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DEFINING EQUATIONS FOR SINGULAR SOLUTIONS AND NUMERICAL APPLICATIONS

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Singularity theory seems to play an important role not only in the theoretical but also in the numerical analysis of bifurcation problems. In this paper we establish a relation between the concept of a universal unfolding and direct methods for the numerical computation of singular points in bifurcation diagrams. In a direct method the unknown singular solution is computed as a regular solution of a so called defining equation. In particular, we discuss a defining equation for a multiple bifurcation point and demonstrate its application to a reaction diffusion system.

1. Introduction

The numerical computation of singular solutions in bifurcation problems has received special attention recently. We refer to [12] for a survey and comparison of numerical methods for turning points. There are by now also various approaches to more difficult singularities (see the papers of this volume), in particular to cusp points [16, 17] and bifurcation points [15, 13, 18,19,1, 9]. Basically, most of these methods consist in setting up a system of equations - we use the term *defining equations* - which has the unknown singularity as a regular solution. Newton's method for the defining equation would then converge locally and quadratically.

In this paper we present a list of defining equations and we want to demonstrate their relation to the concept of a universal unfolding in singularity theory. We consider a system of equations

(1) $\quad T(z,c) = 0$, where $T \in C^\infty(\mathbf{R}^M \times \mathbf{R}^P, \mathbf{R}^N)$, $M \geq N$.

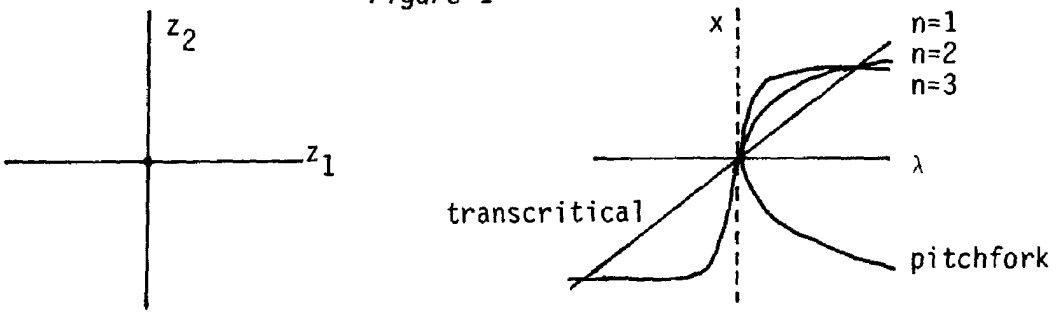
z and c are called the state and the control variable resp. We note that for some of the following definitions and results the operator T need only be defined locally and satisfy less smoothness assumptions. A solution (z_0,c_0) of equation (1) will be called *regular with respect to z* if the Jacobian of T w.r.t. z at (z_0,c_0) has maximum rank, i.e. rank $T_z(z_0,c_0) = N$. Otherwise it is called *singular with respect to z*.

Let (z_0,c_0) be a singular solution of (1) with respect to z. Then one of the fundamental results of singularity theory shows how to obtain in a qualitative way all possible solution sets of (1) in a neighbourhood of z_0 in the state space if c is kept fixed at a value close to c_0. We refer to [6] for a brief account of some ideas and results of standard singularity theory as we use it. The harder parts of the proofs may be found e.g. in [5 , 10]. It should be noted that standard singularity theory is distinct from classical catastrophe theory (which deals with gradient systems $T(z,c) = \nabla_z f(z,c) = 0$, $f \in C^\infty(\mathbb{R}^N \times \mathbb{R}^p, \mathbb{R})$, compare [5 , 14]) and from the "λ-singularity theory" of Golubitsky and Schaeffer [8]. In the approach of [8] there are three types of variables: the state variable x, the bifurcation parameter λ and the control variable c. The (x,λ)-solution branches of a system

$$T(x,\lambda,c) = 0,\ T \in C^\infty(\mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^p, \mathbb{R}^N) \tag{2}$$

are then classified under the restriction that λ-slices are preserved. This turns out to be a refinement of the equivalence classes of singularities which are obtained in the standard theory by setting $z = (x,\lambda)$, $M = N + 1$. For example, the bifurcation points defined by $T_n(x,\lambda) = x(\lambda - x^n) = 0$ $(n \in \mathbb{N})$ are all different in λ-singularity theory, whereas they are equivalent to the simple bifurcation point $T(z_1,z_2) = z_1 z_2 = 0$ in the standard theory.

Figure 1



simple bifurcation point in standard singularity theory

different bifurcation points in λ-singularity theory

Our approach is to compute the bifurcation points of the types in fig. 1 by one and the same defining equation. However, if the particular behaviour of the emanating branches with respect to a bifurcation parameter λ is of interest then one should rather use the defining equations of Spence and Jepson (this volume) which are based on [8].

Our final remark concerns the question whether it is useful to compute more complex singularities at all. Usually, a dynamical system, which has (1) as

its steady state equation, only exhibits drastic changes near the most simple singularities of (1), namely folds (or turning points). As for the higher singularities we rather think of them to play the role of an "organizing center" [7] for the solution diagrams of the steady state equation (1). This aspect has been emphasized in [7 , 1 , 4].

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2. Some fundamentals about singular solutions

For a singular solution (z_0,c_0) of (1) there are at least three important numbers to know:

the *index* $i = M - N$, the *corank* $n = N - \text{rank } T_z(z_0,c_0)$ and

the *codimension* $k \in \mathbb{N} \cup \{\infty\}$.

The codimension measures in some sense the complexity of the singularity and will be explained in detail later on (cf. [6 , V § 2]).

Let (z_0,c_0) be a regular solution of (1) w.r.t. z. Then the solution set of $T(z,c_0) = 0$ in a neighbourhood of z_0 is a smooth $i = M - N$ dimensional manifold. In general, this is no longer true near a singular solution with respect to z. However the solution set of (1) in a neighbourhood of (z_0,c_0) in the complete space $\mathbb{R}^M \times \mathbb{R}^p$ may be smooth again. For example, the equation $z^2 - c = 0$ has a fold w.r.t. z at $z = 0$, $c = 0$ (i.e. a singular solution of index 0) but defines a regular branch in $\mathbb{R} \times \mathbb{R}$. Similarly, $z_1^2 - z_2^2 - c = 0$ has a simple bifurcation point w.r.t. z at $(z_1,z_2) = 0, c = 0$ (i.e. a singular solution of index 1) but defines a regular surface in $\mathbb{R}^2 \times \mathbb{R}$. In what follows, the term "singular" will always mean "singular with respect to the state variable" and we will use the terms "point singularity" if index = 0 and "branch singularity" if index = 1.

The corank n of a singular solution (z_0,c_0) gives the number of equations to which the full system (1) can be reduced by the Liapunov-Schmidt method. The reduced equations are usually called the bifurcation equations. For numerical purposes it is important to note that this reduction may be performed without knowing the null space $N(T_z^o)$ or the range $R(T_z^o)$ (the upper index "o" always indicates the argument (z_0,c_0)).

We start with a decomposition into subspaces

(3) $\mathbb{R}^M = V \oplus W$, $\mathbb{R}^N = X \oplus Y$, where $\dim X = \dim V = N - n$,

and we write $z = (v,w) \in \mathbb{R}^M$, $z_0 = (v_0,w_0)$. From (3) we obtain $\dim Y = n$, $\dim W = M - N + n =: m$. Let $P : \mathbb{R}^N \to X$ be the projector along Y. Our basic assumption is that for some open sets $\Omega \subset V$, $\Gamma \subset W \times \mathbb{R}^p$ the equation

(4) $PT(v,w,c) = 0$, $v \in \Omega$, $(w,c) \in \Gamma$

defines a unique implicit function $v(w,c)$ such that

(5) $PT_v\,(v(w,c),w,c) : V \to X$ is nonsingular.

For example, this is satisfied in some suitable neighbourhoods if $(z_0,c_0) = (v_0,w_0,c_0)$ solves (4) and $PT_v^0 : V \to X$ is nonsingular. In this case $v(w_0,c_0) = v_0$ holds.
The mapping $S : \Omega \times \Gamma \to Y$, defined by

(6) $S(w,c) = (I-P)T(v(w,c),w,c)$

will then be called a *Liapunov-Schmidt reduction of T* w.r.t. (V,W,X,Y).

Theorem 1

Let $(z_0,c_0) = (v_0,w_0,c_0)$ be a solution of (4) where $T \in C^r(\mathbb{R}^M \times \mathbb{R}^p, \mathbb{R}^N)$, $1 \le r \le \infty$ and let $S(w,c)$ be a Liapunov-Schmidt reduction of T with respect to (V,W,X,Y). Further, let $R : V \to X$ be linear and bijective. Then in a neighbourhood $U(z_0,c_0)$ a relation

(7) $\tau(z,c)T(\rho(z,c),c) = (R(v-v_0),\ S(w,c))$, $z = (v,w)$

holds where $\tau(z,c)$ is a C^{r-1}-family of regular $N \times N$-matrices and $\rho \in C^r(U(z_0,c_0),\ U(z_0))$ satisfies $\rho(z_0,c_0) = z_0$, ρ_z^0 nonsingular. Moreover, if (z_0,c_0) is a singular solution of (1) w.r.t. z of corank n then $S(w_0,c_0) = 0$, $S_w(w_0,c_0) = 0$.

Remark: Formula (7) means that in a neighbourhood of a singular solution of corank n the operator T may be decomposed into a regular part R and a singular part S after a parameter dependent change of coordinates in $\mathbb{R}^M$ and $\mathbb{R}^N$ (cf. [8, Lemma 3.13]).

Proof: We drop the control variable c from the proof because it can simply be inserted at each step. By our assumptions the mapping $\sigma(z) = (v_0+R^{-1}PT(z),w)$ satisfies $\sigma(z_0) = z_0, \sigma_z(z_0)$ nonsingular. Hence

$\sigma^{-1}(z) =: \rho(z) = (\rho_1(z),w) \in V \oplus W$ has the same property. By the definition of ρ we have

(8) $\quad R(v-v_0) = PT(\rho(z)),\ z = (v,w).$

Setting $v = v_0$ in (8) we obtain $\rho_1(v_0,w) = v(w)$ from (4) and hence

(9) $\quad S(w) = (I-P)T(\rho(v_0,w)).$

Now let $\tau(z)$ be given by its representation $\begin{pmatrix} I & 0 \\ \tau_{21}(z) & I \end{pmatrix}$ with respect to $X \oplus Y$ where τ_{21} will be defined below.
Then (8) yields

$$\tau(z)T(\rho(z)) = (R(v-v_0),\ \tau_{21}(z)R(v-v_0) + (I-P)T(\rho(v,w))).$$

Expanding the last term to first order in v and using (9) we end up with the relation (7) if we set

$$\tau_{21}(z) = -\int_0^1 (I-P)T_z(\rho(v_0+t(v-v_0),w))\rho_v(v_0+t(v-v_0),w)R^{-1}dt.$$

Finally, $S(w_0,c_0) = 0$, $S_w(w_0,c_0) = 0$ are easy consequences of (7) if (z_0,c_0) is a singular solution of corank n. □

The effect of theorem 1 is to concentrate the singular part of T into a low dimensional mapping $G(w) = S(w,c_0)$. In the following we need some basic notations from singularity theory [6, V]. Let $E_m^n = C^\infty(\mathbb{R}_0^m, \mathbb{R}^n)$ be the linear space of C^∞-germs defined in a neighbourhood of $0 \in \mathbb{R}^m$ with values in $\mathbb{R}^n$. Similarly, $E_m^{n,n} = C^\infty(\mathbb{R}_0^m, \mathbb{R}^{n,n})$ contains the C^∞-germs with values in the space $\mathbb{R}^{n,n}$ of n×n-matrices. Two germs $G_1, G_2 \in E_m^n$ are called *contact equivalent*, if a relation

(10) $\quad G_1(w) = \tau(w)G_2(\rho(w))$

holds for some $\tau \in E_m^{n,n}$, $\rho \in E_m^m$ with $\rho(0) = 0$ and $\rho_w(0), \tau(0)$ nonsingular. This essentially means that the solution sets of $G_1(w) = 0$ and $G_2(w) = 0$ near 0 are diffeomorphic. The result of theorem 1 may then be reformulated as the contact equivalence of the germs $T(z_0+\cdot,c)$ and $R \otimes S(w_0+\cdot,c)$.
A germ $F \in E_{m+1}^n$ is called an *l-parameter unfolding* of $G \in E_m^n$ iff $G(w) = F(w,0)$. It is called a *versal unfolding* of G if every j-parameter unfolding $H \in E_{m+j}^n$ of G satisfies $H(w,\beta) = \tau(w,\beta)\ F(\rho(w,\beta),\psi(\beta))$ for some $\tau \in E_{m+j}^{n,n}$, $\rho \in E_{m+j}^m$, $\psi \in E_j^1$ such that $\tau(w,0) = I, \rho(w,0) = w$ and $\psi(0) = 0$ (i.e. the germs $H(\cdot,\beta)$ and $F(\cdot,\psi(\beta))$ are contact equivalent). A versal unfolding of G with a minimum number of parameters is said to be *universal*.

For the determination of a universal unfolding of G one needs the so called *tangent space*

$$(11) \qquad TG = \{\tau G + G_w\sigma : \tau \in E_m^{n,n},\ \sigma \in E_m^m\} \subset E_m^n.$$

TG is a linear space over $\mathbb{R}$ as well as a module over E_m^1. The number $k = \operatorname{codim} TG = \dim E_m^n/TG \in \mathbb{N} \cup \{\infty\}$ is the *codimension of the germ G* at 0. It is invariant under contact equivalence. Let us assume that G has finite codimension k and let $F(w,\alpha)$ be a k-parameter unfolding of G. Then the fundamental theorem on universal unfoldings [6, V § 3] states that F is universal if and only if the *transversality condition*

$$(12) \qquad TG + \mathbb{R}\{F_{\alpha_1}(\cdot,0),\ldots,F_{\alpha_k}(\cdot,0)\} = E_m^n$$

is satisfied. This condition means that the germs $F_{\alpha_j}(w,0)(j=1,\ldots,k)$ form a basis of E_m^n/TG.

It is worth noting that the codimension of a singularity of (2) in the theory of [8] is always greater than or equal to the standard codimension obtained by setting $z = (x,\lambda)$, $M = N + 1$.

3. Defining equations for singular solutions of low dimensional systems

We want to set up a system of equations which determines singular solutions (z_0,c_0) of (1) of a given corank n and a given codimension k. As we will see in section 5, this task can be reduced by theorem 1 to the determination of a singular solution (w_0,c_0) w.r.t. w of codimension k for a low dimensional system

$$(13) \qquad G(w,c) = 0,\ G \in C^\infty(\mathbb{R}^m \times \mathbb{R}^p, \mathbb{R}^n) \text{ with index } i = m - n \geq 0.$$

The prescribed codimension k suggests that we have to have at least $p \geq k$ parameters in (13) in order to find a singular solution of codimension k. In fact, we assume $p = k$ in (13). This can always be achieved by either fixing some control variables or inserting new ones (these should be of physical relevance for the underlying system).

A square system of equations

$$(D) \qquad D_G(w,c) = 0, \text{ where } D_G \in C^\infty(\mathbb{R}^{m+k}, \mathbb{R}^{m+k})$$

will then be called a *defining equation* for G if it has the following property

(P) P1: (w_0,c_0) is a regular solution of (D) $\Longleftrightarrow$
P2: (w_0,c_0) is a singular solution of $G(w,c) = 0$ w.r.t. w, it is of corank n and $G(w_0+w,c_0+c)$ is a universal unfolding of $G(w_0+w,c_0)$.

This is a rather strong requirement. For example, if we have computed a regular solution (w_0,c_0) of (D) then we are sure that the variation of c around c_0 will exhibit all possible solution pictures (up to diffeomorphisms) in the state space $\mathbf{R}^m$. The introduction of additional parameters in (13) will not create new phenomena. In the following table of defining equations the property (P) is satisfied in the strict sense only in the case of corank 1. For the corank 2 singularities some additional nondegeneracy conditions (A2), (A3) have to be added to P1 in order to make (P) correct.

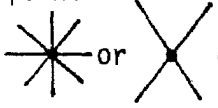
i	n	k	$D_G(w,c)$	name	representative germs $G(w,0)$ near $w = 0$
0	1	k	$(G,G_w,\ldots,G_{wk})$ where $G_{wk} = \frac{\partial^k G}{\partial w^k}$	fold (k=1), cusp (k=2) swallow-tail (k=3) butterfly (k=4)	w^{k+1}
0	2	4	(G,G_w) (A2)		$\begin{pmatrix} w_1^2 \\ w_2^2 \end{pmatrix}$, $\begin{pmatrix} w_1^2 \pm w_2^2 \\ w_1 w_2 \end{pmatrix}$
1	1	1	(G,G_w)	simple bifurcation point or isola center (hermit)  or •	$w_1^2 \pm w_2^2$
1	1	2	$(G,G_w, \det G_{ww})$	cusp curve 	$w_1^2 - w_2^3$
1	2	5	(G,G_w) (A3)	multiple bifurcation point  or •	$\begin{pmatrix} w_1^2 \pm w_2^2 \\ w_2^2 \pm w_3^2 \end{pmatrix}$, $\begin{pmatrix} w_1^2 + w_2^2 - w_3^2 \\ -2w_1 w_3 + w_3^2 \end{pmatrix}$

table 1

(Am) ($m = 2,3$) the homogeneous quadratic $q(w) = \frac{1}{2}G_{ww}(w_0,c_0)w^2$ satisfies $q(\tilde{w}) = 0$, $\tilde{w} \in \mathbb{C}^m$, $\tilde{w} \neq 0 \Rightarrow q_w(\tilde{w})$ has rank 2 over $\mathbb{C}$.

(A2) means that the conic sections $q_i(w) = 0$ ($i=1,2$) are nowhere tangent in $\mathbb{C}^2$ except at 0, or what is the same, q_1 and q_2 have no common factor. Similarly, (A3) means that the quadratic surfaces $q_i(w) = 0$ ($i=1,2$), $w \in \mathbb{C}^3$ are nowhere tangent except at 0. We note that the real version of (A3) is a well known assumption in the study of bifurcation at a double eigenvalue [11, 8, § 5] (the use of (A3) with $\mathbb{R}$ instead of $\mathbb{C}$ is sufficient in [8, § 5] because of the special way in which $\lambda = w_3$ enters into the problem there).
Table 1 shows that a defining equation does usually not determine a unique class but several classes of contact equivalent singularities. These were indicated by some simple representatives in the last column.

The proof of property (P) for all entries of table 1 would be too long, so here we restrict ourselves to the question for which n and m

(14) $D_G(w,c) = (G,G_w)(w,c) = 0$, $G \in C^\infty(\mathbb{R}^m \times \mathbb{R}^k, \mathbb{R}^n)$

is a defining equation. In order to make (14) a square system we need $k = n + nm - m$.

Theorem 2:
Let $n \leq m$, $k = k(n,m) = n + nm - m$ and let $G \in C^\infty(\mathbb{R}^m \times \mathbb{R}^k, \mathbb{R}^n)$. Then P2 implies P1. If P1 is assumed then (w_0,c_0) is a singular solution of (13) w.r.t. w which is of corank n and codimension $\geq k$. If the codimension is equal to k, then $G(w_0 + w, c_0 + c)$ is a universal unfolding of $G(w_0 + w, c_0)$ and the pair (n,m) must be one of the following

(15) either ($n = 1$, $m \in \mathbb{N}$) or ($n = 2$, $m \in \{2,3\}$).

Remark: We have the somewhat surprising result that (14) satisfies the property (P) only for some restricted values of n and m. This should be due to the occurrence of so called modal parameters (cf. [8, § 4,5]).

Proof: Without loss of generality we may assume $(w_0,c_0) = (0,0)$. Let P2 be satisfied. Then obviously $G^0 = 0$ and rank $G^0_w = 0$ hold, hence $D^0_G = 0$. Moreover, we have

$$(16)\qquad D_G'^0 = \begin{pmatrix} G_w^0 & G_c^0 \\ G_{ww}^0 & G_{wc}^0 \end{pmatrix} = \begin{pmatrix} 0 & G_c^0 \\ G_{ww}^0 & G_{wc}^0 \end{pmatrix} .$$

By the transversality condition (12) each $q \in E_m^n$ may be written as

$$(17)\qquad q(w) = \tau(w)G(w,0) + G_w(w,0)\sigma(w) + G_c(w,0)\gamma$$

for some $\tau \in E_m^{n,n}$, $\sigma \in E_m^m$, $\gamma \in \mathbb{R}^k$. Evaluating q and q_w at $w = 0$ yields

$$(18)\qquad \begin{pmatrix} q(0) \\ q_w(0) \end{pmatrix} = \begin{pmatrix} G_c^0\gamma \\ G_{ww}^0\sigma^0 + G_{wc}^0\gamma \end{pmatrix} = D_G'^0 \begin{pmatrix} \sigma^0 \\ \gamma \end{pmatrix} .$$

Since the left hand sides span $\mathbb{R}^{n+nm}$ we obtain that $D_G'^0$ is nonsingular. Assume now that P1 is satisfied. If a relation (17) holds with $q \equiv 0$ then we find $\sigma^0 = 0$, $\gamma = 0$ from (18) and the regularity of $D_G'^0$. Thus we have shown that the functions $G_{cj}(\cdot,0)$ $(j=1,\ldots,k)$ are linearly independent in $E_m^n/TG(\cdot,0)$. The codimension of $G(\cdot,0)$ at 0 is therefore at least k and in case of equality $G(w,c)$ is a universal unfolding of $G(w,0)$ since (12) is satisfied. It remains to prove (15). Let $Q_2 \subset E_m^n$ be the linear subspace of homogeneous quadratics. Each $q \in Q_2$ has a representation (17). From (18) we again find $\sigma^0 = 0, \gamma = 0$ and differentiating (17) twice at $w = 0$ yields

$$(19)\qquad q_{i,ww}^0 = \sum_{j=1}^n \tau_{ij}^0 G_{j,ww}^0 + G_{i,ww}^0 \sigma_w^0 + \sigma_w^{0T} G_{i,ww}^0 \quad (i=1,\ldots,n).$$

We consider this as a linear system for the $n^2 + m^2$ unknowns τ^0 and σ_w^0. Since the left hand sides of (19) span a linear space of dimension $\frac{1}{2}nm(m+1) = \dim Q_2$ we obtain $\frac{1}{2}nm(m+1) \le n^2 + m^2$. But the homogeneous equation (19) also admits the nontrivial solution $\tau^0 = -2I$, $\sigma_w^0 = I$ so that in fact $\frac{1}{2}nm(m+1) \le n^2 + m^2 - 1$. An elementary discussion of this inequality using $n \le m$ then leaves us with the cases given in (15). □

In the case $n = 1$, $m \in \mathbb{N}$ the proof of property (P) is easily completed. Let us assume P1. Now we have $k = k(1,m) = 1$ and from (16) and the regularity of $D_G'^0$ we find that the Hessian G_{ww}^0 is nonsingular. By the Morse lemma $G(w,0)$ is then contact equivalent to a quadratic $\sum_{i=1}^m \varepsilon_i w_i^2$, $\varepsilon_i \in \{-1,1\}$ and hence has codimension 1 (cf. [6, IV § 4]). The assertion P2 then follows from theorem 2.

In the case $n = 2$, $m \in \{2,3\}$ we assume P1 and (Am) and define $F(w) = \frac{1}{2} G_{ww}^0 w^2$, $w \in \mathbb{R}^m$. After some algebraic manipulations, which we omit, the property (Am) turns out to be equivalent to

(20) for each $q \in Q_2$ there exist matrices $A \in \mathbb{R}^{2,2}$, $B \in \mathbb{R}^{m,m}$ such that $q(w) = A\,F(w) + F_w(w)\,Bw$, $w \in \mathbb{R}^m$.

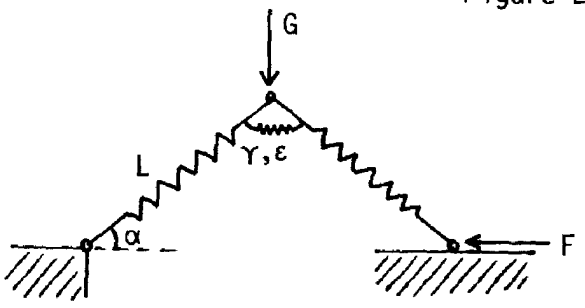
Since F agrees with $G(\cdot,0)$ to second order we obtain from (20)
$q(w) = A\,G(w,0) + G_w(w,0)\,Bw + O(\|w\|^3)$.
This result may be written in a more formal way as $M^n_{2,m} \subset TG(\cdot,0) + M_m \cdot M^n_{2,m}$ where $M^n_{2,m}$ is the module generated by Q_2 in E^n_m and M_m is the maximal ideal in E^1_m which is generated by the germs $w \to w_i$ $(i=1,\ldots,m)$. The lemma of Nakayama [6, IV § 2] then ensures $M^n_{2,m} \subset TG(\cdot,0)$. Therefore, a basis of $E^n_m/M^n_{2,m}$, which consists of $nm + n$ linear germs, also spans $E^n_m/TG(\cdot,0)$. By the regularity of $D^{1,0}_G$ we have $G^0_{ww}\,\gamma = 0$, $\gamma \in \mathbb{R}^m \Rightarrow \gamma = 0$. This proves that the linear functions $p_i(w) = G^0_{ww}\,e^i w$ $(i=1,\ldots,m, e^i = i\text{-th unit vector in } \mathbb{R}^m)$ are linearly independent. Moreover $p_i(\cdot) = F_w(\cdot)e^i = G_w(\cdot,0)e^i + (F_w(\cdot) - G_w(\cdot,0))e^i \in TG(\cdot,0) + M^n_{2,m} \subset TG(\cdot,0)$, $i=1,\ldots,m$ so that finally $\dim E^n_m/TG(\cdot,0) \le nm + n - m = k$. Again theorem 2 completes the proof of P2.

Let us finally notice that the nontrivial solutions $\hat{w} \in \mathbb{R}^3$ of $G_{ww}(w_0,c_0)\hat{w}^2 = 0$ determine the bifurcation directions in the case $m = 3$. Due to (A3) there are either 0,2 or 4 branches passing through w_0.

4. Two applications

Our first example describes the buckling of a spring (fig. 2) and is taken from [14,§13.8] (with the exception of the parameter ε).

Figure 2



G,F : load parameters,
γ,ε : spring constants
α,L ; state variables

The total energy of the system is

$$U(\alpha,L;\ G,F,\gamma,\varepsilon) = \tfrac{1}{2}\gamma(2\alpha)^2 + \tfrac{1}{3}\varepsilon(2\alpha)^3 + (L-1)^2 + FL\cos\alpha + GL\sin\alpha\,.$$

From $U_\alpha = U_L = 0$ we can eliminate L and we find for the stationary states the scalar equation

(21) $$T(\alpha,G,F,\gamma,\varepsilon) = 4\gamma\alpha^2 + 8\varepsilon\alpha^3 + G\cos\alpha - 2F\sin\alpha - GF\cos 2\alpha + (F^2 - \frac{1}{4}G)^2 \sin 2\alpha = 0.$$

This system has a butterfly point w.r.t. α at

(22) $$\alpha = 0;\ G = 0,\ F = \frac{1}{4},\ \gamma = \frac{3}{32},\ \varepsilon = 0 \quad \text{(see [14])},$$

where the four parameters provide a universal unfolding. Figure 3 shows a portion of the solutions in the (α,G,F)-space at fixed values $\gamma = 0.11$, $\varepsilon = 10^{-3}$. It also shows how we approached the butterfly point (22) numerically by solving the defining equations $(T,T_\alpha,\ldots,T_{\alpha k}) = 0$ for increasing k. Starting with a regular solution ($\alpha = 1.8785$, $G = 0$, $F = 0.4$) we computed a branch of regular solutions (r) by varying G. Then we switched to the defining equation of the fold $(T,T_\alpha)(\alpha,G) = 0$ and computed a branch of folds (f) by varying F. Proceeding in this way we obtained a branch of cusps (c) and swallow tails (s) which finally ends at the butterfly point (b).

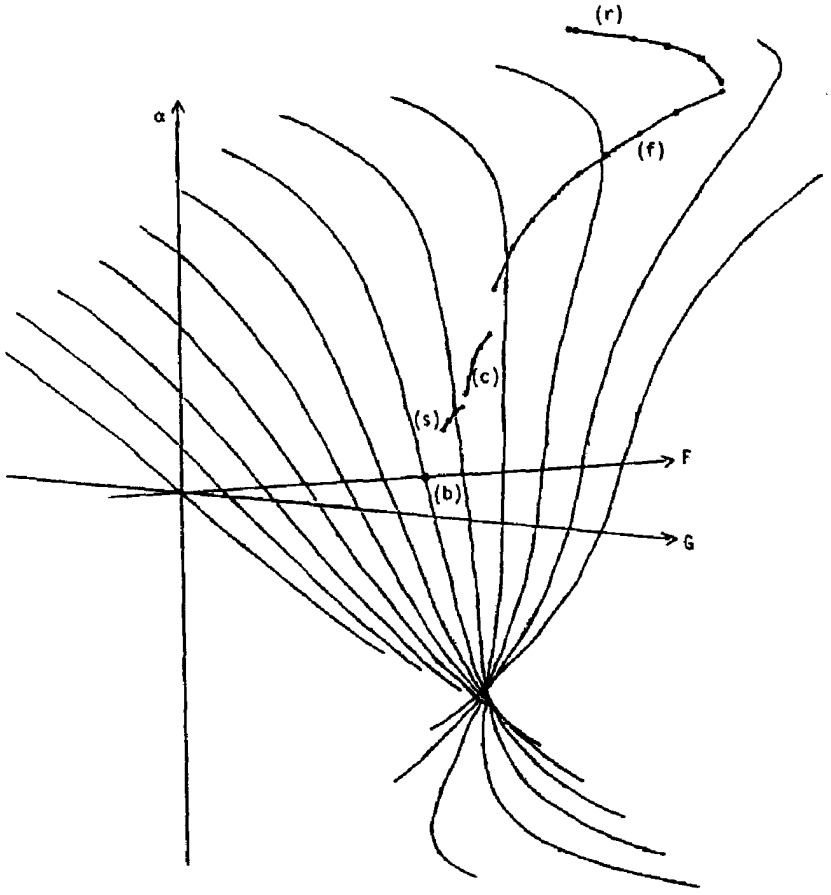


Figure 3

the jumps between the curves (r), (f), (c) and (s) are caused by the switching to the next defining equation

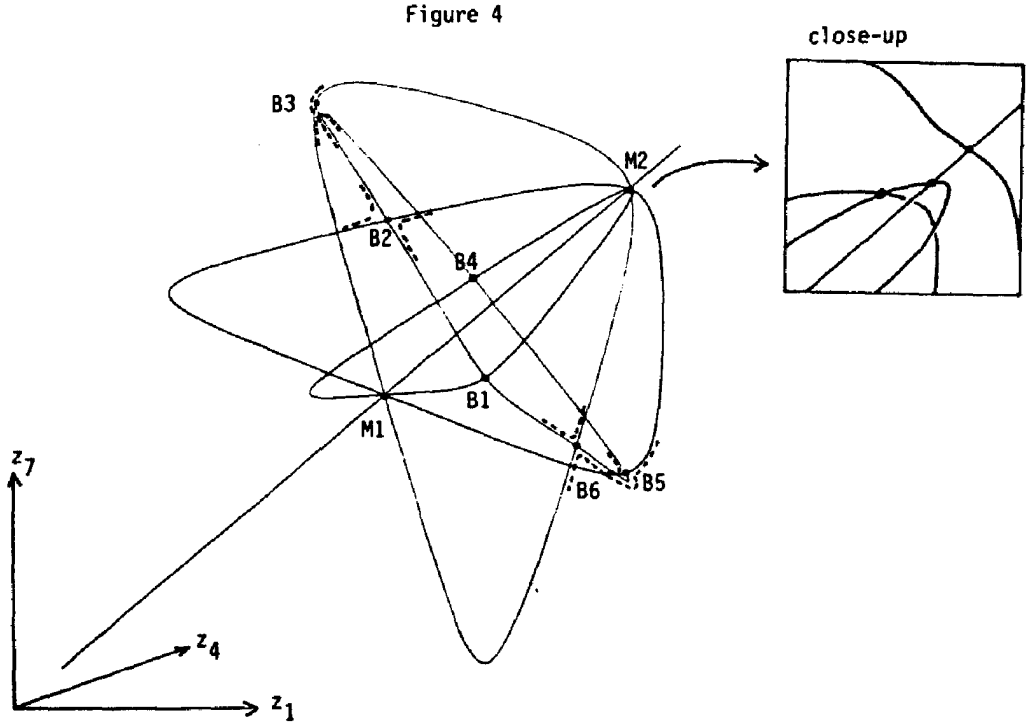
Our second example is an N-cell model with diffusion and reaction as discussed in detail in [2, 3]. The steady state equations are of the following form

$$(23)\qquad D_j(z_j-z_{j-1}) - D_{j+1}(z_{j+1}-z_j) + d_j z_j = h_j g(c_o-z_j,\lambda,\mu),\ j=1,\ldots,N$$
$$z_o = z_{N+1} = 0 \quad \text{where } z_j = c_o - c_j$$

and c_j (resp. c_o) = substrate concentration in the j-th cell (resp. outer reservoir), $D_j(d_j)$ = diffusion constant between the j-th cell and the (j-1)-th cell (the outer reservoir), h_j = thickness of the j-th cell, $g(x,\lambda,\mu) = 10^{\mu}x(1+x+\lambda x^2)^{-1}$ = reaction rate of an inhibited Michaelis-Menten process. The cells with numbers 0 and N+1 should be interpreted as part of the reservoir. Since we are interested in the branches generated by varying λ we set $z = (z_1,\ldots,z_N,\lambda)$, $c = (D_1,\ldots,D_{N+1},d_1,\ldots,d_N,h_1,\ldots,h_N,\mu)$ and write (23) in the form (1) with M = N+1.

Here we consider a special case of 7 cells where 3 cells are in contact with the outer reservoir ($D_j = 0.3$(j=2,...,7), $D_1 = D_8 = 1$, $d_4 = 2$, $d_j = 0$ otherwise, $h_4 = 2$, $h_j = 1$ otherwise, $c_o = 4$, $\mu = 1.4$). A three-dimensional view of the numerical solution branches in the (z_1,z_4,z_7)-space is shown in fig. 4.

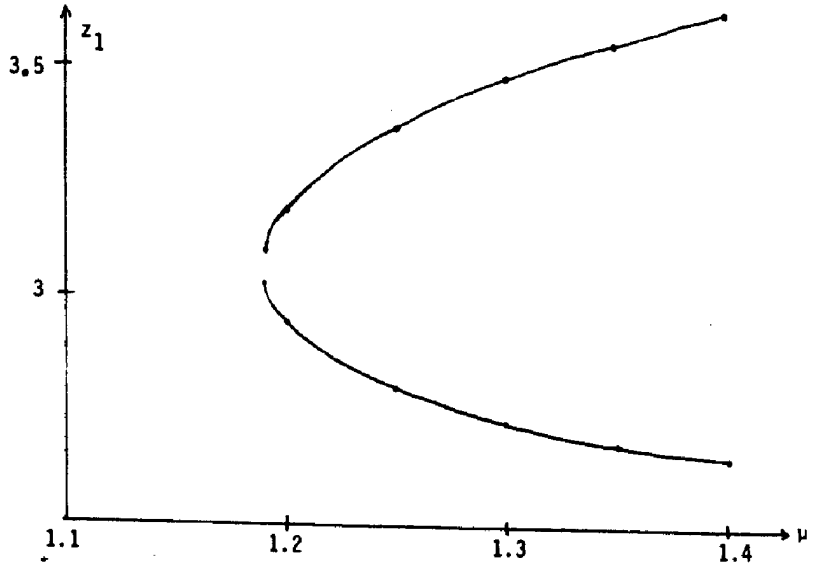
Figure 4



The numerical results suggest 6 simple bifurcation points (B1 - B6) and 2 multiple bifurcation points (M1, M2). However, a closer look at the

continuation procedure near these points reveals that only B1 and B4 are bifurcation points (which we have computed by the defining equations of section 3) whereas the others are actually separated as indicated by the dotted lines in fig. 4. Moreover, near M1 and M2 there are in fact 3 closely spaced simple bifurcation points as shown in the close up of fig. 4. These could only be determined by using very good initial guesses for the defining equation. A more detailed explanation of the branching structure in fig. 4 which uses the inherent symmetries in equation (23) is given in [4].
By table 1 we expect to find true multiple bifurcation points near M1, M2 if we let 5 parameters vary in the system (23). We used $c_1 = d_1$, $c_2 = d_4$ and the perturbations $c_3 z_4$, $c_4 z_7$, $c_5 z_1$ in the equations (23) with the numbers 1, 4, 7 respectively. Newton's method for the defining equation was then successful when started near M1, M2 and multiple bifurcation points with 4 bifurcation directions were detected (see section 5 for details of the reduction process). By varying the parameter μ we then found an upper and a lower branch of multiple bifurcation points (fig. 5). These seem to coalesce at a new singularity the type of which we do not know at present.

Figure 5



5. The reduction process

In order to compute a singular solution of the system (1) which is of codimension $k = p$ we apply the defining equations from table 1 to a Liapunov-Schmidt reduction $S(w,c)$ of T w.r.t. (V,W,X,Y), i.e. we solve

(24) $\quad D_S(u) = D_S(w,c) = 0,\ u = (w,c) \in W \oplus \mathbb{R}^k\ (\cong \mathbb{R}^{m+k})$.

If D_S has the property (P) and if the assumptions of theorem 1 hold then theorem 1 can be used to prove the following: (w_0,c_0) is a regular solution of (24) $\Leftrightarrow$ $(z_0,c_0) = (v(w_0,c_0),w_0,c_0)$ is a singular solution of (1) of corank n and $T(z_0+z,c_0+c)$ is a universal unfolding of $T(z_0+z,c_0)$.

We used a two stage process for the numerical solution of (24). This will only be briefly outlined here since less costly methods are available for special singularities [12, 9, 19]. In particular, in [9] singular solutions of corank 1 and of codimension 1 but of arbitrary index (these have the defining equation $(G,G_w) = o$, compare section 3) are obtained in an efficient way by solving (1) together with a set of M+1-N scalar equations which characterize the points where rank $T_z = N - 1$.

Suppose D_S involves the derivatives $S, S_w,\ldots,S_{wr}$ (r=1 in most cases), then one Newton step for the system (24) needs S(u) and the derivatives $S_{wju}(u)(j=0,\ldots,r)$. We always used coordinate subspaces for V,W,X,Y and a few Newton steps for (4) in order to obtain a good approximation to v(w,c)=v(u) and hence to S(u) from (6). Differentiating (6) with respect to w and u shows that S_{wju} is of the form

$$(25) \qquad S_{wju} = (I-P)(T_v\, v_{wju} + \kappa_j),\ j = 0,\ldots,r.$$

Here we have suppressed the arguments and denoted by κ_j all terms which involve only lower order derivatives of the implicit function v(u). The expressions for κ_j get more and more complicated, for example $\kappa_0 = T_u$, $\kappa_1 = T_{wv}v_u + T_{vv}v_w v_u + T_{uv}v_w + T_{uw}$. The derivatives v_{wju} are computed from the linear systems

$$(26) \qquad (PT_v)\ v_{wju} = -P\kappa_j\ (j = 0,\ldots,r)$$

which are obtained by differentiating $PT(v(u),u) = 0$. It is worth noting that the same matrix $PT_v(v(u),u)$ appears in all systems (26) so that one LU-factorization is sufficient. Moreover, our reduction process is essentially independent of the special form of the defining equation (24).

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