6 Calculating Branching Behavior of Boundary-Value Problems

The main topic of this chapter is the calculation of branching behavior of the one-parameter family of two-point boundary-value problems

\[ \dot{y} = f(t, y, \lambda), \quad r(y(a), y(b)) = 0. \]  

As usual, the variable \( y(t) \) consists of \( n \) scalar functions \( y_1(t), \ldots, y_n(t) \). The right-hand side \( f(t, y, \lambda) \) is a vector function; the boundary conditions [the second equation (6.1)] consist of \( n \) scalar equations,

\[
\begin{align*}
    r_1(y_1(a), \ldots, y_n(a), y_1(b), \ldots, y_n(b)) &= 0 \\
    &\vdots \\
    r_n(y_1(a), \ldots, y_n(a), y_1(b), \ldots, y_n(b)) &= 0
\end{align*}
\]

The independent variable \( t \) \( (a \leq t \leq b) \) need not be time; accordingly, the derivative with respect to \( t \) is denoted by a prime \( ' \) rather than a dot: \( \dot{y} = \frac{dy}{dt} \). The bifurcation parameter \( \lambda \) can occur in the boundary conditions:

\[ r(y(a), y(b), \lambda) = 0. \]

However, because the methods discussed in this chapter are not affected by the dependence of \( r \) on \( \lambda \), the notation \( r(y(a), y(b)) \) of equation (6.1) will be retained.

The methods for boundary-value problems resemble methods explained in the previous chapter. Following [Sey77], our approach stays in the infinite-dimensional space of ODEs and lets standard software take care of the transition to the finite-dimensional world of numerical approximation. Most of the methods discussed in this chapter are not dependent on any particular solution procedure or software. As an alternative to the methods set out in this chapter, the methods of the preceding chapter can be applied, provided equation (6.1) is discretized first. As an example of such a discretization, see the PDE model Example 5.6 (in Section 5.4.4), which was transformed into a system of algebraic equations.

In addition to ODE boundary-value problems, we shall study certain classes of PDEs, mainly to investigate stability. Solutions of equation (6.1) can be stationary states of certain classes of PDEs, the long-term temporal behavior of which is of interest.
6.1 Enlarged Boundary-Value Problems

Specific tasks (such as continuation or branch switching) can be reformulated into boundary-value problems of the general type

\[ Y'(t, Y) = F(t, Y), \quad R(Y(a), Y(b)) = 0. \] (6.2)

Typically, equation (6.2) includes equation (6.1) as a subsystem. Because solvers for two-point boundary-value problems of type (6.2) are well established, we consider that the specific task is solved whenever we succeed in

1. formulating an equation of type (6.2) that is equivalent to the specific task, and
2. constructing a reasonable initial guess to the solution.

In this section we use two examples to explain elementary ways of constructing a boundary-value problem of the general type (6.2).

The most widely applicable enlarged boundary-value problem is

\[ \begin{align*}
\left( \begin{array}{c}
y \\
\lambda
\end{array} \right)' &= \begin{pmatrix} f(t, y, \lambda) \\ 0 \end{pmatrix}, \\
\begin{pmatrix} r(y(a), y(b)) \\ y_k(a) - \eta \end{pmatrix} &= 0.
\end{align*} \] (6.3)

The system (6.3) of dimension \( n+1 \) is of type (6.2), with vector function \( Y = (y, \lambda) \). Equation (6.3) is applied in the same way the related equation (4.16) is applied for continuation of systems of equations. In particular, equation (6.3) is appropriate for passing turning points. Prescribing a suitable index \( k \) and a value of \( \eta \) enables the calculation of \( \lambda \) as a dependent variable. The “trivial” differential equation \( \lambda' = 0 \) characterizes \( \lambda \) as constant. Solving equation (6.3) automatically yields a value of \( \lambda \) that matches the underlying \( k \) and \( \eta \). Concerning the choice of \( k \) and \( \eta \), the strategy outlined in Section 4.5.3 is applied. If one of the \( n \) boundary conditions (\( r_j \), say) is of the form of an initial condition for \( y_{\nu} \)

\[ r_j = y_{\nu}(a) - \text{constant} = 0, \]

the index \( k \) must be different from \( \nu \) in order to avoid a contradiction. A strategy such as equation (4.18), evaluated for \( y(a) \), prevents \( k \) from conflicting with an initial condition. Choosing \( k = n + 1 \) in equation (6.3), the parameter \( \lambda \) becomes the control parameter.

Example 6.1 Brusselator with Diffusion

We reconsider the Brusselator model [see equation (5.53) in Section 5.6.5] now without neglecting the diffusion. Concentrating on the steady-state situation \( \dot{X} = \dot{Y} = 0 \) yields two differential equations of the second order, namely,

\[ \begin{align*}
0 &= A + X^2 Y - BX - X + D_1 \frac{\partial^2 X}{\partial x^2}, \\
0 &= BX - X^2 Y + D_2 \frac{\partial^2 Y}{\partial x^2}.
\end{align*} \] (6.4)
These ordinary differential equations describe the spatial dependence of the two chemicals $X$ and $Y$ along a reactor with length $L$, $0 \leq x \leq L$. We impose fixed boundary conditions,

\[
X = A \quad \text{for } x = 0, \ x = L, \\
Y = B/A \quad \text{for } x = 0, \ x = L.
\]

Scaling the independent variable according to $t := x/L$ and writing $\lambda := L^2$ lead to the system of four ODEs of the first order

\[
\begin{align*}
    &y_1' = y_2, \\
    &y_2' = -\lambda[A + y_1^2 y_3 - (B + 1)y_1]/D_1, \\
    &y_3' = y_4, \\
    &y_4' = -\lambda[By_1 - y_1^2 y_3]/D_2,
\end{align*}
\]

with boundary conditions

\[
y_1(0) = y_1(1) = A, \ y_3(0) = y_3(1) = B/A \quad (6.5b)
\]

(Exercise 6.1). We adopt the constants

\[
D_1 = 0.0016, \quad D_2 = 0.008, \quad A = 2, \quad B = 4.6
\]

from [KuRM78]. As equation (6.5a) shows, the independent variable $t$ in equation (6.1) need not occur explicitly in the right-hand side; the right-hand side of equation (6.5a) is of the form $f(y, \lambda)$.

Because the boundary conditions in equation (6.5b) include two initial conditions (imposed on $y_1$ and $y_3$), the index $k$ in equation (6.3) can take only the values $k = 2$ or $k = 4$. In order to extend equation (6.5) to the system of equation (6.3), define $y_5 = \lambda$ and attach the differential equation and boundary condition

\[
y_5' = 0, \quad y_k(0) = \eta. \quad (6.5c)
\]

Writing the boundary conditions in the form used in equations (6.1), (6.2), or (6.3) yields

\[
\begin{align*}
    &y_1(0) - A = 0, \\
    &y_1(1) - A = 0, \\
    &y_3(0) - B/A = 0, \\
    &y_3(1) - B/A = 0, \\
    &y_k(0) - \eta = 0.
\end{align*}
\]

(6.5d)

This concludes the formal preparations that transform the original problem, equation (6.4), into the standard forms of equation (6.1) or (6.2).

After having implemented the right-hand side of equation (6.5a) together with $y_5' = 0$ in a routine for $\mathbf{F}$, and equation (6.5d) in a routine for $\mathbf{R}$,
the next step is to call SOLVER in order to calculate solutions and trace branches. The specific Brusselator model equation (6.5) has a great number of solutions [KuRM78]; some are shown in the bifurcation diagram of Figure 6.1. One nontrivial bifurcation point is found in Figure 6.1 for $L = 0.1698$, $y_2(0) = 6.275$. The closed branches have been calculated by using the $k - \eta$ strategy in equations (4.18), (4.19), or (4.23).

The above Brusselator has served as a first example illustrating the transformation from a particular model into the two-point boundary-value problem, equation (6.1) or (6.3), in standard form. The second example represents a different class of solutions—namely, the time-dependent periodic solutions.

**Example 6.2 Forced Duffing Equation**

We reconsider the Duffing equation (2.9) introduced in Section 2.3,

$$\ddot{u} + 0.04\dot{u} - 0.2u + 8u^3/15 = 0.4 \cos \omega t .$$

The harmonic forcing term on the right-hand side provokes a response of the system (beam, electric current). We confine ourselves to harmonic oscillations $u(t)$, which have the same period $T$ as the excitation,

$$T = \frac{2\pi}{\omega} .$$

(6.6)
Hence, harmonic oscillations obey the boundary conditions
\[ u(0) = u(T), \quad \dot{u}(0) = \dot{u}(T). \]

(For subharmonic oscillations, see Section 7.7.)

Because the period \( T \) varies with \( \omega \), the integration interval \( 0 \leq t \leq T \) must be adapted whenever \( \omega \) is changed. This is inconvenient when nodes of a numerical solution procedure must also be adapted, so we transform the integration interval to unit length, thereby shifting the dependence on \( \omega \) to the right-hand side of the differential equation. The normalized time \( \tilde{t} \) satisfies
\[ T \tilde{t} = t, \quad 0 \leq \tilde{t} \leq 1. \]  

(6.7)

The transformation
\[ y_1(t) := u(t), \quad y_2(t) := \dot{u}(t) \]  

(6.8)

leads to the first-order system
\[ y'_1 = Ty_2, \]
\[ y'_2 = T(-0.04y_2 + 0.2y_1 - 8y_1^3/15 + 0.4 \cos 2\pi \tilde{t}) \]  

(6.9)

with boundary conditions
\[ y_1(0) - y_1(1) = 0, \]
\[ y_2(0) - y_2(1) = 0. \]
Redefining the normalized time by $t$ we obtain a boundary-value problem of the standard form in equation (6.1). With $y_3 := \omega$, the corresponding extended system equations (6.2) and (6.3) is

\begin{align}
    y_1' &= 2\pi y_2/y_3, \\
    y_2' &= 2\pi (-0.04y_2 + 0.2y_1 - 8y_1^3/15 + 0.4 \cos 2\pi t)/y_3, \\
    y_3' &= 0, \\
    y_1(0) - y_1(1) &= 0, \\
    y_2(0) - y_2(1) &= 0, \\
    y_k(0) - \eta &= 0.
\end{align}

(6.10)

Fig. 6.3. Example 6.2, $(u, \dot{u})$-plane for $\omega = 0.053$, symmetric oscillation

Harmonic solutions can be calculated by solving equation (6.10). With appropriate choices for $k$ and $\eta$, the bifurcation diagram in Figure 2.7 results. The branching behavior is rich for small values of $\omega$. As Figure 6.2 shows, there are many branches, turning points, and bifurcation points for values of the parameter $\omega < 0.5$. The solid curve in this branching diagram represents oscillations with phase diagrams being symmetric with respect to the origin (Figure 6.3). For decreasing $\omega$, each loop of this “main” branch attaches a further wiggle to the oscillation. The wiggles indicate that the small-amplitude oscillation around any of the stable equilibria (Section 2.3) takes much time to collect enough energy before a transition to the other attracting basin is possible; compare the phase diagram in Figure 6.3 and
the time dependence in Figure 6.4 ($\omega = 0.053$). At first glance, the many wiggles might give the impression that such solutions are not harmonic; but they do have period $T$.

Each of the closed branches in Figure 6.2 (dashed and dotted curves) is attached to the main branch via two pitchfork bifurcations. Accordingly, the phase diagrams of these “secondary” branches are asymmetric with respect to the origin; Figure 6.5 shows one such phase plot. The closed branch drawn in a dashed line (Figure 6.2) appears to have sharp corners, and one might expect difficulties in tracing this particular branch. The plotted behavior refers only to the dependence $y_1(0)$ versus $\lambda$; the corresponding graph of $y_2(0)$ behaves more smoothly (see Figure 6.6). Accordingly, a local parameterization does not encounter difficulties in finding an appropriate index $k$. The closed branch depicted in Figure 6.6 illustrates how difficult it is to decide when the tracing of the branch is completed. As outlined in Section 4.9, it is not easy to implement a criterion that recognizes safely that a part of a branch is already known. Note that all of the Figures 6.2 through 6.6 depict harmonic solutions.

For periodic oscillations it is interesting to know the amplitude. The amplitude can often be measured sufficiently accurately from related plots (as in Figures 6.3, 6.4, and 6.5). If more accuracy is required, one must resort to numerical approximations. The amplitude of an oscillation can be calculated with high accuracy as part of the solution procedure [BeS80]. As an alternative, the amplitude can be approximated after the solution is cal-
Fig. 6.5. Example 6.2, \((u, \dot{u})\)-plane for \(\omega = 0.12861\), asymmetric oscillation

culated. To this end, a spline that approximates the current solution can be constructed. Evaluating the zeros of the derivative of the spline yields the values of the amplitude (Exercise 6.3). A table of 20 bifurcation points of the above Duffing equation with accurate values of the amplitude can be found in [BeS80]. The above Duffing equation also exhibits subharmonic oscillations; then the period of the system is an integral multiple of the period of the external frequency. The period-adding behavior has been investigated in [EnL91]. Note that periodic oscillations can also be calculated by methods other than applying shooting. For example, Fourier expansion methods have shown good results. For an application to bifurcation, see [Del92].

## 6.2 Calculation of Bifurcation Points

The calculation of bifurcation points in boundary-value problems follows along the lines outlined in the previous chapter. We establish a general direct method and deduce a bifurcation test function on the ODE level.

The linearization of equation (6.1) with respect to \(y\) is the boundary-value problem

\[
\begin{align*}
\mathbf{h}' &= f_y(t, y, \lambda)\mathbf{h}, \\
A\mathbf{h}(a) + B\mathbf{h}(b) &= 0.
\end{align*}
\]  \hfill (6.11)

The vector-valued function \(\mathbf{h}(t)\) corresponds to the \(\mathbf{h}\) of Chapter 5. \(A\) and \(B\) are the \(n^2\) matrices of the linearization of the boundary conditions,
6.2 Calculation of Bifurcation Points

Fig. 6.6. Example 6.2: Closed branch $u$ versus $\omega$ (top), $\dot{u}$ versus $\omega$ (bottom)

\[ A := \frac{\partial r(y(a), y(b))}{\partial y(a)}, \quad B := \frac{\partial r(y(a), y(b))}{\partial y(b)}. \]  \hspace{1cm} (6.12)

Note that $A$ and $B$ in general vary with $y$. But, since $A$ and $B$ are frequently constant matrices, we suppress the dependence on $y$ for the sake of convenience. Evaluated at a bifurcation point $(y_0, \lambda_0)$, the linearized problem in equation (6.11) has a nontrivial solution $h \neq 0$. For $(y, \lambda) \neq (y_0, \lambda_0)$, the only solution to equation (6.11) is $h = 0$. Along the lines set out in the previous chapter, we impose the equation
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\[ h_k(a) = 1 \]

on equation (6.11); this initial condition enforces \( h \neq 0 \). Hence, a bifurcation point is characterized by

\[ \zeta(y, \lambda) := h_k(a) - 1 = 0 \]

for a solution \( h \) to equation (6.11), which depends on \( (y, \lambda) \). This characteristic feature formally replaces the \((n+1)\)st boundary condition of equation (6.3). In this way the value \( \lambda_0 \) of a branch point is fixed as a solution of

\[
\begin{pmatrix}
  y' \\
  \lambda'
\end{pmatrix} = \begin{pmatrix}
  f(t, y, \lambda) \\
  0
\end{pmatrix}, \quad \begin{pmatrix}
  r(y(a), y(b)) \\
  \zeta(y, \lambda)
\end{pmatrix} = 0.
\]

(6.13)

One way of implementing this equation is to attach the linearization equation (6.11), which is implicitly included in \( \zeta = 0 \). This leads to the branching system of ODEs \([\text{Sey77}], [\text{Sey79a}]\),

\[
\begin{pmatrix}
  y' \\
  \lambda'
\end{pmatrix} = \begin{pmatrix}
  f(t, y, \lambda) \\
  0
\end{pmatrix}, \quad \begin{pmatrix}
  r(y(a), y(b)) \\
  \zeta(y, \lambda)
\end{pmatrix} = 0.
\]

(6.14)

The boundary-value problem (6.14) is of the standard form in equation (6.2) and thus is amenable to SOLVER. Because the branching system involves \( 2n + 1 \) components, storage requirements grow rapidly with \( n \). This usually restricts equation (6.14) to small or moderate values of \( n \). The index \( k \) is the same as the \( k \) of the previous section and the previous chapter. In particular, indices that refer to an initial condition in the boundary conditions of equation (6.1) are not feasible (Exercise 6.5). Other implementations of equation (6.13) lead to an indirect method (to be described next) or to a semidirect method (Exercise 6.7). The branching system of equation (6.14) applies to both simple bifurcation and turning points; it also applies to Hopf bifurcation and other bifurcation points. Because equation (6.14) includes equation (5.21) as a special case, we can regard equation (6.14) as a most general extended system devoted to the calculation of bifurcation points. Before we discuss such topics as the calculation of an initial guess, we study an example.

**Example 6.3 Catalytic Reaction**

Heat and mass transfer within a porous catalyst particle can be described by the boundary-value problem

\[
\frac{d^2 y}{dx^2} + \frac{a}{x} \frac{dy}{dx} = \vartheta^2 y^m \exp \left[ \frac{\gamma \beta (1 - y)}{1 + \beta (1 - y)} \right].
\]

(6.15)

The meaning of the variables (see [HLMK68]) is

- \( y \): dimensionless concentration;
- \( x \): dimensionless coordinate;
6.2 Calculation of Bifurcation Points

\( a \): coefficient defining shape of particle (\( a = 0 \): flat plate; \( a = 1 \): cylindrical; \( a = 2 \): spherical);

\( \vartheta \): Thiele modulus;

\( \gamma \): dimensionless energy of activation; and

\( \beta \): dimensionless parameter of heat evolution.

The boundary conditions are
\[
\frac{dy(0)}{dx} = 0, \quad y(1) = 1.
\]

We choose the simple case of a flat particle (\( a = 0 \)) with first-order reaction (\( m = 1 \)) and take as a bifurcation parameter the modified Thiele modulus \( \lambda := \vartheta^2 \).

The resulting first-order system is
\[
y_1' = y_2, \\
y_2' = \lambda y_1 e(y_1), \\
y_1(1) = 1, \quad y_2(0) = 0.
\] (6.16)

Here \( e(y) \) serves as an abbreviation of the exponential term,
\[
e(y_1) = \exp \left[ \frac{\gamma \beta (1 - y_1) / (1 + \beta (1 - y_1))}{1} \right].
\]

The Jacobian matrix \( f_y \) associated with equation (6.16) is
\[
f_y(t, y, \lambda) = \begin{pmatrix} 0 & \frac{de}{dy_1} y_1 & 1 \\ \lambda \left[ e(y_1) + \frac{de}{dy_1} y_1 \right] & 0 & 0 \end{pmatrix}.
\]

We write \( y_3 = \lambda, \ y_4 = h_1, \ y_5 = h_2 \) and obtain for the linearized system
\[
h_1' = y_4' = h_2 = y_5, \\
h_2' = y_5' = y_3 y_4 \left[ e(y_1) + \frac{de}{dy_1} y_1 \right].
\]

Because the boundary conditions are linear (Exercise 6.6), the boundary conditions of the linearization can be written down immediately as
\[
h_1(1) = 0, \quad h_2(0) = 0.
\]

Collecting all parts, one obtains the branching system
\[
y_1' = y_2, \\
y_2' = y_1 y_3 e(y_1), \\
y_3' = 0, \\
y_4' = y_5, \\
y_5' = y_3 y_4 e(y_1)[1 - y_1 \gamma \beta (1 + \beta (1 - y_1))^{-2}], \\
y_1(1) = 1, \quad y_2(0) = 0, \\
y_4(1) = 0, \quad y_5(0) = 0, \quad y_4(0) = 1 \quad (k = 1).
\] (6.17)
For $\gamma = 20$, $\beta = 0.4$, and positive values of $\lambda$, there is a branch that exhibits hysteresis behavior; see the bifurcation diagram in Figure 6.7. During the course of the continuation, the two turning points have been calculated by solving the branching system (6.17). The resulting values are

$$\lambda_0 = 0.07793, \quad y_0(0) = 0.2273,$$

$$\lambda_0 = 0.13756, \quad y_0(0) = 0.7928.$$ 

For values of $\lambda$ between these two critical values, there are three different concentrations (see Figure 6.8). Only the upper and lower profiles are stable.

Section 5.9 showed how the hysteresis behavior varies with $\gamma$ (see Figures 5.21 and 5.22). The critical boundaries of Figure 5.21 are obtained by continuation of the branching system of equation (6.17) with respect to $\gamma$ or by indirect methods (see Section 5.9). For completeness we remark that for $\lambda < 0$ another branch can be found. These solutions are not physical because concentrations become negative or larger than one. From a mathematical point of view, however, the new branch is interesting because it branches off to infinity for $\lambda \to 0$.

Next we discuss how to calculate initial approximations, and how to define bifurcation test functions. Consider the situation that $(\bar{y}, \bar{\lambda})$ is a solution to equation (6.1), calculated not far from a bifurcation point $(y_0, \lambda_0)$. The linearized boundary-value problem equation (6.11) has only the trivial solution if evaluated about $(\bar{y}, \bar{\lambda}) \neq (y_0, \lambda_0)$. As in the methods described in Section
5.4.1, the $l$th boundary condition (for an index $l$, $1 \leq l \leq n$) is removed to obtain a solvable system,

$$
\begin{align*}
\mathbf{h}' &= \mathbf{f}_{\mathbf{y}}(t, \bar{\mathbf{y}}, \bar{\mathbf{\lambda}})\mathbf{h}, \\
(I - e_l e_l^\top)(A\mathbf{h}(a) + B\mathbf{h}(b)) &= 0, \quad h_k(a) = 1.
\end{align*}
$$

(6.18)

We denote the solution to equation (6.18) by $\bar{\mathbf{h}}$. This vector function serves as the concluding part of the initial approximation $(\bar{\mathbf{y}}, \bar{\mathbf{\lambda}}, \bar{\mathbf{h}})$ of the solution $(\mathbf{y}_0, \lambda_0, \mathbf{h}_0)$ to the branching system of equation (6.14). One way of calculating $\bar{\mathbf{h}}$ is to solve the boundary-value problem

$$
\begin{align*}
\begin{pmatrix}
\mathbf{y} \\
\lambda \\
\mathbf{h}
\end{pmatrix}' &= \begin{pmatrix}
\mathbf{f}(t, \mathbf{y}, \lambda) \\
0 \\
\mathbf{f}_{\mathbf{y}}(t, \mathbf{y}, \lambda)\mathbf{h}
\end{pmatrix}, \\
\begin{pmatrix}
\mathbf{y}(a) - \bar{\mathbf{y}}(a) \\
\lambda - \bar{\lambda} \\
h_k(a) - 1
\end{pmatrix} &= 0, \\
(I - e_l e_l^\top)(A\mathbf{h}(a) + B\mathbf{h}(b)) &= 0,
\end{align*}
$$

(6.19)

which differs from equation (6.14) only in the boundary conditions. Solving equation (6.19) is not problematic because it is a linear problem; the nonlinear part is not effective because its solution $\bar{\mathbf{y}}$ is already calculated. In the following section, we see how $\bar{\mathbf{h}}$ can be approximated more efficiently.

By construction, the value of the removed boundary condition is a bifurcation test function $\tau$,

$$
\tau := e_l^\top(A\mathbf{h}(a) + B\mathbf{h}(b)).
$$

(6.20)
One possibility for calculating $\tau$ is to use $h(a), h(b)$ from equation (6.19); a more economical way to calculate $\tau$ is presented in the next section. As in Chapter 5, the test function depends on the choice of the indices $l$ and $k$. As in the method in Exercise 5.12, the branching system of equation (6.14) can be embedded in a set of boundary-value problems parameterized by $\tau$ from equation (6.20).

On the accuracy that can be obtained efficiently by using equation (6.14), see Section 5.4.1. The same observations are valid in the ODE situation. The singularity in the case of bifurcation points can be overcome by following a proposal in [Moo80] (see Section 5.7.2). Alternatively, underlying symmetries can be exploited to remove the singularity.

As indicated earlier, the entire Chapter 5 can be seen as a special case of Chapter 6; just consider all $y_i$ as constant and identify $r$ with the $f$ of Chapter 5. Numerical algorithms for the bifurcation analysis of the more difficult infinite case of the ODE boundary-value problems of this chapter have been treated much less frequently than those for the finite-dimensional situation of Chapter 5. It is interesting to note that several of the basic ideas of algorithms and methods were first proposed for ODE boundary-value problems. This was done in the widely distributed report of 1977 [Sey77], which was the author’s dissertation. In this work, the branching system of equation (6.14) was introduced, as well as the test function equation (6.20), the vector $\vec{h}$, and the step control equation (4.23). In the same year (1977) the influential paper of Keller [Kel77] was published, and the dissertation of Abbott [Abb77] was completed. These two papers considered the finite-dimensional case. Several years of generalizations, specializations, and applications followed, and many further methods have been proposed. Today, the numerical treatment of bifurcations, and continuation methods can be considered as being on a sophisticated level.

### 6.3 Stepping Down for an Implementation

Although from a theoretical point of view $h$ and $\tau$ can be satisfactorily defined and calculated via ODE boundary-value problems, this approach is not practical. Notice that equation (6.19) represents a boundary-value problem of the double size. In order to construct an efficient implementation, we temporarily step down from the ODE level to a finite-dimensional approximation. The vector function $h(t)$ can be approximated for discrete values of $t_j$, which will suffice for both branch switching and calculating $\tau$.

Information required for evaluating $h$ and $\tau$ is hidden in the data calculated during the approximation of a solution $y$ to equation (6.1) or (6.3). It is possible to reveal this information, thereby benefiting from data that are available without extra cost. Different methods incorporated in SOLVER produce data in different ways. Accordingly, the analysis of revealing $h$ and $\tau$ depends on the type of method applied to solve equation (6.1) or (6.3). To discuss an example, let us assume that SOLVER is based on multiple shoo-
Assume that $y$ was calculated by multiple shooting. In a shooting implementation in condensed form, an $n^2$ iteration matrix, which is the core of the internal Newton iteration, is established [StB80]. This iteration matrix is

$$
E := A + BG_{m-1} \cdot \ldots \cdot G_1.
$$

(6.21)

The matrices $A$ and $B$ are those of the linearized boundary conditions equation (6.12). The matrices $G_j$ are defined as

$$
G_j = G(t_{j+1}),
$$

(6.22)

where $G(t)$ solves the matrix initial-value problem

$$
G' = f_y(t, y, \lambda)G, \quad G(t_j) = I.
$$

Here $a = t_1 < t_2 < \ldots < t_m = b$ are the nodes of multiple shooting ($m = 2$ for simple shooting). When SOLVER terminates, the internal iteration matrix $E$ and the matrices $G_j$ can be made available without extra cost. As in the method in Section 5.4.1, we replace the $l$th row of $E$ by the $k$th unit vector to obtain the matrix $E_{lk}$. This can be formally written as

$$
E_{lk} := (I - e_l e^*_k)E + e_l e^*_k;
$$

(6.23)

compare equation (5.23). The matrix $E_{lk}$ depends on the solution $(y, \lambda)$ or $(\bar{y}, \bar{\lambda})$, at which $E$ was evaluated. If the indices $l$ and $k$ are chosen in a way such that $E_{lk}$ is nonsingular (not problematic), then equation (6.18) has a unique solution $h(t)$. The initial vector $h(a)$ is the solution of the linear equation

$$
E_{lk} h(a) = e_l.
$$

(6.24)

Test functions $\tau = \tau_{lk}$ are given by the scalar product of $h(a)$ with the $l$th row of $E$,

$$
\tau_{lk} = e^*_l E h(a).
$$

(6.25)

Because SOLVER outputs $y$ at the discrete shooting nodes, $y(t_j)$, it is sufficient to calculate $h$ at the same points $t_j$. This is furnished by

$$
h(t_j) = G_{j-1} h(t_{j-1}) \quad \text{for } j = 2, \ldots, m.
$$

(6.26)

Summarizing, the bifurcation test function $\tau$ can be calculated by solving one linear system, equation (6.24), and evaluating one scalar product, equation (6.25). This amount of work compares favorably to solving boundary-value problem equation (6.19). Because the matrices $A$, $B$, and $G_j$ are approximated by numerical differentiation, the iteration matrix $E$ is subjected to discretization errors. This affects the accuracy of $h$ and $\tau$. The remarks in Section 5.1 are valid here too—that is, the accuracy of $\tau$ depends on the strategy of rank-one approximations in SOLVER and on the history of previous continuation steps. Further simplifications are possible that exploit decompositions of $E$. 
6.4 Branch Switching and Symmetry

We end the excursion to a finite-dimensional approximation and come back to the ODE level. Concerning branch switching, approaches similar to those described earlier are valid. We confine ourselves to a brief list of suitable boundary-value problems; for motivations and illustrating figures, see Section 5.6.

Predictors \( \tilde{z} \) can be based on interpolation,

\[
\tilde{z}(t) := \tilde{y}_0(t) \pm |\delta| \tilde{h}_0(t).
\]  

(6.27)

Here \( \tilde{y}_0(t) \) and \( \tilde{h}_0(t) \) are linear interpolations based on the values of \( y \) and \( h \) obtained at two solutions not far from a bifurcation point. Equation (5.46) holds true for boundary-value problems; in equation (5.46b) the Jacobian \( f_y \) is replaced by the matrix \( E \). The distance \( \delta \) is given by equation (5.45); in this formula, \( y_k \) is evaluated at \( t = a \). If \( h \) is approximated as described in the previous section, the predictor \( \tilde{z} \) is given only at the discrete nodes \( t_j \). This is no disadvantage because SOLVER does not require more.

The boundary-value problem that establishes a parallel computation of two distinct solutions is written in standard form, equation (6.2), with \( Y = (y, \lambda, z) \),

\[
Y' = F(t, Y) = \begin{pmatrix} f(t, y, \lambda) \\ 0 \\ f(t, z, \lambda) \end{pmatrix},
\]

\[
R(Y(a), Y(b), \delta) = \begin{pmatrix} r(y(a), y(b)) \\ z_k(a) - y_k(a) - \delta \\ r(z(a), z(b)) \end{pmatrix} = 0.
\]  

(6.28)

The initial approximation is \( (\tilde{y}_0, \tilde{\lambda}_0, \tilde{z}) \). We shall prefer equations of the simple dimension \( n + 1 \) to the dimension \( 2n + 1 \) of equation (6.28). As mentioned in Chapter 5, the method of parallel computation is most attractive when an analytic expression for \( y \) is known and inserted. Another possibility to obtain a “small" system is given by equation (6.3), initial approximation and \( \eta \) are

\[
(y, \lambda) = (z, \tilde{\lambda}_0), \quad \eta = \tilde{z}_k(a).
\]  

(6.29)

Better selective properties are obtained by exploiting symmetry breaking. To classify and investigate symmetries in the solution, consider a reflection \( \tilde{y}_i(t) \) of \( y_i(t) \). For example,

\[
\tilde{y}_i(t) := y_i(a + b - t)
\]

defines the reflection with respect to the line \( t = \frac{1}{2}(a + b) \). We define the component \( y_i \) to be symmetric if

\[
\tilde{y}_i(t) = y_i(t)
\]
holds for all \( t \) in the interval \( a \leq t \leq b \). The type of symmetry depends on the reflection and can be different in the components of the vector \( \mathbf{y} \). We shall say that a boundary-value problem supports symmetry if it is solved by \( \tilde{\mathbf{y}} \) whenever it is solved by \( \mathbf{y} \).

In particular, two kinds of symmetries occur frequently in bifurcation problems: even functions (6.30a) and odd functions (6.30b):

\[
y_i(t) = \tilde{y}_i(t) \quad \text{for} \quad \tilde{y}_i(t) := y_i(a + b - t) , \tag{6.30a}
\]

\[
y_i(t) = \bar{y}_i(t) \quad \text{for} \quad \bar{y}_i(t) := -y_i(a + b - t) . \tag{6.30b}
\]

In equation (6.30b) the reflection is with respect to the point \((y, t) = (0, \frac{1}{2}(a + b))\). Note that a component \( y_i \) can be odd while another component of the same solution is even. Two other types of symmetry are characteristic for bifurcations of periodic solutions with period \( b - a \):

\[
y_i(t) = \bar{y}_i(t) \quad \text{for} \quad \bar{y}_i(t) := -y_i\left(t + \frac{b-a}{2}\right) , \tag{6.30c}
\]

\[
y_i(t) = \tilde{y}_i(t) \quad \text{for} \quad \tilde{y}_i(t) := y_i\left(t + \frac{b-a}{2}\right) . \tag{6.30d}
\]

A periodic solution of type (6.30d) actually has a period \( \frac{1}{2}(b - a) \).

For a practical evaluation of symmetry, we first check a current solution to see whether its components are symmetric. Because it is not practical to check the above criteria for all \( t \) in the interval \( a \leq t \leq b \), we confine ourselves to \( t = a \). This establishes necessary criteria for the onset of symmetries. For a small error tolerance \( \epsilon_1 \) (not smaller than the error tolerance of SOLVER) we check the criteria

\[
|y_i(b) - y_i(a)| < \epsilon_1 , \tag{6.31a}
\]

\[
|y_i(b) + y_i(a)| < \epsilon_1 , \tag{6.31b}
\]

\[
|y_i(a) + y_i\left(\frac{a+b}{2}\right)| < \epsilon_1 , \tag{6.31c}
\]

\[
|y_i(a) - y_i\left(\frac{a+b}{2}\right)| < \epsilon_1 . \tag{6.31d}
\]

If for one index \( i \) (say \( k \)) one of the inequalities holds, we assume a symmetry of the corresponding type in (6.30). The next question is whether this symmetry is broken in the component \( z_k \) of the emanating solution. Because the emanating solution \( \mathbf{z} \) is yet unknown, we resort to the predictor \( \tilde{\mathbf{z}} \) from equation (6.27). For a symmetric \( \mathbf{z} \), the following value of \( \gamma \) is zero:

\[
\gamma := \tilde{z}_k(b) - \tilde{z}_k(a) \quad \text{in case (6.31a)} ,
\]

\[
\gamma := \tilde{z}_k(b) + \tilde{z}_k(a) \quad \text{in case (6.31b)} , \tag{6.32}
\]

\[
\gamma := \tilde{z}_k(a) + \tilde{z}_k\left(\frac{a+b}{2}\right) \quad \text{in case (6.31c)} ,
\]

\[
\gamma := \tilde{z}_k(a) - \tilde{z}_k\left(\frac{a+b}{2}\right) \quad \text{in case (6.31d)} .
\]

Hence, asymmetry of \( \mathbf{z} \) manifests itself by

\[
|\gamma| > \epsilon_2 ; \tag{6.33}
\]
here we choose an error tolerance $\epsilon_2$ slightly larger than $\epsilon_1$. Numerical experience indicates that the test criteria (6.31) through (6.33) reliably detect a symmetry breaking. This success is to be expected, because $\bar{z}$ is close to an emanating solution in case of pitchfork bifurcations—that is, in particular the $\mathbb{Z}_2$ symmetry breaking can be detected in advance during branch tracing. This requires monitoring both $\tau$ and $h$. The above test for symmetry breaking is easily automated. Note that the test is based on solutions instead of on equations.

Assume now that for $i = k$ one of the criteria in equation (6.31) holds and that equation (6.33) is satisfied. For each kind of symmetry breaking there is a corresponding boundary-value problem with an appropriate selective boundary condition:

$$
\left( \begin{array}{c}
y \\
\lambda
\end{array} \right)' = \left( \begin{array}{c}
f(t, y, \lambda) \\
0
\end{array} \right), \quad \left( \begin{array}{c}
r(y(a), y(b)) \\
r_{n+1}
\end{array} \right) = 0
$$

(6.34)

with $\gamma \neq 0$ from equation (6.32) and the boundary condition

$$
r_{n+1} := y_k(b) - y_k(a) - \gamma \quad \text{in case (6.31a)},
$$

$$
r_{n+1} := y_k(b) + y_k(a) - \gamma \quad \text{in case (6.31b)},
$$

$$
r_{n+1} := y_k(a) + y_k(\frac{a+b}{2}) - \gamma \quad \text{in case (6.31c)},
$$

$$
r_{n+1} := y_k(a) - y_k(\frac{a+b}{2}) - \gamma \quad \text{in case (6.31d)}.
$$

The initial approximation is $(\bar{z}, \bar{\lambda}_0)$. In cases (6.31c) and (6.31d) the boundary-value problem is a three-point boundary-value problem; a transformation to a two-point boundary-value problem is possible [Sey83a]. Case (6.30d) refers to period doubling; this can be seen by setting $T = \frac{1}{2}(b - a)$. The corresponding bifurcation means there is a transition from period $T$ to period $2T$. This kind of bifurcation will be discussed in Chapter 7.

The above numerical test for symmetry breaking dispenses with an analytical investigation of equation (6.1), which can be cumbersome (Exercise 6.10). There is no guarantee that the criteria in equation (6.31) detect all the relevant regularities. For example, equation (6.31b) fails if equation (6.30b) is generalized to

$$
y_i(a + b - t) + \vartheta = \vartheta - y_i(t)
$$

for a nonzero value of $\vartheta$. Fortunately, if such a $y_i$ is solution of a second-order differential equation, the derivative or antiderivative is even and equation (6.31a) works.

Example 6.4 Superconductivity Within a Slab

In [Odeh67] a model of a superconducting slab in a parallel magnetic field is discussed. The Ginzburg–Landau equations are equivalent to the boundary-value problem of two second-order ODEs

$$
\Theta'' = \Theta(\Theta^2 - 1 + \lambda \Psi^2) \kappa^2,
$$

$$
\Psi'' = \Theta^2 \Psi
$$

(6.35)
Fig. 6.9. Example 6.4; antisymmetric solutions for $\lambda = 0.6647$. $\Theta(t)$ and $\Theta'(t)$ (top), $\Psi(t)$ and $\Psi'(t)$ (bottom)

for $0 \leq t \leq d$, $\Theta'(0) = \Theta'(d) = 0$, $\Psi'(0) = \Psi'(d) = 1$.

The meaning of the variables is

- $\Theta$: an order parameter that characterizes different superconducting states;
- $\Psi$: potential of the magnetic field;
- $\lambda$: square of external field;
- $d$: thickness of the slab ($d = 5$); and
- $\kappa$: Ginzburg–Landau parameter ($\kappa = 1$).
Investigation of the above boundary-value problem reveals that it supports symmetry. To see this, define the “antisymmetric” counterparts\[\tilde{\Theta}(t) := \Theta(d - t), \quad \tilde{\Psi}(t) := -\Psi(d - t)\]
and realize that the signs are the same after differentiating twice with respect to \(t\). Hence, \(\tilde{\Theta}\) and \(\tilde{\Psi}\) satisfy the differential equations (6.35) if \(\Theta\) and \(\Psi\) do. Analyzing the boundary conditions, as, for example,
\[\tilde{\Theta}'(0) = -\Theta'(d) = 0,\]
shows that \(\tilde{\Theta}\) and \(\tilde{\Psi}\) satisfy the boundary conditions. Hence, equation (6.35) supports even \(\Theta\) and odd \(\Psi\). This does not imply that solutions must be even or odd. In fact, equation (6.35) has asymmetric solutions. See the solution in Figure 6.9, which depicts both the solutions \(\Theta, \Psi\) and \(\tilde{\Theta}, \tilde{\Psi}\) for the parameter value \(\lambda = 0.6647\).

![Figure 6.10](image)

**Fig. 6.10.** Example 6.4, bifurcation diagram, \(y_3(0)\) versus \(\lambda\)

In order to calculate solutions, we rewrite the boundary-value problem as a first-order system. Denoting \(y_1 = \Theta, \ y_2 = \Theta', \ y_3 = \Psi, \) and \(y_4 = \Psi'\) yields
\[
\begin{align*}
  y'_1 &= y_2, \\
  y'_2 &= y_1(y_1^2 - 1 + \lambda y_3^2), \\
  y'_3 &= y_4, \\
  y'_4 &= y_1^2 y_3, \\
  y_2(0) &= y_2(5) = 0, \quad y_4(0) = y_4(5) = 1.
\end{align*}
\]
Solutions are summarized in the bifurcation diagram in Figure 6.10. A branch of asymmetric solutions branches off a branch of symmetric solutions at a pitchfork bifurcation point. The data of the pitchfork point and four turning points (TP) are listed in Table 6.1. The values in that table have been calculated by solving the branching system. The solution profiles of the bifurcation point are shown in Figure 6.11; notice the symmetries. This bifurcation point is straddled between the two turning points with asymmetric solutions, which are depicted in Figure 6.9. Compare Figures 6.9 and 6.11 to see how this straddling becomes evident in the solution profiles.

<table>
<thead>
<tr>
<th>$\lambda_0$</th>
<th>$\Theta_0(0)$</th>
<th>$\Psi_0(0)$</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.66294</td>
<td>0.08996</td>
<td>−2.687</td>
<td>TP, asymmetric sol.</td>
</tr>
<tr>
<td>0.66294</td>
<td>0.8461</td>
<td>−1.016</td>
<td>TP, asymmetric sol.</td>
</tr>
<tr>
<td>0.91196</td>
<td>0.5853</td>
<td>−1.407</td>
<td>Pitchfork bif. point</td>
</tr>
<tr>
<td>0.92070</td>
<td>0.5214</td>
<td>−1.496</td>
<td>TP, symmetric sol.</td>
</tr>
<tr>
<td>0.84769</td>
<td>0.1923</td>
<td>−2.095</td>
<td>TP, symmetric sol.</td>
</tr>
</tbody>
</table>

The boundary-value problem equation (6.34) is designed to calculate asymmetric solutions. For the sake of completeness, we mention that boundary-value problems can be reformulated in a way that admits only symmetric solutions. We illustrate this possibility by means of the above example. Symmetric solutions to equation (6.35) satisfy

$$\Theta'(\frac{d}{2}) = 0, \quad \Psi'(\frac{d}{2}) = 0$$

(see Figure 6.11). This allows one to reduce the integration interval from $0 \leq t \leq d$ to $0 \leq t \leq \frac{d}{2}$, or, generally, $a \leq t \leq \frac{a + b}{2}$.

Replacing the previous boundary conditions at $t = d$ by the midpoint conditions leads to the new boundary conditions

$$\Theta'(0) = 0, \quad \Psi'(0) = 1, \quad \Theta'(\frac{d}{2}) = 0, \quad \Psi'(\frac{d}{2}) = 0.$$

Solving a corresponding boundary-value problem yields the symmetric solutions supported by this example. Note that for this modified boundary-value problem the symmetry-breaking bifurcation does not exist.

Let us discuss the matter in more general terms. The “space” of symmetric functions is a (small) subspace of the space of all functions. The smaller space reflects certain assumptions that are imposed on the underlying model (here it is the assumption of symmetry). Relaxing a restricting assumption
means enlarging the space of admissible functions. As a result, the bifurcation behavior may become richer. Another example of this phenomenon will be presented in Example 7.6 in Section 7.4.1.
6.5 Trivial Bifurcation

Before modern computers and powerful numerical methods became generally available, a substantial part of the bifurcation research concentrated on problems where one basic solution $y^B$ is known analytically for all $\lambda$. This drastic restriction is theoretically equivalent to the assumption

$$f(t, 0, \lambda) = 0, \ r(0, 0) = 0. \quad (6.37)$$

This can be seen by applying the transformation

$$y^* = y - y^B$$

to the original problem (Exercise 6.10). We refer to bifurcations from the trivial solution $y = 0$ as trivial bifurcations or primary bifurcations.

In principle, all the methods described so far apply to trivial bifurcation; some of the relevant methods simplify significantly. The branching system equation (6.14) reduces to

$$\begin{pmatrix} h \\ \lambda \end{pmatrix}' = \begin{pmatrix} f_y(t, 0, \lambda) & h \\ 0 & 0 \end{pmatrix} \begin{pmatrix} Ah(a) + Bh(b) \\ h_k(a) - 1 \end{pmatrix} = 0. \quad (6.38)$$

In contrast to equation (6.14), this boundary-value problem of the simple dimension must be considered an efficient tool for calculating bifurcation points, at least as far as storage requirements are concerned. The Jacobian $f_y$, however, is still required analytically. Indirect methods simplify drastically in the case of trivial bifurcations [Sey81b]; they are a recommended alternative to solving equation (6.38). Note that the techniques reported here and in Section 6.2 are readily applied to linear eigenvalue problems—namely, to the calculation of eigenvalues and eigenvectors.

The assumption in equation (6.37) often enables a simple analytical evaluation of bifurcation points. Although we generally put emphasis on numerical methods, let us take a break and carry out such a hand calculation.

Example 6.5

Consider the simple second-order boundary-value problem

$$-u'' + u^3 = \lambda u, \quad u(0) = u(\pi) = 0. \quad (6.39)$$

Clearly, equation (6.37) is satisfied. For the left-hand operator $F(u) := -u'' + u^3$ the linearization is obtained from

$$F(u + v) - F(u) = -v'' + 3u^2v + v^2(3u + v).$$

The linear part is $-v'' + 3u^2v$. Hence, the linearization around $u = 0$ is the eigenvalue problem

$$-v'' = \lambda v, \quad v(0) = v(\pi) = 0.$$
Because both $\cos(\sqrt{\lambda}t)$ and $\sin(\sqrt{\lambda}t)$ solve the linearized differential equation, and the general solution of the equation must be of the form

$$v(t) = c_1 \cos \sqrt{\lambda}t + c_2 \sin \sqrt{\lambda}t.$$

The constants and eigenvalues are determined by the boundary conditions. We obtain $c_1 = 0$ and $\sin(\sqrt{\lambda}t) = 0$, which fixes the eigenvalues

$$\lambda = j^2, \quad j = 1, 2, 3, \ldots.$$

In this example, all the eigenvalues are bifurcation points. Simple eigenvalues of the linearization are always bifurcation points of the nonlinear problem. We remark in passing that the emanating solutions of equation (6.39) can be calculated analytically in terms of elliptic functions [Sey75]. □

We close this section by investigating a more demanding example:

**Example 6.6  Buckling of a Rod**

Consider a rod of length $L$ that is subject to end loading (load $P > 0$). The shape of the rod is described by the tangent angle $u(x)$ as a function of the material points $x$ on the rod in its originally straight position [Olm77]. The variation of the angle with $x$ is zero at the ends of the rod,

$$u'(0) = u'(L) = 0.$$  \hfill (6.40a)

A deformation of the rod depends on the pressure $P$, on the stiffness $K$ of the rod material, and on compressibility effects. Neglecting the latter effects, the tangent angle satisfies the differential equation

$$u'' + \frac{P}{K} \sin(u) = 0.$$  \hfill (6.40b)

This is the famous Euler buckling problem [Eul52]; a finite-element analog is discussed in Exercise 2.14. Euler showed that the undeformed state $u = 0$ is the only solution for $P/K$ less than the first eigenvalue of the linearization,

$$\frac{P}{K} < \left( \frac{\pi}{L} \right)^2.$$

A bent state is stable for values of $P/K$ exceeding this critical value. Solutions in closed form can be found in [Sta71].

A rod with nonlinear compressibility properties is discussed in [Olm77]; the differential equation is

$$u'' + \frac{P}{K} \exp[C(P \cos u(x)) - C(0)] \sin u = 0$$  \hfill (6.41)

with $C(\zeta)$ chosen to be

$$C(\zeta) = \frac{1}{5} \tanh[5(3 - 5\zeta + 2\zeta^2)].$$
In order to make it fit into the analytical framework of [Olm77], this problem was simplified by fixing a unit load \( P = 1 \). This means varying the stiffness \( K \) or the parameter

\[
\lambda := \frac{\exp(-C(0))}{K} = \frac{0.81873\ldots}{K}
\]

in the boundary-value problem

\[
u'' + \lambda \exp[C(\cos(u))] \sin(u) = 0, \quad u'(0) = u'(L) = 0.
\] (6.42)

We follow this simplification in order to obtain comparable results; numerical methods can handle the original problem, equation (6.41), taking \( \lambda = P \) as the parameter.

The boundary-value problem equation (6.42) has been solved for \( L = 2 \). Figure 6.12 shows a bifurcation diagram. The eigenvalues of the linearization (Exercise 6.15) can be calculated numerically by solving equation (6.38). Alternatively, approximations \( \tilde{\lambda}_0, \tilde{h}_0 \) are obtained effectively by the method of Section 6.3, which simplifies significantly in case of trivial bifurcation. Starting from these approximations, the emanating branch is traced by means of the boundary-value problem (6.3). This reveals that the nontrivial branches locally branch off to the left, but globally the branches “soon” turn back to the right. The related turning points are easily obtained as by-products of the continuation; the methods indicated in Exercises 5.7 through 5.9 apply without change to boundary-value problems. The turning point with the smallest value of \( \lambda \) is

\[
\lambda_0 = 2.242, \quad u(0) = 0.7293.
\]
6.6 Testing Stability

This section looks at the stability of solutions to boundary-value problems. Recall the situation encountered with nonlinear equations

\[ 0 = f(y, \lambda). \]

If this equation represents equilibria of a system of ODEs, the dynamic behavior is governed by the *evolution equation*

\[ \dot{y} = \frac{dy}{dt} = f(y, \lambda). \]

The situation of second-order ODE boundary-value problems

\[ 0 = y'' - f(x, y, y', \lambda), \quad r(y(a), y(b), y'(a), y'(b)) = 0 \quad (6.43) \]

is analogous. Assume that equation (6.43) represents a stationary solution of a partial differential equation with the independent space variable \( x \) varying in the interval \( a \leq x \leq b \). An evolution equation corresponding to second-order differential equations with linear boundary conditions is the system of PDEs

\[
\begin{align*}
\frac{\partial y}{\partial t} &= D \frac{\partial^2 y}{\partial x^2} + f(x, y, \frac{\partial y}{\partial x}, \lambda), \\
A_0 y(a, t) + A_1 \frac{\partial y(a, t)}{\partial x} &= c_a, \\
B_0 y(b, t) + B_1 \frac{\partial y(b, t)}{\partial x} &= c_b.
\end{align*} \quad (6.44)
\]

Prominent examples of this class are reaction-diffusion systems, see Section 3.5.3. Solutions to equation (6.44) depend on both time \( t \) and space variable \( x, y(x, t) \) for \( a \leq x \leq b, t \geq 0 \). The matrices \( D, A_0, A_1, B_0, \) and \( B_1 \) are of size \( n^2 \), and \( c_a \) and \( c_b \) are \( n \)-vectors, fixing linear boundary conditions for \( x = a \) and \( x = b \). Often, the matrices are diagonal. With

\[ y' = \frac{\partial y}{\partial x}, \quad y'' = \frac{\partial^2 y}{\partial x^2}, \]

we write the ODE problem that represents the steady states of equation (6.44) in a form similar to equation (6.43),

\[
\begin{align*}
0 &= Dy'' + f(x, y, y', \lambda), \\
A_0 y(a) + A_1 y'(a) &= c_a, \\
B_0 y(b) + B_1 y'(b) &= c_b.
\end{align*} \quad (6.45)
\]

The Brusselator model is an example for the pair of equations (6.44) and (6.45). The full PDE problem of the Brusselator is listed in equation (5.53); the steady-state problem is in equation (6.4).
6.6.1 Elementary Approaches

It makes sense to investigate the stability of a solution $y_s(x)$ of the steady-state problem equation (6.45) that has the evolution equation (6.44) as background. Clearly, $y(x,t) = y_s(x)$ is a solution to the full system in equation (6.44) for all $t$. The question is whether nearby solutions approach the steady state or leave its neighborhood. Testing the stability of a steady state is cumbersome [HeP81], [PeOH81], [JeR82], [RoH83], [KuH84a], [Sey85a]. In Section 3.5.4 we have discussed a linear stability analysis for homogeneous solutions of reaction-diffusion problems. In what follows we describe some numerical strategies.

One method for testing a steady state for stability simulates the dynamic behavior. To this end, $y_s(x)$ is taken as an initial profile for $t = 0$. Then equation (6.44) is solved numerically as an initial-value problem starting from $y(x,0) = y_s(x)$ or from an artificially perturbed $\tilde{y}_s$. Initial deviations eventually die out or grow. Stability is indicated when $y(x,t)$, for increasing $t$, converges to $y_s(x)$ or remains close. On the other hand, instability is signaled when $y(x,t)$ takes values that are significantly distinct from the initial profile. The difficulty with simulation lies in the uncertainty about how to perturb $\tilde{y}_s$ and which value of $t_f$ to carry out the integration.

A second method is based on a semidiscretization in the space variable —namely, the method of lines. This can also be used for a simulation. But now our aim is to set up a framework for an eigenvalue analysis. For example, perform a simple discretization using the standard difference quotients

$$
\frac{\partial^2 y(x)}{\partial x^2} \approx \frac{y(x + \Delta) - 2y(x) + y(x - \Delta)}{\Delta^2},
$$

$$
\frac{\partial y(x)}{\partial x} \approx \frac{y(x + \Delta) - y(x - \Delta)}{2\Delta},
$$

(6.46)

for a small increment $\Delta$. This is easily organized by imposing an equidistant grid on the interval $a \leq x \leq b$, using $N$ interior grid points,

$$
\Delta := \frac{b - a}{N + 1}, \quad x_j := a + j\Delta \quad \text{for } j = 0, 1, \ldots, n + 1.
$$

(6.47)

The components $y_i(x,t)$ of $y(x,t)$ are approximated along the discrete “lines” $x = x_j$. This gives rise to $nN$ scalar functions

$$
y_i(x_j,t),
$$

which depend on time only. Introducing an $nN$-vector $Y$ by

$$
Y_\nu(t) := y_i(x_j,t) \text{ with } \nu = (j - 1)n + i, \quad i = 1, \ldots, n, \; j = 1, \ldots, N
$$

(6.48)
and inserting the difference quotients (6.46) into equation (6.44) yields an ordinary differential equation $\dot{Y} = F(Y, \lambda)$. The generation of $F(Y, \lambda)$ is best done by computer; some care in implementing the boundary conditions is required (Exercise 6.17). After the ODE system in standard form is constituted, eigenvalue-based methods for checking the stability apply [Neu93a].

This second approach may be attractive because it is more deterministic than simulation is, but there are many difficulties to overcome. An equidistant grid with a constant spacing $\Delta$ is not adequate for many applications. Steep gradients in the $y_s(x)$ profile call for a non-equidistant grid. Also, to keep the dimension small, difference quotients of an order higher than the second-order discretizations equation (6.46) are preferred. Such improvements lead to highly complex algorithms. In any case, the dimension $nN$ will be large, and the evaluation of the eigenvalues of the Jacobian of $F$ is mostly too expensive. For alternatives, see Section 5.1. One must frequently resort to a small value of $N$, hoping that the stability of the stationary PDE solution is reflected by a coarse ODE approximation.

Summarizing, we point out that it requires much effort to test the stability of a solution that was the straightforward result of some ODE solver. Consequently, during continuation stability is tested only occasionally, in order to save on cost.

6.6.2 Inertial Manifolds

The above approach has set up a system of ODEs to approximate the PDE solution. The better the approximation, the more trustworthy a prediction of stability or bifurcation will be. The method of inertial manifolds has been applied successfully for a bifurcation and stability analysis [Foi88], [Tém90], [KeJT91], [JoT92], [MaJ92]. This class of methods handles, for example, evolution equations of the type

$$u_t + Au + F(u) = 0.$$  \hspace{1cm} (6.49)

Here $A$ is a linear differentiation operator such as $Au = -\gamma u_{xx}$ and $F(u)$ stands for other terms. An example of this type of equation is the reaction-diffusion problem

$$u_t - \gamma u_{xx} + u^3 - u = 0$$  \hspace{1cm} (6.50)

with boundary conditions $u(0, t) = u(\pi, t) = 0$. The linear operator $Au$ acts on an appropriate function space that has a complete orthonormal basis consisting of eigenfunctions $w_1, w_2, w_3, \ldots$ of $A$, observing the given boundary conditions. Example 6.5 has revealed for the operator $Au = -\gamma u_{xx}$ of equation (6.50) the eigenfunctions $w_k(x) = \sin kx$.

An approximation to $u$ is sought in the form of the truncated series

$$p(x, t) := \sum_{j=1}^{l} a_j(t)w_j(x).$$  \hspace{1cm} (6.51)
Let us denote by $P_l$ the projection onto $\text{span}\{w_1, \ldots, w_l\}$, $p = P_l u$, which implies $q := u - p = (\text{id} - P_l)u$. This allows one to split equation (6.49) into two equations by multiplying with $P_l$ and the complementary $(\text{id} - P_l)$,

\begin{align*}
  p_t + Ap + P_l F(p + q) &= 0, \\
  q_t + Aq + (\text{id} - P_l) F(p + q) &= 0.
\end{align*}

(6.52)

The first part in equation (6.52) is an equation for the $l$ lower modes, and the second equation takes care of the infinite number of higher modes. Traditionally, Galerkin-type methods discard the higher modes completely and solve the finite-dimensional part

\begin{align*}
  p_t + Ap + P_l F(p) &= 0;
\end{align*}

no correction term is applied in the argument of $F$. Frequently, this truncation is too severe to accurately predict the long term behavior of $u(t)$. Inertial manifold methods solve

\begin{align*}
  p_t + Ap + P_l F(p + \psi_m(p)) &= 0,
\end{align*}

(6.53)

constructing an approximate inertial manifold $\tilde{q} = \psi_m(p)$ such that $\tilde{q}$ captures the essence of the truncated dynamics. The function $\tilde{q} = \psi_m(p)$ serves as a correction term in the argument of $F$, $u \approx p + \tilde{q}$. Constructing $\psi_m(p)$ can be accomplished by taking $m > l$ further eigenfunctions $w_{l+1}, \ldots, w_m$ into consideration, for $m > l$. This defines a projection $Q$ onto $\text{span}\{w_{l+1}, \ldots, w_m\}$, $\tilde{q} = Qu$. For convenience, we rewrite $\tilde{q}$ as $q$. The truncated dynamics $q = \psi_m(p)$ is then defined by

\begin{align*}
  q_t + Aq + QF(p + q) &= 0.
\end{align*}

(6.54)

A crude approximation for $q$ will suffice. Take, for example, an implicit Euler integration step, with

\begin{align*}
  q_t \approx \frac{q - q_0}{\Delta t},
\end{align*}

and start from the trivial approximation $q_0 = 0$, which corresponds to the traditional Galerkin approach. We obtain an implicit equation for $q$

\begin{align*}
  q + \Delta t A q + \Delta t QF(p + q) &= 0,
\end{align*}

which can be written

\begin{align*}
  q = -(I + \Delta t A)^{-1} \Delta t QF(p + q).
\end{align*}

This equation is regarded a fixed point equation; the fixed point iteration converges for suitably chosen $\Delta t$. Carrying out only one iteration, starting again from $q = 0$, yields as approximate inertial manifold

\begin{align*}
  q = \psi_m(p) := -\Delta t (1 + \Delta t A)^{-1} QF(p).
\end{align*}

(6.55)
This establishes the higher modes \( q (\bar{q}) \) as functions of the lower modes \( p \).

For \( m \to \infty \), \( \psi_m(p) \) approaches the inertial manifold \( \psi(p) \), and \( Q \) approaches \( \text{id} - P_1 \). Hence, equation (6.54) approximates the second equation in equation (6.52), and the function \( q = \psi_m(p) \) in equation (6.53) can be seen as a correction term that improves the accuracy of this equation. Typically, equation (6.53) represents a system of \( l \) ODEs for the functions \( a_j(t) \). For instance, for \( l = 2, m = 4 \) the above approach means to express the higher modes \( a_3, a_4 \) by the lower ones, \( a_3 = a_3(a_1, a_2), a_4 = a_4(a_1, a_2) \). The reader is encouraged to try this on equation (6.50). The inertial manifold methods, when applicable, have shown remarkably accurate results using a smaller \( l \) than required for traditional Galerkin-type methods.

### 6.7 Hopf Bifurcation in PDEs

The stability of solutions to ODE boundary-value problems can be lost in similar ways, as is common with solutions to equations \( f(y, \lambda) = 0 \). The way a critical eigenvalue crosses the imaginary axis is crucial [JoS72], [CrR77].

Consider the PDE in equation (6.44) and a solution \( y_s(x) \) to the steady-state equations (6.45). Let us denote the difference between \( y_s(x) \) and a solution \( y(x, t) \) to equation (6.44) by \( \tilde{d} \),

\[
y(x, t) = y_s(x) + \tilde{d}(x, t).
\]

(For a constant \( y_s \) see Section 3.5.4.) Substituting \( y \) into the PDE in equation (6.44) leads to

\[
\frac{\partial \tilde{d}}{\partial t} = D y''_s + D \tilde{d}'' + f(x, y_s + \tilde{d}, y'_s + \tilde{d}', \lambda).
\]

Linearizing \( f \) about \( y_s, y'_s \) yields the linearized PDE

\[
\frac{\partial d}{\partial t} = D d'' + f_y(x, y_s, y'_s, \lambda) d + f_y'(x, y_s, y'_s, \lambda) d',
\]

\[
A_0 d(a, t) + A_1 d'(a, t) = 0, \quad (6.56)
\]

\[
B_0 d(b, t) + B_1 d'(b, t) = 0.
\]

For \( y \approx y_s \), the linear PDE in equation (6.56) reflects the dynamics of the solutions to equation (6.44) that are close to \( y_s(x) \). This analysis parallels the ODE stability analysis outlined in Section 1.2 and in Section 5.7.4. Compare also the analysis of pattern formation in Section 3.5.4. The ansatz

\[
d(x, t) = e^{\mu t} w(x),
\]

substituted into equation (6.56), yields the ODE eigenvalue problem
\[ \mu w = Dw'' + f_y(x, y_s, y'_s, \lambda)w + f_{y'}(x, y_s, y'_s, \lambda)w', \]
\[
A_0w(a) + A_1w'(a) = 0, \\
B_0w(b) + B_1w'(b) = 0.
\]

For complex \( \mu \) and \( w \), this boundary-value problem is equivalent to two boundary-value problems for real variables. The two real systems are obtained by substituting
\[ \mu = \alpha + i\beta, \quad w(x) = h(x) + ig(x) \]
into equation (6.57). After collecting real and imaginary parts we have
\[
Dh'' + f_y(x, y_s, y'_s, \lambda)h + f_{y'}(x, y_s, y'_s, \lambda)h' = \alpha h - \beta g, \\
Dg'' + f_y(x, y_s, y'_s, \lambda)g + f_{y'}(x, y_s, y'_s, \lambda)g' = \beta h + \alpha g, \\
A_0h(a) + A_1h'(a) = 0, \\
B_0h(b) + B_1h'(b) = 0, \\
A_0g(a) + A_1g'(a) = 0, \\
B_0g(b) + B_1g'(b) = 0.
\]

This coupled system consists of \( 2n \) second-order ODEs with boundary conditions. The difficulty with the ODE eigenvalue problem in equation (6.58) is that it has an infinite number of eigenvalues. Hence, it can hardly be calculated whether, for instance, all eigenvalues have negative real parts. Bifurcation points are characterized in the usual way: The \( \alpha \) and \( \beta \) depend on \( \lambda \), and for one of the \( \alpha \) we have \( \alpha(\lambda_0) = 0 \) at the parameter value \( \lambda_0 \) of a bifurcation point. In the real case, \( \beta(\lambda_0) = 0 \), we encounter a turning point or a stationary bifurcation point. In the imaginary case, \( \beta(\lambda_0) \neq 0 \), we have a Hopf bifurcation.

This situation enables us to set up direct methods for calculating bifurcation points. As in the branching system in equation (6.14), we keep the solution \( y_s(x) \) available by attaching equation (6.45) to equation (6.58). The \( \alpha \) terms in equation (6.58) can be dropped because \( \alpha(\lambda_0) = 0 \). For the stationary bifurcation, the \( \beta \) terms are also dropped. In the latter case, the two systems in equation (6.58) are identical, and one can be removed (the \( g \) system, say). Imposing a normalizing equation such as \( h_k(a) = 1 \), and attaching the trivial differential equation \( \lambda' = 0 \), reproduces the branching system in equation (6.14), here written for second-order ODEs. This shows that the bifurcation points calculated by equation (6.14) are candidates for gain or loss of stability. We conclude that it is sufficient to test stability only once on either side of a bifurcation point.

The direct method for calculating Hopf points is now easily set up. Because \( \beta(\lambda_0) \neq 0 \) is an unknown constant, we set up the trivial differential equation \( \beta' = 0 \). Imposing a normalizing condition on \( g(a) \) and collecting all equations, one has
\[ Dy'' + f(x, y, y', \lambda) = 0, \]
Calculating Branching Behavior of Boundary-Value Problems

\[ Dh'' + f_y(x, y', y, \lambda)h + f_{y'}(x, y, y', \lambda)h' = -\beta g, \]
\[ Dg'' + f_y(x, y, y', \lambda)g + f_{y'}(x, y, y', \lambda)g' = \beta h, \]
\[ \lambda' = 0, \quad \beta' = 0, \]
\[ A_0y(a) + A_1y'(a) = c_a, \quad B_0y(b) + B_1y'(b) = c_b, \quad (6.59) \]
\[ A_0h(a) + A_1h'(a) = 0, \quad B_0h(b) + B_1h'(b) = 0, \]
\[ A_0g(a) + A_1g'(a) = 0, \quad B_0g(b) + B_1g'(b) = 0, \]
\[ h_k(a) = 1, \quad g_k(a) = 1. \]

In order to use standard software for ODEs, each of the second-order systems is transformed into a system of \( 2n \) first-order ODEs. Hence, altogether, equation (6.59) represents a first-order boundary-value problem consisting of \( 6n + 2 \) differential equations. Numerical results with \( n = 2 \) are reported in [KuH84a]. Severe problems in finding reasonable initial approximations were indicated.

The above approach can be generalized to PDEs with more than one space variable. For ease of notation, we suppress boundary conditions and write down the equations for the PDE

\[ \frac{\partial y}{\partial t} = \nabla^2 y + f(x, y, \lambda). \]

Here the independent space variable \( x \) is two-dimensional or three-dimensional. For Hopf bifurcation, the system that corresponds to equation (6.59) is based on

\[ \nabla^2 y + f(x, y, \lambda) = 0, \]
\[ \nabla^2 h + f_y(x, y, \lambda)h = -\beta g, \quad (6.60) \]
\[ \nabla^2 g + f_y(x, y, \lambda)g = \beta h. \]

The system reduces in the case of stationary bifurcation (\( \beta = 0 \)). A general reference on numerical bifurcation in reaction-diffusion equations is [Mei00].

Example 6.7 Nonstationary Heat and Mass Transfer

A nonstationary heat and mass transfer inside a porous catalyst particle can be described by the two parabolic PDEs [KuH84a], [RoH83]:

\[ Lw \frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} - \frac{\lambda c}{\gamma \beta} \exp \left( \frac{\Theta}{1 + \Theta/\gamma} \right), \]
\[ \frac{\partial \Theta}{\partial t} = \frac{\partial^2 \Theta}{\partial x^2} + \lambda c \cdot \exp \left( \frac{\Theta}{1 + \Theta/\gamma} \right), \quad (6.61a) \]

with boundary conditions

\[ \frac{\partial c(0, t)}{\partial x} = \frac{\partial \Theta(0, t)}{\partial x} = 0, \]
\[ c(1, t) = 1, \quad \Theta(1, t) = 0. \quad (6.61b) \]
The steady state satisfies the boundary-value problem

\[ c'' = \frac{\lambda c}{\gamma \beta} \exp \left( \frac{\Theta}{1 + \Theta/\gamma} \right), \]
\[ \Theta'' = -\lambda c \cdot \exp \left( \frac{\Theta}{1 + \Theta/\gamma} \right), \]
\[ c'(0) = 0, \quad c(1) = 1, \quad \Theta'(0) = 0, \quad \Theta(1) = 0. \]

After evaluating the Jacobian \( f_y \), the remaining parts of equation (6.59) can be easily written down. Denoting the exponential terms

\[ E_0 := \exp \left( \frac{\Theta}{1 + \Theta/\gamma} \right), \]
\[ E_1 := \frac{c}{(1 + \Theta/\gamma)^2} E_0, \]

one obtains

\[ h''_1 = \frac{\lambda}{\gamma \beta} E_0 h_1 - \frac{\lambda}{\gamma \beta} E_1 h_2 = -\beta \cdot \text{Lw} \cdot g_1, \]
\[ h''_2 + \lambda E_0 h_1 + \lambda E_1 h_2 = -\beta g_2, \]
\[ g''_1 = \frac{\lambda}{\gamma \beta} E_0 g_1 - \frac{\lambda}{\gamma \beta} E_1 g_2 = \beta h_1, \]
\[ g''_2 + \lambda E_0 g_1 + \lambda E_1 g_2 = \beta h_2, \]
\[ h'_1(0) = h_1(1) = h'_2(0) = h_2(1) = 0, \]
\[ g'_1(0) = g_1(1) = g'_2(0) = g_2(1) = 0. \]

The coupling with the steady state is hidden in the exponential terms. Writing down the 14 first-order differential equations explicitly is beyond the scope of this book. Such systems are seldom written down explicitly because they can be conveniently set up in a computer working with \( n^2 \)-matrices and subvectors. In order to give an impression of how the system equation (6.59) can be organized, we write down the components of the resulting extended vector \( Y \):

\[ Y_1 = c, \quad Y_2 = c', \quad Y_3 = \Theta, \quad Y_4 = \Theta', \]
\[ Y_5 = h_1, \quad Y_6 = h'_1, \quad Y_7 = h_2, \quad Y_8 = h'_2, \]
\[ Y_9 = g_1, \quad Y_{10} = g'_1, \quad Y_{11} = g_2, \quad Y_{12} = g'_2, \]
\[ Y_{13} = \lambda, \quad Y_{14} = \beta. \]
6.8 Computation of Heteroclinic and Homoclinic Orbits

The computation of heteroclinic or homoclinic orbits leads to boundary-value problems of a specific kind. The derivation of such boundary-value problems is the topic of this section. For an illustration of a homoclinic orbit see Figure 2.29, and Figure 6.13a depicts a heteroclinic orbit. We assume an autonomous system of ODEs

\[ \dot{y} = f(y) \]

and postpone possible parameters until later. To explain basic ideas, we start with a simple planar scenario, where a heteroclinic orbit of the differential equation connects two saddles \( y^{s_1}, y^{s_2} \). Figure 6.13a shows a related phase portrait, including the lines of the eigenspaces.

It takes an infinite time for a particle to follow the ideal heteroclinic trajectory from one stationary solution to the other, \(-\infty < t < \infty\). In practice, a trajectory can only be approximated for a finite time interval of length \( T \). Since we have assumed an autonomous ODE, the interval of the truncated problem can be taken as \( 0 \leq t \leq T \). The aim is to calculate an orbit \( \tilde{y}(t) \) that approximates the heteroclinic orbit in that \( \tilde{y}(0) \) is close to \( y^{s_1} \), and \( \tilde{y}(T) \) is close to \( y^{s_2} \), for a large prescribed value of \( T \). Since the heteroclinic orbit enters or leaves the stationary solutions tangentially to the eigenspaces, it is reasonable to try to find an orbit \( \tilde{y}(t) \) that starts and ends on the relevant eigenspace close to the saddles (Figure 6.13b). This amounts to formulate boundary conditions

\[
\begin{align*}
\tilde{y}(0) &= y^{s_1} + \varepsilon_1 w^{11}, \\
\tilde{y}(T) &= y^{s_2} + \varepsilon_2 w^{21}.
\end{align*}
\]

(6.62)
In equation (6.62), $w^{11}$ is the vector tangent to the unstable manifold of $y^{s1}$, $w^{21}$ defines the stable manifold of $y^{s2}$, and $\varepsilon_1$ and $\varepsilon_2$ measure the distances from the start and end points of $\bar{y}$ to the saddles. The trajectory $\bar{y}$ can be seen as being parameterized by $\varepsilon_1$, $\varepsilon_2$, which is a parameterization by “irregularity” or “discrepancy” following the lines of Section 5.6.6 and Section 6.4. We expect $\varepsilon_1$ and $\varepsilon_2$ to be close to 0 for large $T$.

In order that a solution of the differential equation with boundary conditions equation (6.62) exists, the problem must have enough free parameters to be flexible. The number $n_p$ of necessary free parameters depends on $n$ and the type of the stationary solutions $y^{s1}, y^{s2}$. We arrange the free parameters in a parameter vector $\Lambda = (\lambda_1, ..., \lambda_{n_p})$ and shall see what $n_p$ might be. That is, we study a differential equation of the form $y' = f(y, \Lambda)$. Transforming the integration interval to $0 \leq t \leq 1$ leads to

$$y' = Tf(y, \Lambda).$$

(6.63)

For this differential equation we need boundary conditions for $y(0)$ and $y(1)$ in the spirit of equation (6.62). For general stationary solutions, the boundary conditions are more involved, taking into account higher-dimensional stable manifolds and unstable manifolds. We describe this more general setting next. For ease of notation, we drop the overbar on the approximation $\bar{y}$.

Assume that the Jacobian $f_y(y^{s1}, \Lambda)$ has $n_1$ real positive eigenvalues $\mu_{1k}$ with $n_1$ eigenvectors $w^{1k}$ ($k = 1, ..., n_1$). For an easy setting suppose (as in [DoKK91]) that the remaining $n - n_1$ eigenvalues have negative real parts. Then the unstable eigenspace belonging to $y^{s1}$ consists of all linear combinations

$$y^{s1} + \sum_{k=1}^{n_1} c_{1k} w^{1k},$$

for coefficients $c_{11}, ..., c_{1n_1}$. Demanding the start point $y(0)$ to be on this eigenspace gives the boundary condition for $y(0)$ that replaces the planar saddle situation in equation (6.62). For this saddle, $n_1 = 1$, and $c_{11}$ is included in $\varepsilon_1$. This outlines the general idea.

For the other stationary solution $y^{s2}$ we assume similar conditions to describe the stable manifold: Let $n_2$ be the number of real negative eigenvalues $\mu_{2k}$ and eigenvectors $w^{2k}$ of the matrix $f_y(y^{s2}, \Lambda)$, $k = 1, ..., n_2$. The other $n - n_2$ eigenvalues are assumed to be “unstable,” having positive real parts. We collect the defining equations:

$$f(y^{s1}, \Lambda) = 0,$$

(6.64a)

$$f(y^{s2}, \Lambda) = 0,$$

(6.64b)

$$f_y(y^{s1}, \Lambda)w^{1k} = \mu_{1k}w^{1k}, \quad k = 1, ..., n_1,$$

(6.64c)

$$f_y(y^{s2}, \Lambda)w^{2k} = \mu_{2k}w^{2k}, \quad k = 1, ..., n_2,$$

(6.64d)

$$\|w^{1k}\| = 1, \quad k = 1, ..., n_1,$$

(6.64e)
These equations define the unstable manifold of \( y^{s1} \) and the stable manifold of \( y^{s2} \). The equations (6.64e/f) normalize the eigenvectors to unit length, using the Euclidean norm; other normalizing conditions may also be used. The following equations formulate the boundary conditions, which specify \( y(0) \) to lie on the unstable manifold of \( y^{s1} \), and \( y(1) \) to arrive on the stable manifold of \( y^{s2} \):

\[
y(0) = y^{s1} + \varepsilon_1 \sum_{k=1}^{n_1} c_{1k} w^{1k}, \tag{6.65a}
\]

\[
y(1) = y^{s2} + \varepsilon_2 \sum_{k=1}^{n_2} c_{2k} w^{2k}. \tag{6.65b}
\]

To give \( \varepsilon_1 \) and \( \varepsilon_2 \) a unique meaning, the coefficients \( c_{1k} \) and \( c_{2k} \) must be normalized,

\[
\sum_{k=1}^{n_1} c_{1k}^2 = 1, \tag{6.65c}
\]

\[
\sum_{k=1}^{n_2} c_{2k}^2 = 1. \tag{6.65d}
\]

Finally, a phase condition is required, because the differential equation (6.63) is autonomous. This topic will be explained in Section 7.1. As an example of a phase condition one may choose

\[
f_1(y(0), \Lambda) = 0. \tag{6.66}
\]

The equations (6.64), (6.65), and (6.66) consist of

\[n + n + nn_1 + nn_2 + n_1 + n_2 + n + n + 1 + 1 + 1\]

scalar equations. By substituting \( y^{s1} \) and \( y^{s2} \) from equation (6.65a/b) into equation (6.64) \( 2n \) of the equations can be replaced. Additional \( n \) of the equations are needed as boundary conditions for the differential equation for \( y(t) \) in equation (6.63). The remaining number of equations is

\[n + 3 + (n + 1)(n_1 + n_2). \tag{6.67}\]

The unknown variables are the reals \( A_1, ..., A_{n_1}, c_{11}, ..., c_{1n_1}, c_{21}, ..., c_{2n_2}, \varepsilon_1, \varepsilon_2, \mu_{11}, ..., \mu_{1n_1}, \mu_{21}, ..., \mu_{2n_2} \), the vectors \( w^{1k} (k = 1, ..., n_1) \) and \( w^{2k} (k = 1, ..., n_2) \). Altogether we have

\[2 + n_p + (n + 2)(n_1 + n_2) \tag{6.68}\]

scalar variables. The counting of the constraints in equation (6.67) and of the variables in equation (6.68) does not include \( y \), for which we have the
differential equation with boundary conditions. The numbers in equations (6.67) and (6.68) must match, which leads to the relation

$$1 + n = n_1 + n_2 + n_p.$$  

(6.69)

This equation fixes the number $n_p$ of free parameters needed to define an orbit as illustrated in Figure 6.13b. In order to have a branch of such orbits, another free parameter is needed. This introduces our $\lambda$, and the differential equation is then

$$y' = T \mathbf{f}(y, \Lambda, \lambda),$$

(6.70)

where $\Lambda$ consists of $n + 1 - n_1 - n_2$ free parameters.

The above involved set of equations is solved numerically. If analytic information on stationary solutions and eigenvectors is available, the number of equations in equation (6.67) can be reduced. It is straightforward to reduce the above method such that homoclinic orbits are approximated (Exercise 6.18). For references on this and related methods on global bifurcation, see for example [Beyn90a], [Beyn90b], [Kuz90], [DokKK91], [FrD91], [ChK94], [Moo95], [BaLS96], [Kuz98], [OlCK03]. Test functions and other techniques described in this book are extended and applied frequently.

Example 6.8 Fisher’s Model

This equation was discussed in Section 3.5.1; see Example 3.6. The ODE system ($n = 2$) is

$$y_1' = y_2,$$

$$y_2' = -\lambda y_2 - \zeta y_1 (1 - y_1).$$

The heteroclinic orbit starts from the saddle $(y_1, y_2) = (1, 0)$; we have $n_1 = 1$. The other stationary solution $(0, 0)$ is for $\lambda > 2\sqrt{\zeta}$ a stable node, hence $n_2 = 2$. The count of free parameters $n_p$ of equation (6.69) is $n_p = 0$. No free parameter is required for a heteroclinic orbit, $\zeta > 0$ and $\lambda > 2\sqrt{\zeta}$ can be fixed constants. A branch of heteroclinic orbit is obtained when one parameter, say $\lambda$, is varied. □

Exercises

Exercise 6.1

(a) Derive equations (6.5a) and (6.5b) from equation (6.4).

(b) What are the boundary conditions that replace those in equation (6.5b) when zero flux is considered,

$$\frac{\partial X}{\partial x} = \frac{\partial Y}{\partial x} = 0 \quad \text{for } x = 0, x = L?$$
(c) Write down explicitly the functions $f_i$ and $r_i$ ($i = 1, \ldots, 4$) from equation (6.1) that define equations (6.5a) and (6.5b).

(d) Calculate all first-order partial derivatives of $f_i$ and $r_i$ with respect to $y_j$ ($i, j = 1, \ldots, 4$) and arrange them in matrices. Notice that the derivatives of $r$ include $2n^2$ entries.

(e) Which constant solution satisfies equations (6.5a) and (6.5b)? Where is this solution found in Figure 6.1?

**Exercise 6.2**
Derive in detail boundary-value problem equation (6.10). Start from the original Duffing equation and use equations (6.7) and (6.8).

**Exercise 6.3**
*(Project.)* Assume that a periodic oscillation has been calculated with a vector of initial values $y(0)$ and period $T$. The right-hand side of the differential equation is $f$. Suppose further that $N$ values $y(t_j)$ at equidistant nodes $t_j$ are required (for plotting purposes, say), together with an approximation of the amplitude. Design and implement an algorithm that calculates the required approximations. To this end, modify an integration routine with step control (as, for instance, an RKF method; see Appendix A.6) as follows: Each function evaluation of $f$ is to be used to calculate locally cubic splines [StB80], [DaB08]. Establish formulas that calculate the extrema of the splines. Use the splines also for calculating the desired approximations of $y(t_j)$; in this way the step control need not be manipulated.

**Exercise 6.4**
Establish the linearized boundary-value problems in equation (6.11) for the Brusselator in equation (6.5) and the Duffing equation in equation (6.9).

**Exercise 6.5**
Show that a boundary condition $r_j = y_\nu(a) - \text{constant} = 0$ implies $h_\nu(a) = 0$.

**Exercise 6.6**
Boundary conditions are frequently linear, $r = \tilde{A}y(a) + \tilde{B}y(b) - c$, with an $n$-vector $c$ and matrices $\tilde{A}$ and $\tilde{B}$.

(a) What are the boundary conditions of the linearization?

(b) What are $\tilde{A}$, $\tilde{B}$, and $c$ in the case of periodic boundary conditions?

**Exercise 6.7**
*(Laborious Project.)* Construct a direct method for calculating bifurcation points as follows: Implement a special shooting code that solves equation (6.13), exploiting equation (6.24) and $E \cdot h(a) = 0$ internally.

**Exercise 6.8**
For each of the cases (6.30a) through (6.30d), sketch an example.
Exercise 6.9
Assume that $u(t)$ and $v(t)$ are two scalar variables defined for $-1 \leq t \leq 1$. $u(t)$ is supposed to be odd, and $v(t)$ is even. What can be said about $u', \, v', \, u'', \, v'', \, u^2, \, uv$?

Exercise 6.10
Show that the Brusselator model equation (6.4) supports even solutions. (Hint: Substitute $X^* = X - A$, $Y^* = Y - B/A$, and investigate the resulting system in $X^*, Y^*$.)

Exercise 6.11
Show that the Duffing equation (6.9) supports a symmetry of the type in equation (6.30c).

Exercise 6.12
Consider a periodic solution of a second-order oscillator [such as the Duffing equation in equation (6.9)] and its graphical representation in a phase plane. What can be said about the graphs of $u(t)$ and $\tilde{u}(t)$ when there is a symmetry of the type of equation (6.30c)?

Exercise 6.13
Find the trivial solution(s) of the superconductivity example in equation (6.35).

Exercise 6.14
For the boundary-value problem
\[-u'' + u^3 = \lambda u, \quad u(0) = u(\pi), \quad u'(0) = u'(\pi)\]
calculate the eigenvalues of the linearization about $u = 0$.

Exercise 6.15
Consider the buckling rod problem in equations (6.40a) and (6.40b). Calculate the eigenvalues of the linearization about $u = 0$. Show that the linearization of equation (6.42) has the same eigenvalues.

Exercise 6.16
Consider stationary solutions ($u_t = 0$) of the Kuramoto–Sivashinsky equation (3.30). Show that bifurcations from the trivial solution $u \equiv 0$ can only take place for $\gamma = 4j^2, \, j = 1, 2, 3, \ldots$.

Exercise 6.17
Assume that the scalar dependent variable $u(x, t)$ satisfies the boundary conditions of equation (6.44) (consider $A_0, \, A_1, \, B_0, \, B_1$ to be scalars). Suppose further that the standard difference quotients in equation (6.46) with equidistant spacing are applied with $N > 1$. 
(a) Show that
\[
\frac{\partial u(a, t)}{\partial x} = \frac{1}{2\Delta} \left[ -3u(a, t) + 4u(x_1, t) - u(x_2, t) \right] + O(\Delta^2).
\]

(b) Use (a) to show that
\[
\frac{\partial u(b, t)}{\partial x} \approx \frac{2\Delta c_b - A_1(4u(x_1, t) - u(x_2, t))}{(2\Delta A_0 - 3A_1)}.
\]

(c) Show the analog
\[
u(x_i, t) \approx \frac{2\Delta c_i + B_1(4u(x_{i+1}, t) - u(x_{i-1}, t))}{(2\Delta B_0 + 3B_1)}.
\]

(d) How can these expressions be used to generate the differential equation
\[
\dot{Y} = F(Y, \lambda) \text{ that belongs to equation (6.48)?}
\]

**Exercise 6.18**
Specialize the method outlined in Section 6.8 to the computation of a homoclinic orbit.
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