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Note

Finding Singular Points of Two-Point Boundary Value Problems

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1. INTRODUCTION

A number of physically important systems display multiple solutions (see [1] and the references therein). It is of interest to know the dependence of the number of solutions on the parameters in the model. The most powerful techniques for accomplishing this task are the singularity and bifurcation theories [2–4]. These theories require the calculation of special singular solutions. Consider a system described by an algebraic equation

$$F(y, \mathbf{p}) = 0 \tag{1}$$

where y is a scalar variable describing the state of the system and $\mathbf{p}$ is a vector of parameters. A solution is defined to be a singularity of codimension k if it satisfies Eq. (1) and the conditions

$$\frac{d^iF}{dy^i} = 0, \qquad i = 1, 2,..., k \tag{2}$$

$$\frac{d^{k+1}F}{dy^{k+1}} \neq 0. \tag{3}$$

Singularities of codimension 1, 2, 3, 4 are called fold, cusp, swallowtail, and butterfly, respectively. Under certain restrictions, a system has $k+1$ local solutions in some neighborhood of a singularity of codimension k. A technique proposed by Bröcker and Lander [5] and extended by Balakotaiah and Luss [4] enables the use of the singular points to divide the global parameter space $\mathbf{p}$ into regions containing different numbers of solutions.

Singularities of differential equations may be found either directly or by studying the set of algebraic equations resulting from discretization. The direct approach

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uses the Liapunov–Schmidt reduction technique [3] applied to the differential equation and is difficult to apply from a computational standpoint, while the discretized form of a differential equation may not retain all the features of the original equation [6].

We present here a systematic method of finding singularities of a two-point boundary value problem with unmixed boundary conditions. It is based on a technique developed by Michelsen and Villadsen [7] and Kubicek and Hlavacek [8] to compute branching (fold) points and extended by Eaton and Gustafson [9] to find cusp points. These previous efforts used geometric features of the bifurcation diagrams to define the singularities. This made the extension to higher codimension singularities rather cumbersome and difficult. We extend the method so that it can find directly singularities of higher codimension.

2. Determination of a Singular Point of Codimension k

Consider the two-point boundary value problem

$$\frac{d^2y}{dx^2}=f\left(x, y, \frac{dy}{dx}, \mathbf{p}\right), \qquad 0<x<1, \tag{4}$$

$$a_1 y(0)+b_1\frac{dy}{dx}(0)=d_1 \qquad (|a_1|+|b_1|>0), \tag{5}$$

$$a_2 y(1)+b_2\frac{dy}{dx}(1)=d_2 \qquad (|a_2|+|b_2|>0). \tag{6}$$

The shooting method proposed by Keller [10] can be used to solve this problem. In this method, the boundary value problem is converted into an initial value problem by introducing a scalar variable s:

$$\frac{d^2u}{dx^2}=f\left(x, u, \frac{du}{dx}, \mathbf{p}\right) \qquad 0<x<1 \tag{7}$$

$$u(0)=b_1 s-c_1 d_1 \tag{8}$$

$$\frac{du}{dx}(0)=c_0 d_1-a_1 s \tag{9}$$

where we choose c_0 and c_1 such that

$$b_1 c_0-a_1 c_1=1. \tag{10}$$

The second boundary condition is written as an algebraic equation in s:

$$F(s, \mathbf{p}) \triangleq a_2 u(1, s)+b_2\frac{du}{dx}(1, s)-d_2=0. \tag{11}$$

For any assumed value of s we can evaluate the profile $u(x, s)$ as well as the function F by integrating the initial value problem defined by Eqs. (7–9). When F vanishes for a certain s, the corresponding profile $u(x, s)$ is a solution to the boundary value problem. Thus, the solution of the boundary value problem is reduced to finding the zeros of the algebraic equation (11). A singular point of codimension k is found by solving simultaneously Eq. (11) and the k equations

$$\frac{d^iF}{ds^i} = a_2 q_i(1, s) + b_2 \frac{dq_i}{dx}(1, s) = 0 \qquad (i = 1, 2, ..., k) \tag{12}$$

where

$$q_i(x, s) = \frac{d^i u(x, s)}{ds^i}.$$

The functions $q_i(x, s)$ can be found by solving the initial value problems that are obtained when Eqs. (7–9) are differentiated with respect to s:

$$\frac{d^2 q_i}{dx^2} = \frac{d^i}{ds^i}\left[f\left(x, u(x, s), \frac{du}{dx}(x, s), \mathbf{p}\right)\right]$$

$$\triangleq g_i\left(x, u, \frac{du}{dx}, q_1, \frac{dq_1}{dx}, ..., q_i, \frac{dq_i}{dx}, \mathbf{p}\right) \tag{13}$$

$$q_1(0) = b_1; \qquad q_i(0) = 0, \qquad i \geqslant 2 \tag{14}$$

$$\frac{dq_1}{dx}(0) = a_1; \qquad \frac{dq_i}{dx}(0) = 0, \qquad i \geqslant 2. \tag{15}$$

Thus, finding a singular point of codimension k requires the integration of $(k+1)$ initial value problems Eqs. (7–9) and (13–15) and solution of $k+1$ algebraic Eqs. (11) and (12).

We now illustrate the procedure with a specific example.

3. Example

A nonisothermal Langmuir–Hinshelwood reaction occurring in a symmetric catalyst pellet satisfies the dimensionless equation

$$\frac{d^2y}{dx^2} + \frac{n}{x}\frac{dy}{dx} = \frac{\phi^2 y}{(1+Ky)^2} \exp\left\{\gamma\left(1 - \frac{1}{1+\beta(1-y)}\right)\right\} \triangleq h(y, \mathbf{p}) \tag{16}$$

where $\mathbf{p}^T = (\beta, \gamma, K, \phi)$ and the geometric factor n equals to 0, 1, 2 for planar, cylindrical, and spherical geometries, respectively. The boundary conitions are

$$\frac{dy}{dx}(0) = 0 \tag{17}$$

$$y(1) = 1. \tag{18}$$

Brown, Schmitz, and Tsotsis [11] found two butterfly points in the corresponding lumped-parameter system, indicating that two separate regions with five solutions exist in the parameter space. To calculate the butterfly points of the distributed model, boundary condition (18) was chosen as the algebraic equation. Thus,

$$F(s, \mathbf{p}) \triangleq u(1, s) - 1 = 0. \tag{19}$$

We take $b_1 = c_0 = 1$ and $a_1 = c_1 = 0$. To find a butterfly singularity we solve Eq. (19) and the four equations

$$\frac{d^iF}{ds^i} = q_i(1, s) = 0 \qquad (i = 1, 2, 3, 4). \tag{20}$$

Values of $u(1, s)$ and $q_i(1, s)$ are obtained by solving the following five initial value problems:

$$\frac{d^2u}{dx^2} + \frac{n}{x}\frac{du}{dx} = h(u, \mathbf{p}) \tag{21}$$

$$u(0) = s \tag{22}$$

$$\frac{du}{dx}(0) = 0 \tag{23}$$

$$\frac{d^2q_i}{dx^2} + \frac{n}{x}\frac{dq_i}{dx} = g_i\left(u, \frac{du}{dx}, q_1, \frac{dq_1}{dx}, \ldots, q_i, \frac{dq_i}{dx}, \mathbf{p}\right) \tag{24}$$

$$q_1(0) = 1; \qquad q_i(0) = 0 \qquad (i = 2, 3, 4) \tag{25}$$

$$\frac{dq_i}{dx}(0) = 0; \qquad i = 1, 2, 3, 4 \tag{26}$$

where

$$\begin{aligned}
g_1 &= \frac{dh}{du} q_1 \\
g_2 &= \frac{d^2h}{du^2} q_1^2 + \frac{dh}{du} q_2 \\
g_3 &= \frac{d^3h}{du^3} q_1^3 + 3\frac{d^2h}{du^2} q_1 q_2 + \frac{dh}{du} q_3 \\
g_4 &= \frac{d^4h}{du^4} q_1^4 + 6\frac{d^3h}{du^3} q_1^2 q_2 + \frac{d^2h}{du^2}(3q_2^2 + 4q_1q_3) + \frac{dh}{du} q_4.
\end{aligned} \tag{27}$$

TABLE I

Butterfly Points for Nonisothermal Langmuir-Hinshelwood Reaction in a Catalyst Pellet

Geometry	s	β	γ	K	ϕ
Slab ($n=0$)	0.5970	6.466	3.524	4.271	1.282
	0.0684	−0.906	0.259	98.436	89.760
Cylinder ($n=1$)	0.552	6.983	3.601	4.407	1.900
	0.042	−0.926	0.215	137.260	180.940
Sphere ($n=2$)	0.505	7.530	3.672	4.558	2.415
	0.022	−0.945	0.172	212.030	345.870

Note that the scalar variable in this problem corresponds to the concentration of the reactant at the center of the catalyst pellet.

The initial value problems were integrated by a standard Gear package. The resulting algebraic equations were solved by a modified Newton–Raphson method in which the Jacobian matrix was computed numerically. Two butterfly points were found for each of the standard geometries, i.e., infinite slab, infinite cylinder, and sphere. The results are listed in Table I.

4. Finding Singularities for Problems with a Distinguished Parameter

In many physical problems it is important to know the dependence of the steady state solution on a distinguished parameter (bifurcation variable), say λ. The steady state equation in such a case is written as

$$F(y, \lambda, \mathbf{p}^*) = 0 \tag{28}$$

where $\mathbf{p}^*$ is a vector of parameters which are independent of λ. The graph of y versus λ for a fixed $\mathbf{p}^*$ is called a bifurcation diagram. Parameter regions with different types of bifurcation diagrams coalesce at singular points of Eq. (28). These degenerate points are defined by various equalities and inequalities involving partial derivatives of F with respect to y and λ [3]. For example, a pitchfork singularity is defined by

$$F = \frac{\partial F}{\partial y} = \frac{\partial^2 F}{\partial y^2} = \frac{\partial F}{\partial \lambda} = 0 \tag{29a}$$

$$\left(\frac{\partial^3 F}{\partial y^3}\right)\left(\frac{\partial^2 F}{\partial y \partial \lambda}\right) \neq 0 \tag{29b}$$

The technique described in Section 2 may be used to calculte the partial derivatives with respect to λ. To illustrate this consider the boundary value problem

$$\frac{d^2y}{dx^2}=f\left(x, y, \frac{dy}{dx}, \lambda, \mathbf{p}^*\right) \tag{30}$$

and assume (for simplicity) that the boundary conditions do not involve λ and are given by Eqs. (5) and (6). Equation (11) is now rewritten as

$$F(s, \lambda, \mathbf{p}^*) \triangleq a_2 u(1, s, \lambda)+b_2 \frac{du}{dx}(1, s, \lambda)-d_2=0. \tag{31}$$

The partial derivatives are calculated from the relation

$$\frac{\partial^{i+j}F}{\partial s^i \partial \lambda^j} \triangleq a_2 q_{i,j}(1, s, \lambda)+b_2 \frac{dq_{i,j}(1, s, \lambda)}{dx} \tag{32}$$

where

$$q_{i,j}=\frac{\partial^{i+j}u(x, s, \lambda)}{\partial s^i \partial \lambda^j} \tag{33}$$

are found by solving the initial-value problems that are obtained by differentiating Eqs. (5), (6), and (30) w.r.t. s and λ, i.e.,

$$\frac{d^2q_{i,j}}{dx^2}=\frac{\partial^{i+j}}{\partial s^i \partial \lambda^j}\left[f\left(x, u(x, s, \lambda), \frac{du}{dx}(x, s, \lambda), \lambda, \mathbf{p}^*\right)\right] \tag{34}$$

$$q_{1,0}(0)=b_1 \qquad q_{i,j}(0)=0 \qquad i \geqslant 2 \text{ or } j \geqslant 1 \tag{35}$$

$$\frac{dq_{1,0}}{dx}(0)=a_1 \qquad \frac{dq_{i,j}}{dx}(0)=0 \qquad i \geqslant 2 \text{ or } j \geqslant 1. \tag{36}$$

5. Remarks

The proposed technique may be use to compute any singularity for a system described by a two-point boundary value problem which may be solved by the shooting technique. Extensions are possible for systems described by several differential equations but containing only a single intrinsic state variable [12] as well as to systems described by partial differential equations. The computed singular points may be used to divide the parameter space into regions with qualitatively different bifurcation diagrams. Further details may be found in [6].

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