aligned} \tag{3.8}$$

where $x = (u, \lambda)$, $u \in \mathrm{R}^n$, $\lambda \in \mathrm{R}^{n_\lambda}$, and $\tau \in \mathrm{R}^{n_\mu}$. Here λ denotes the control parameters with respect to which g has a local extremum, and μ denotes the remaining control parameters, for which

$$\tau_i = f_{\mu_i}^* p + g_{\mu i} q \neq 0, \quad i = 1, \ldots, n_\mu.$$

Let $F(x, \omega) \equiv \begin{pmatrix} f(x) \\ g(x) - \omega \end{pmatrix}$. Then $F_x = \begin{pmatrix} f_x \\ g_x \end{pmatrix}$ and $F_x^* = (f_x^* \quad g_x^*)$. Since $\mathrm{Rank}(f_x) = n$ and $f_x^* p + g_x^* q = 0$, it follows that $\mathrm{Rank}(F_x) = n$ also. Define $\psi \equiv \begin{pmatrix} p \\ q \end{pmatrix}$. Then (3.8) becomes

$$\begin{aligned} &F(x, \omega) = 0, \\ &F_x^* \psi = 0, \\ &\psi^* \psi - 1 = 0, \end{aligned} \tag{3.9a}$$

$$\tau = F_\mu^* \psi \ . \tag{3.9b}$$

First (3.9a) is solved for $x \in \mathrm{R}^{n+n_\lambda}$, $\psi \in \mathrm{R}^{n+1}$, and $\omega \in \mathrm{R}$. Thereafter (3.9b) is used to evaluate τ. Recall that in the successive continuation algorithm we seek zeroes of the components τ_i of τ.

The Jacobian matrix at a solution (x_0, ψ_0, ω_0) of (3.9a) is

$$\begin{pmatrix} F_x^0 & O & \gamma \\ (F_x^* \psi)_x^0 & (F_x^0)^* & 0 \\ 0^* & 2\psi_0^* & 0 \end{pmatrix},$$

where $\gamma \equiv F_\omega^0 = (0, 0, \ldots, 0, -1)^* \in \mathrm{R}^{n+1}$. The linear operator $(F_x^* \psi)_x^0$ acts upon a vector $x \in R^{n+n_\lambda}$ as follows:

$$(F_x^* \psi)_x^0 x = (F_{xx}^0 x)^* \psi_0 \ .$$

The linear systems in Newton's method applied to (3.9a) are then of the form

$$\begin{pmatrix} A & O & \gamma \\ C & A^* & 0 \\ 0^* & \psi^* & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} f \\ g \\ h \end{pmatrix} \ . \tag{3.10}$$

As noted above, the $n + 1$ by $n + n_\lambda$ matrix $A \equiv F_x^0$ has rank n. We have $N(A^*) = \mathrm{Span}\{\psi\}$. Let $N(A) = \mathrm{Span}\{\phi_i\}_{i=1}^{n_\lambda}$. The first equation in (3.10) is $Ax = f - \gamma z$. Thus we must have

$$z = \frac{\psi^* f}{\psi^* \gamma} \ .$$

The solution x to

$$Ax = f - \frac{\psi^* f}{\psi^* \gamma} \gamma$$

has the form

$$x = x_p + \sum_{i=1}^{n_\lambda} \alpha_i \phi_i .$$

A particular solution x_p is easily found, as are the null vectors $\{\phi_i\}_{i=1}^{n_\lambda}$ of A and ψ of A^* as will be shown below. The second equation of (3.10) then reads, upon left multiplication by ϕ_i^*,

$$\phi_i^* C(x_p + \sum_{j=1}^{n_\lambda} \alpha_j \phi_j) = \phi_i^* g \ ,$$

which can be rewritten as

$$\sum_{j=1}^{n_\lambda} (\phi_i^* C \phi_j) \alpha_j = \phi_i^* g - \phi_i^* C x_p, \quad i = 1, \ldots, n_\lambda \ . \tag{3.11}$$

Upon solving the linear Eqs. (3.11) for the $\{\alpha_i\}_{i=1}^{n_\lambda}$ one can evaluate $x = x_p + \sum_{i=1}^{n_\lambda} \alpha_i \phi_i$. Now find a particular solution y_p to

$$A^* y = g - Cx \quad .$$

Finally we have $y = y_p + \beta\psi$, where by the third equation in (3.10), $\psi^*(y_p + \beta\psi) = h$, from which

$$\beta = \frac{h - \psi^* y_p}{\psi^* \psi} \quad .$$

In practice we use pseudoarclength continuation which adds one more dimension to (3.10). But this inflated system can be solved efficiently as discussed earlier in Sec. 2.3.

The solution algorithm above also establishes the nonsingularity of the matrix in (3.10) provided that

(1) The matrix f_x^0 has full rank.
(2) The n_λ by n_λ matrix in (3.11) is nonsingular. We call this matrix Q. Its entries are

$$Q_{i,j} \equiv \phi_i^* C \phi_j = \phi_i^* (F_x^* \psi)_x^0 \phi_j = \phi_i^* (F_{xx}^0 \phi_j)^* \psi_0 = \psi_0^* F_{xx}^0 \phi_j \phi_i .$$

(3) The inner product $\psi^* \gamma$ is nonzero.

By the implicit function theorem we can then locally continue the solution (x, ψ, ω) of (3.9a) using any one of the μ_i as continuation parameter. (In practice we use of course pseudoarclength continuation in order to be able to compute around folds with respect to μ_i).

Condition (1) is our basic assumption. It is easily seen that condition (3) is satisfied. If not, then the last component ($= q$) of ψ must be zero and by (3.8) we then have $(f_x^* \; g_x^*)\begin{pmatrix} \tilde{\psi} \\ 0 \end{pmatrix} = 0$ where $\tilde{\psi} \in \mathrm{R}^n$ is not zero. Thus $f_x^* \tilde{\psi} = 0$, which contradicts the assumption that f_x has full rank.

Finally, Condition (2) is satisfied if the given extremum of the objective function $g(x)$ on the manifold $f(x) = 0$ at the point $x = x_0$ corresponds to a strict quadratic extremum. In fact, in this case Q is positive (or negative) definite. To see this, let $x(s)$ be any solution path to $F(x, \omega) = 0$ that passes through x_0. From differentiating $F(x(s), \omega(s)) = 0$ we have $F_x \dot{x} + F_\omega \dot{\omega} = 0$. At x_0 we have $\dot{\omega} = 0$ so that $F_x^0 \dot{x}_0 = 0$, and therefore $\dot{x}_0 = \sum_{i=0}^{n} \alpha_i \phi_i$. Taking the second derivative gives

$$F_{xx}\dot{x}\dot{x} + F_x \ddot{x} + 2F_{x\omega}\dot{x}\dot{\omega} + F_{\omega\omega}\dot{\omega}\dot{\omega} + F_\omega \ddot{\omega} = 0 \quad .$$

Evaluation at x_0, using $\dot{\omega}_0 = 0$, and multiplication on the left by ψ^* results in

$$\psi^* F_{xx}^0 \dot{x}_0 \dot{x}_0 + \psi^* F_\omega^0 \ddot{\omega}_0 = 0 \quad .$$

We already know that $\psi^* F_\omega^0 = \psi^* \gamma \neq 0$. Thus

$$\ddot{\omega}_0 = \frac{\psi^* F_{xx}^0 (\sum \alpha_i \phi_i)(\sum \alpha_i \phi_i)}{\psi^* F_\omega^0} = \frac{\alpha^* Q \alpha}{\psi^* F_\omega^0} ,$$

and for a strict quadratic extremum this must be nonzero for all nonzero choices of α.

Computation of the null vectors

The null vectors $\{\phi_i\}_{i=1}^{n_\lambda}$ of A and ψ of A^* can be computed efficiently by a generalization of a procedure given earlier. Assume that the $n + 1$ by $n + n_\lambda$ matrix A has been decomposed by Gauss elimination with row and column interchanges into $A = P\hat{L}\hat{U}Q$, where P and Q are permutation matrices. P has dimensions $n + 1$ by $n + 1$, Q is $n + n_\lambda$ by $n + n_\lambda$, and

$$\hat{L} = \begin{pmatrix} L & 0 \\ l^* & 1 \end{pmatrix} , \quad \hat{U} = \begin{pmatrix} U & R \\ 0^* & 0^* \end{pmatrix} ,$$

where L and U are n by n and R is n by n_λ. L is lower triangular with 1's along the main diagonal and U is upper triangular with nonzero entries along the main diagonal. Thus both L and U are nonsingular. Then each ϕ_i is a solution of $P\hat{L}\hat{U}Q\,\phi_i = 0$, or equivalently, since P and $\hat{L}$ are nonsingular, of

$$\begin{pmatrix} U & R \\ 0^* & 0^* \end{pmatrix} \begin{pmatrix} v_i \\ -e_i \end{pmatrix} \begin{pmatrix} 0 \\ 0 \end{pmatrix} ,$$

where $\begin{pmatrix} v_i \\ -e_i \end{pmatrix} \equiv Q\phi_i$. Choose $e_i \in \mathrm{R}^{n_\lambda}$ to be the ith unit vector. Find each v_i from backsubstitution in $Uv_i = R\,e_i =$ the ith column of R. Then $\phi_i = Q^* \begin{pmatrix} v_i \\ -e_i \end{pmatrix}$. Note that if A has already been decomposed (for computing x_p) then only one additional backsolve is needed for each ϕ_i.

We find ψ in one backsolve as in Sec. 2.1: From $A^*\psi = 0$ we have $Q^* \hat{U}^* \hat{L}^* P^* \psi = 0$, or since Q is nonsingular

$$\begin{pmatrix} U^* & 0 \\ R^* & 0 \end{pmatrix} \begin{pmatrix} L^* & l \\ 0^* & 1 \end{pmatrix} \begin{pmatrix} w \\ \nu \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} ,$$

where $\begin{pmatrix} w \\ \nu \end{pmatrix} \equiv P^*\psi$. Since U^* is nonsingular we must have

$$\begin{pmatrix} L^* & l \\ 0^* & 1 \end{pmatrix} \begin{pmatrix} w \\ \nu \end{pmatrix} = \begin{pmatrix} 0 \\ \nu \end{pmatrix} ,$$

Take $\nu = -1$. Then w is found from $L^* w = 1$. Finally $\psi = P \begin{pmatrix} w \\ -1 \end{pmatrix}$.

Particular solutions x_p and y_p to $Ax = \ldots$, and $A^*y = \ldots$ can also be computed using the decomposition above (cf. Sec. 2.1).

3.3. *The projected gradient method*

Another optimization algorithm that requires the continuation path to remain on the equilibrium manifold $f(x) = 0$ is the *projected gradient method*. In this method the direction of the branch is taken to be the direction of steepest descent. This leads to the following system of equations:

$$\begin{aligned} x &= x_0 + \alpha(g_x^0)^* + (f_x^0)^*\beta, \\ f(x) &= 0, \\ (x - x_0)^*\dot{x}_0 - \Delta s &= 0, \end{aligned}$$

which can be rewritten as

$$\begin{aligned} f(x_0 + \alpha(g_x^0)^* + (f_x^0)^*\beta) &= 0, \\ \alpha g_x^0 \dot{x}_0 + \dot{x}_0^*(f_x^0)^*\beta - \Delta s &= 0, \end{aligned} \qquad (3.12)$$

and which is to be solved for $\beta \in \mathrm{R}^n$ and $\alpha \in \mathrm{R}$. Newton's method for (3.12) is

$$\begin{pmatrix} f_x^0(f_x^0)^* & f_x^0(g_x^0)^* \\ (f_x^0\dot{x}_0)^* & g_x^0\dot{x}_0 \end{pmatrix} \begin{pmatrix} \Delta\beta \\ \Delta\alpha \end{pmatrix} = - \begin{pmatrix} f(x_0 + \alpha(g_x^0)^* + (f_x^0)^*\beta) \\ \alpha g_x^0\dot{x}_0 + \dot{x}_0^*(f_x^0)^*\beta - \Delta s \end{pmatrix} .$$

The new direction vector $\dot{x}$ is given by

$$\dot{x} = \dot{\alpha}(g_x^0)^* + (f_x^0)^*\dot{\beta} ,$$

where $\dot{\alpha}$ and $\dot{\beta}$ are obtained from

$$\begin{pmatrix} f_x^0(f_x^0)^* & f_x^0(g_x^0)^* \\ (f_x^0\dot{x}_0)^* & g_x^0\dot{x}_0 \end{pmatrix} \begin{pmatrix} \dot{\beta} \\ \dot{\alpha} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} . \qquad (3.13)$$

This takes only one extra backsubstitution at the end of the Newton iterations. The normalization used in (3.13) is $\dot{x}^*\dot{x}_0^* = 1$. Rescale $(\dot{\beta}, \dot{\alpha})$ so that $\| \dot{x} \|^2 \equiv \dot{x}^*\dot{x} = 1$.

Efficient implementation

The linear systems in Newton's method are of the form

$$\begin{pmatrix} AA^* & c \\ b^* & d \end{pmatrix} \begin{pmatrix} \hat{x} \\ \hat{z} \end{pmatrix} = \begin{pmatrix} \hat{f} \\ \hat{h} \end{pmatrix} , \qquad (3.14)$$

where

$$A = f_x^0 = (f_u^0 \quad f_{\lambda_1}^0 \quad f_{\lambda_2}^0 \quad \ldots \quad f_{\lambda_{n_\lambda}}^0).$$

We assume again that A has full rank ($= n$). As already mentioned, this poses no real restriction if the system $f(x) = 0$ is generic. Thus AA^* is nonsingular and (3.14) can be solved by the algorithm for bordered systems given earlier. The bordering algorithm requires the solution of two subsystems of the form

$$AA^*x = f .$$

This can be done efficiently as follows: First determine the decomposition

$$A = P\hat{L}\hat{U}Q ,$$

where $\hat{L}$ is n by n and lower triangular with 1's on the main diagonal, and $\hat{U} = (U \quad R)$ is n by $n + n_\lambda$ with U upper triangular and nonsingular. As before, the null vectors $\{\phi_i\}_{i=1}^{n_\lambda}$ of A and a particular solution y_p of

$$Ay = f$$

can be computed efficiently. Then $y = y_p + \sum_{i=1}^{n_\lambda} \alpha_j\phi_j$, and x is the solution to

$$A^*x = y = y_p + \sum_{i=1}^{n_\lambda} \alpha_j\phi_j . \qquad (3.15)$$

The right-hand side must be in the range of A^*. This is equivalent to requiring that

$$\sum_{i=1}^{n_\lambda} \alpha_j\phi_i^*\phi_j = -\phi_i^*y_p, \quad i = 1, \ldots, n_\lambda .$$

This system is nonsingular and can be solved for $\{\alpha_i\}_{i=1}^{n_\lambda}$. Now y can be evaluated and the overdetermined system (3.15) is uniquely solvable for x.

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References

Aronson, D. G., Chory, M. A., Hall, G. R. & McGehee, R. P. [1982] "Bifurcations from an invariant circle for two parametcr families of maps of the plane: A computer-assisted study," *Comm. Math. Phys.* **83**, 303-353.

Beyn, W.-J. [1990] "Numerical methods for dynamical systems," in *Proceedings of the SERC Summer School at Lancaster (UK)* (Oxford University Press).

Chan, T. N. [1983] M. Comp. Sci. Thesis, Concordia University, Montréal.

Dellwo, D., Keller, H. B., Matkowsky, B. J. & Reiss, E. L. [1982] "On the birth of isolas," *SIAM J. Appl. Math.* **42** (5), 956-963.

Doedel, E. J. [1981] "AUTO: A program for the automatic bifurcation analysis of autonomous systems," *Cong. Num. 30*, 265-284 (Proc. 10th Manitoba Conf. Num. Math. and Comp., Univ. Manitoba, Winnipeg, Canada).

Doedel, E. J. [1984] "The computer-aided bifurcation analysis of predator-prey models," *J. Math. Biol.* **20**, 1-14.

Doedel, E. J., Jepson, A. D. & Keller, H. B. [1984] "Numerical methods for Hopf bifurcation and continuation of periodic solution paths," in *Computing Methods in Applied Sciences and Engineering VI*, ed. Glowinski, R. & Lions, J. L. (North Holland, Amsterdam), pp. 127-136.

Doedel, E. J., Keller, H. B. & Kernévez, J. P. [1991] "Numerical analysis and control of bifurcation problems: (II) Bifurcation in infinite dimensions," *Int. J. Bifurcation and Chaos* **1** (4), (to appear).

Doedel, E. J. & Kernévez, J. P. [1986] "AUTO: Software for continuation and bifurcation problems in ordinary differential equations," *Applied Mathemaics Report*, California Institute of Technology, 226 pages.

Doedel, E. J. & Kernévez, J. P. [1987] "Optimization in bifurcation problems, Part I: Theory and illustration," *Lecture Notes in Control and Information Sciences* **102** (Springer-Verlag), pp. 181-190.

Doedel, E. J. & Kernévez, J. P. [1987] "Optimization in bifurcation problems, Part II: Numerical method and applications," *Lecture Notes in Control and Information Sciences* **102** (Springer-Verlag), pp. 191-203.

Fairgrieve, T. F. & Jepson, A. D. "O. K. Floquet multipliers," to appear in *SIAM J. Numer. Anal.*

Fier, J. M. [1985] "Fold continuation and the flow between rotating, coaxial disks," Thesis, Part I, California Institute of Technology, Pasadena CA.

Griewank, A. & Reddien, G. W. [1983] "The calculation of Hopf points by a direct method," *IMA J. Numer. Anal.* **3**, 295-303.

Griewank, A. & Reddien, G. W. [1984] "Characterization and computation of generalized turning points," *SIAM J. Numer. Anal.* **21** (1), 176-185.

Jepson, A. & Spence, A. [1985] "Folds in solutions of two parameter systems and their calculation: Part I," *SIAM J. Numer. Anal.* **22** (2), 347-368.

Keller, H. B. [1977] "Numerical solution of bifurcation and nonlinear eigenvalue problems," in *Applications of Bifurcation Theory*, ed. Rabinowitz, P. H. (Academic Press), 359-384.

Keller, H. B. [1978] "Global homotopies and Newton methods," in *Recent Advances in Numerical Analysis*, (Academic Press), pp. 73-94.

Keller, H. B. [1987] "Lectures on numerical methods in bifurcation problems," Notes by Nandakumaran, A. K. & Ramaswamy, M., Indian Institute of Science, Bangalore (Springer-Verlag).

Kernévez, J. P. [1980] *Enzyme Mathematics* (North-Holland, Amsterdam).

Kevrekidis, I. G., Aris, R., Schmidt, L. D. & Pelikan, S. [1985] "Numerical computation of invariant circles of maps," *Physica* **16D**, 243-251.

Kubíček, M. & Marek, M. [1983] *Computational Methods in Bifurcation Theory and Dissipative Structures* (Springer-Verlag).

Rheinboldt, W. C. [1982] "Computation of critical boundaries on equilibrium manifolds," *SIAM J. Numer. Anal.* **19** (3), 653-669.

Rheinboldt, W. C. [1986] "Numerical analysis of parametrized nonlinear equations," University of Arkansas Lecture Notes in the Mathematical Sciences (Wiley-Interscience).

Seoane, M. L., Doedel, E. J. & Kernévez, J. P. [1991] "A method for the localization and continuation of isola centers and bifurcation points," (submitted to *Int. J. Bifurcation and Chaos*)

Seydel, R. [1988] *From Equilibrium to Chaos. Practical Bifurcation and Stability Analysis* (Elsevier, New York).

Seydel, R. [1991] "Tutorial on continuation," *Int. J. Bifurcation and Chaos* **1** (1), 3-11.

Taylor, M. A. & Kevrekidis, I. G. [1990] "Interactive AUTO: A graphical interface for AUTO86," Technical Report, *Department of Chemical Engineering*, (Princeton University).

van Veldhuizen, M. [1987] "A new algorithm for the numerical approximation of an invariant curve," *SIAM J. Sc. Stat. Comp.* **8** (6), 951-962.