JOURNAL OF COMPUTATIONAL PHYSICS 50, 171–177 (1983)

Note

Calculation of Critical Branching Points in Two-Parameter Bifurcation Problems*

1. Introduction

In certain nonlinear eigenvalue problems exhibiting two-parameter dependence, one encounters the phenomenon of a critical branching point: a parameter point for which a change in the secondary (e.g., energy) parameter causes a loss of branching in the primary (e.g., eigenvalue) parameter. Problems of this type arise for example in models of thermal ignition, in the theory of stellar structure, in chemical kinetics, and elsewhere. See for example the discussion in [1].

Numerical computation of the critical branching point has been achieved [2] through the solution of an associated linear eigenvalue boundary problem. We present here an alternate technique based upon an extension of the work in [1]. In particular, we extend the approach of [1] from a single parameter dependence to two-parameter dependence. This, furthermore, allows us to then solve simultaneously for both the primary and secondary critical parameter values in an exact criticality scheme. In the latter, we use an implicit calculus an order higher than that used in [1]. We have applied our method in [3] to a problem of thermal ignition similar to that treated in [1] and [2] in order to compare several models in explosion theory. In the present paper we emphasize the essentials of the numerical method (not given in [3]), for its potential use elsewhere, as an extension of the method of [1]. For convenience we shall use for the most part the nomenclature of [1], which treated the one-parameter second-order ordinary differential equation $y'' = f(x, y, y', \delta)$.

2. The Method

Consider the two-parameter ordinary differential equation

$$y'' = f(x, y, y', \delta, \varepsilon), \qquad 0 < x < 1, \tag{1}$$

subject to the boundary conditions

$$y'(0) = 0, \qquad \alpha_1 y(1) + \beta_1 y'(1) = \gamma_1. \tag{2}$$

* Partially supported by National Science Foundation Grant MCS 80–12220.

0021-9991/83 $3.00

581/50/1-12

We have tacitly assumed for simplicity that the original boundary value problem has been, by scale change if necessary, set to the interval $-1 < x < 1$, and that the solution is symmetric and takes its maximum at the origin.

Branching is then often represented in the form of bifurcation curves of δ versus η, where

$$\eta = \| y \|_\infty \equiv y(0). \tag{3}$$

Here we may assume that the solutions are all nonnegative. See Fig. 1 for a qualitative picture of three situations which can occur. The family of curves $\delta(\eta)$ of the (primary) eigenvalue parameter δ is also a function of the (secondary) parameter ε: $\delta = \delta(\eta, \varepsilon)$. The condition for a branching point is

$$\left.\frac{\partial \delta}{\partial \eta}\right|_\varepsilon = 0. \tag{4}$$

In addition, the critical branching point must satisfy

$$\left.\frac{\partial^2 \delta}{\partial \eta^2}\right|_\varepsilon = 0. \tag{5}$$

The difficulty in determining branching points lies in the fact that we cannot obtain an explicit representation for $\delta(\eta, \varepsilon)$. Instead, we have an implicit representation through the solution of (1), (2). Hence we must obtain expressions for (4) and (5) through the rules for differentiation of implicit functions (see, for example, [4]).

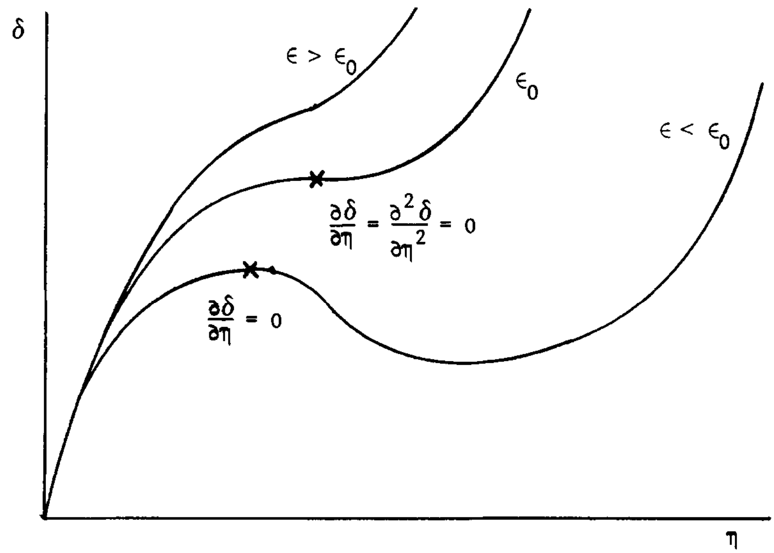

FIG. 1. Bifurcation diagram indicating a curve containing the critical branching point ($\varepsilon = \varepsilon_0$), a curve containing a branching point ($\varepsilon < \varepsilon_0$), and a curve containing no branching point ($\varepsilon > \varepsilon_0$).

Equation (1) may be solved as a split boundary value problem using a standard shooting method. This requires in addition to the initial condition specified in (2), the condition

$$y(0) = \eta. \tag{6}$$

With η, δ, and ε specified (by initial guesses), (1) is integrated to $x = 1$. If the specified parameter values represent a consistent solution to (1), (2), then the boundary condition at $x = 1$ will be satisfied; i.e.,

$$F_1(\delta, \eta, \varepsilon) \equiv \alpha_1\, y(1, \delta, \eta, \varepsilon) + \beta_1\, y'(1, \delta, \eta, \varepsilon) - \gamma_1 = 0. \tag{7}$$

Since all solutions of (1), (2) satisfy (7), the equation

$$F_1(\delta(\eta, \varepsilon), \eta, \varepsilon) = 0 \tag{8}$$

can be considered as an implicit representation of the bifurcation diagram. Then by implicit differentiation:

$$\left.\frac{\partial \delta}{\partial \eta}\right|_{\varepsilon} = -\frac{(\partial F_1/\partial \eta)|_{\delta,\varepsilon}}{(\partial F_1/\partial \delta)|_{\eta,\varepsilon}} \tag{9}$$

and

$$\left.\frac{\partial^2 \delta}{\partial \eta^2}\right|_{\varepsilon} = \left[\frac{\partial F_1}{\partial \eta}\frac{\partial^2 F_1}{\partial \eta \partial \delta} - \frac{\partial F_1}{\partial \delta}\frac{\partial^2 F_1}{\partial \eta^2} - \frac{\partial \delta}{\partial \eta}\left(\frac{\partial^2 F_1}{\partial \delta \partial \eta}\frac{\partial F_1}{\partial \delta} - \frac{\partial F_1}{\partial \eta}\frac{\partial^2 F_1}{\partial \delta^2}\right)\right] \Big/ \left(\frac{\partial F_1}{\partial \delta}\right)^2, \tag{10}$$

where the variables held constant in the partial derivatives on the right-hand side of (10) are clear. In Eqs. (9) and (10) it is assumed that $\partial F_1/\partial \delta$ is nonvanishing. Combining (4) and (5) with (9) and (10) gives

$$F_2(\delta, \eta, \varepsilon) \equiv \partial F_1/\partial \eta = 0 \tag{11}$$

and

$$F_3(\delta, \eta, \varepsilon) = \frac{\partial F_1}{\partial \eta}\frac{\partial^2 F_1}{\partial \eta \partial \delta} - \frac{\partial F_1}{\partial \delta}\frac{\partial^2 F_1}{\partial \eta^2} - \frac{\partial \delta}{\partial \eta}\left(\frac{\partial^2 F_1}{\partial \delta \partial \eta}\frac{\partial F_1}{\partial \delta} - \frac{\partial F_1}{\partial \eta}\frac{\partial^2 F_1}{\partial \delta^2}\right) = 0. \tag{12}$$

The parameter values at the critical branching point are obtained by the simultaneous solution of (8), (11), and (12). It should perhaps be noted at this time that we need the third term in (12) for the correct evaluation of the Jacobian in (17) at noncritical parameter values.

The right-hand sides of (11) and (12) are obtained by differentiating (7), which gives

$$\frac{\partial F_1}{\partial \eta} = \alpha_1 \frac{\partial y}{\partial \eta} + \beta_1 \frac{\partial y'}{\partial \eta}, \tag{13a}$$

$$\frac{\partial F_1}{\partial \delta} = \alpha_1 \frac{\partial y}{\partial \delta} + \beta_1 \frac{\partial y'}{\partial \delta}, \tag{13b}$$

$$\frac{\partial^2 F_1}{\partial \eta^2} = \alpha_1 \frac{\partial^2 y}{\partial \eta^2} + \beta_1 \frac{\partial^2 y'}{\partial \eta^2}, \tag{13c}$$

$$\frac{\partial^2 F_1}{\partial \delta \partial \eta} = \alpha_1 \frac{\partial^2 y}{\partial \delta \partial \eta} + \beta_1 \frac{\partial^2 y'}{\partial \delta \partial \eta}, \tag{13d}$$

$$\frac{\partial^2 F_1}{\partial \delta^2} = \alpha_1 \frac{\partial^2 y}{\partial \delta^2} + \beta_1 \frac{\partial^2 y'}{\partial \delta^2}. \tag{13e}$$

Define the following variables:

$$\Omega_1 \equiv \frac{\partial y}{\partial \eta} \Rightarrow \Omega_1' = \frac{\partial y'}{\partial \eta}, \tag{14a}$$

$$\psi_1 \equiv \frac{\partial y}{\partial \delta} \Rightarrow \psi_1' = \frac{\partial y'}{\partial \delta}, \tag{14b}$$

$$\Omega_2 \equiv \frac{\partial^2 y}{\partial \eta^2} \Rightarrow \Omega_2' = \frac{\partial^2 y'}{\partial \eta^2}, \tag{14c}$$

$$\phi \equiv \frac{\partial^2 y}{\partial \delta \partial \eta} \Rightarrow \phi' = \frac{\partial^2 y'}{\partial \delta \partial \eta}, \tag{14d}$$

$$\psi_2 \equiv \frac{\partial^2 y}{\partial \delta^2} \Rightarrow \psi_2' = \frac{\partial^2 y'}{\partial \delta^2}. \tag{14e}$$

The variables defined in (14a)–(14e) are obtained by differentiating (1). This results in the following auxiliary ordinary differential equations which must be integrated along with (1);

$$\Omega_1'' = \frac{\partial f}{\partial y} \Omega_1 + \frac{\partial f}{\partial y'} \Omega_1', \tag{15a}$$

$$\psi_1'' = \frac{\partial f}{\partial y} \psi_1 + \frac{\partial f}{\partial y'} \psi_1' + \frac{\partial f}{\partial \delta}, \tag{15b}$$

$$\begin{aligned} \Omega_2'' = {} & \frac{\partial^2 f}{\partial y^2} \Omega_1^2 + 2 \frac{\partial^2 f}{\partial y \partial y'} \Omega_1' \Omega_1 + \frac{\partial^2 f}{\partial y'^2} (\Omega_1')^2 \\ & + \frac{\partial f}{\partial y} \Omega_2 + \frac{\partial f}{\partial y'} \Omega_2', \end{aligned} \tag{15c}$$

$$\begin{aligned} \phi'' = {} & \left[\frac{\partial^2 f}{\partial y^2} \psi_1 + \frac{\partial^2 f}{\partial y' \partial y} \psi_1' + \frac{\partial^2 f}{\partial \delta \partial y} \right] \Omega_1 + \frac{\partial f}{\partial y} \phi \\ & + \left[\frac{\partial^2 f}{\partial y \partial y'} \psi_1 + \frac{\partial^2 f}{\partial y'^2} \psi_1' + \frac{\partial^2 f}{\partial \delta \partial y'} \right] \Omega_1' + \frac{\partial f}{\partial y'} \phi', \end{aligned} \tag{15d}$$

$$\psi_2'' = \left[\frac{\partial^2 f}{\partial y^2}\psi_1 + \frac{\partial^2 f}{\partial y \partial y'}\psi_1' + \frac{\partial^2 f}{\partial \delta \partial y}\right]\psi_1 + \frac{\partial f}{\partial y}\psi_2$$
$$+ \left[\frac{\partial^2 f}{\partial y' \partial y}\psi_1 + \frac{\partial^2 f}{\partial y'^2}\psi_1' + \frac{\partial^2 f}{\partial \delta \partial y'}\right]\psi_1' + \frac{\partial f}{\partial y'}\psi_2'$$
$$+ \frac{\partial^2 f}{\partial y \partial \delta}\psi_1 + \frac{\partial^2 f}{\partial y' \partial \delta}\psi_1' + \frac{\partial^2 f}{\partial \delta^2}. \tag{15e}$$

The initial conditions for these auxiliary equations are derived by differentiating the initial conditions for (1) and (2) and are given by

$$\Omega_1(0) = 1; \qquad \Omega_1'(0) = 0, \tag{16a}$$
$$\psi_1(0) = \psi_1'(0) = 0, \tag{16b}$$
$$\Omega_2(0) = \Omega_2'(0) = 0, \tag{16c}$$
$$\phi(0) = \phi'(0) = 0, \tag{16d}$$
$$\psi_2(0) = \psi_2'(0) = 0. \tag{16e}$$

The solution of (8), (11), and (12) is then obtained by the Newton–Raphson technique, i.e.,

$$\begin{bmatrix} \frac{\partial F_1}{\partial \eta} & \frac{\partial F_1}{\partial \delta} & \frac{\partial F_1}{\partial \varepsilon} \\ \frac{\partial F_2}{\partial \eta} & \frac{\partial F_2}{\partial \delta} & \frac{\partial F_2}{\partial \varepsilon} \\ \frac{\partial F_3}{\partial \eta} & \frac{\partial F_3}{\partial \delta} & \frac{\partial F_3}{\partial \varepsilon} \end{bmatrix} \times \begin{bmatrix} \Delta\eta \\ \Delta\delta \\ \Delta\varepsilon \end{bmatrix} = - \begin{bmatrix} F_1(\delta^i, \eta^i, \varepsilon^i) \\ F_2(\delta^i, \eta^i, \varepsilon^i) \\ F_3(\delta^i, \eta^i, \varepsilon^i) \end{bmatrix}, \tag{17}$$

where the superscript i denotes the iteration, and the parameter values are updated by

$$\eta^{i+1} = \eta^i + \Delta\eta, \tag{18}$$

and similarly for δ and ε. Equation (17) is solved by a simple Gaussian elimination procedure. It is assumed that the Jacobian matrix in (17) is nonsingular.

It is possible by the methods employed above to evaluate the terms in the Jacobian matrix by integrating additional auxiliary equations. The main drawback to doing this is the difficulty of performing the required differentiations of F_3. We chose instead to evaluate the derivatives in this matrix numerically using a simple second-order finite difference scheme. It should be noted that any errors in evaluating these terms affect only the rate of convergence of the iteration, and not the accuracy of the final solution. The accuracy of the solution is determined by the accuracy achieved in integrating the ordinary differential equation system and by the iteration tolerance.

TABLE I

Critical Branching Point Parameter Values

Geometry	δ	η	ε
$j=0$	1.307374	4.896548	0.245780
$j=1$	3.006301	5.943244	0.242106
$j=2$	5.041112	7.184944	0.238797

3. Example

As an example of our scheme, it was applied in [3] to the thermal explosion problem treated in [1, 2]. Also see [3] for a more complete discussion of several other competing explosion models treated, and the implications to the explosion theory. As in [1, 2, 3], the dimensionless steady state heat conduction equation for a semi-infinite slab ($j=0$), an infinite circular cylinder ($j=1$), or a sphere ($j=2$), with an Arrhenius type heat source, can be written

$$y'' + \frac{j}{x} y' + \delta \exp[y/(1+\varepsilon y)] = 0, \qquad 0 < x < 1, \tag{19}$$

subject to the boundary conditions

$$\begin{gathered} y'(0) = 0, \\ \alpha_1 y(1) + \beta_1 y'(1) = \gamma_1. \end{gathered} \tag{20}$$

Our code employs a standard Gear package for integrating the ODE system, and by setting tolerances appropriately, we can obtain accuracies well beyond those justified by any such physical model.

Presented in Table I are the results for the critical branching point parameters of (19) for the cases $j=0, 1, 2$, and with the outer boundary condition $y(1)=0$. These figures are accurate to six significant digits and improve all previously found.

TABLE II

Course of Iteration for Geometry $j=0$

δ	η	ε
1.500000	5.000000	0.250000
1.326116	4.656040	0.248303
1.309016	4.901870	0.245962
1.307368	4.896481	0.245780
1.307374	4.896548	0.245780

Without our general method as put forth herein, extending that of [1], it would be extremely tedious to attempt to find the critical dimensionless activation energy parameter ε (and then the corresponding δ and η) by trial and error.

The rate of convergence of the iterations was unaffected by the approximations used in the Jacobian matrix. From ballpark initial guesses, as shown in Table II for the case $j = 0$, in all three cases $j = 0, 1, 2$ convergence was obtained to the desired accuracy in five or six iterations. This compares favorably to that found in [1].

4. Remarks

In principle our method is general and can be extended to multiple primary and secondary parameters. However, the physical meanings of criticality, the analytical considerations, and the numerical schemes will all be more complicated. Similarly, and perhaps more easily, one can consider more dependent variables (i.e., the R^n case). In all cases the method can fail if the associated initial value problems exhibit numerical instability.

References

1. M. Kubicek and V. Hlavacek, *J. Comput. Phys.* **17** (1975), 79.
2. W. Kordylewski, *Int. J. Numer. Methods Eng.* **17** (1981), 1081.
3. K. Gustafson and B. Eaton, *Z. Angew. Math. Phys.* **33** (1982), 392.
4. R. Courant and F. John, "Introduction to Calculus and Analysis," Vol. 2, Wiley, New York, 1974.

Received: April 14, 1982

Brian Eaton and Karl Gustafson

Department of Chemical Engineering,
Department of Mathematics,
University of Colorado,
Boulder, Colorado 80309