NUMERICAL ANALYSIS OF SINGULARITIES IN A DIFFUSION REACTION MODEL

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Abstract: In a recent paper, Bigge and Bohl [2] found some interesting bifurcation diagrams for a discrete diffusion reaction model. We give an interpretation of their results from the view of singularity theory and we will also indicate how this theory may be used to set up numerical methods for singular solutions such as bifurcation points or isolated points.

1. Introduction. This paper is intended to show how singularity theory (e.g. [4, 5, 6]) may help to understand bifurcation diagrams that have been obtained numerically for a finite dimensional system of N equations in N+1 variables

(1) $T(z) = 0,\ T : \mathbb{R}^{N+1} \to \mathbb{R}^N$, z = state variable.

In contrast to the standard situation in the theory we assume that we do neither know the singularity of (1) (i.e. a point $z_0 \in \mathbb{R}^{N+1}$ such that $T(z_0) = 0$, rank $(T'(z_0)) < N$) nor do we know its type. Moreover, we are usually not even given a system (1) which has a singularity, but rather a parametrized system of equations

(2) $T(z,c) = 0,\ T : \mathbb{R}^{N+1} \times \mathbb{R}^P \to \mathbb{R}^N$, c = control variable

for which solution diagrams have been computed for various values of c. The problem then is to guess from these data the type of a singularity z_0 of $T(z,c_0) = 0$, where c_0 is close to the numerical c-values. The choice of a correct singularity depends on its universal unfolding (cf. [5,6]) which should generate in a qualitative way the bifurcation pictures which have been observed numerically. Once a proper singularity is detected we can use the theory of unfolding to predict further types of solution curves of the system (2) and try to find them numerically by varying c.

We will illustrate this process for a specific example recently discussed in [2]

(3)
$$x_1 = x_N = 0 \text{ and for } i = 2,\dots,N-1$$
$$h^{-2}(-x_{i-1} + 2x_i - x_{i+1}) + \nu h^{-1}(x_i - x_{i-1}) = 10^{\mu}(\beta - x_i)\exp\left(-\frac{\lambda}{1+x_i}\right)$$

where $h = (N-1)^{-1}$. We put (3) into the form (2) by setting

(4) $z = (x_1, x_2, \dots, x_N, \lambda),\ c = (\nu,\mu,\beta)$.

The system (3) may either be viewed as a discrete cell model with diffusion and an exothermic reaction or as a discretization of a corresponding boundary value problem ([2, 3]). Our special singularity proposed here is based on the results of [2] and should also appear in the more general equations described therein.
Finally, we show how the above interplay of singularity theory and numerical computations can be made more rigorous. The crucial point here is to actually compute a singularity as a solution of a so called defining equation (cf. the inflated systems for bifurcation points in [7, 10]). In the case of bifurcation points and isolated points we will present some defining equations and show their relation to singularity theory.

Acknowledgement: I am particularly indebted to Dipl. Math. J. Bigge for providing me with several solution branches of the example (3) which are not contained in [2].

2. Finding and analysing the singularity in the discrete model

Let us first recall some solution branches of (3) from [2] as given in figure 1 for the values $N = 11$, $\nu = 0$, $\mu = 7$ and $\mu = 12$, $\beta = 1$.

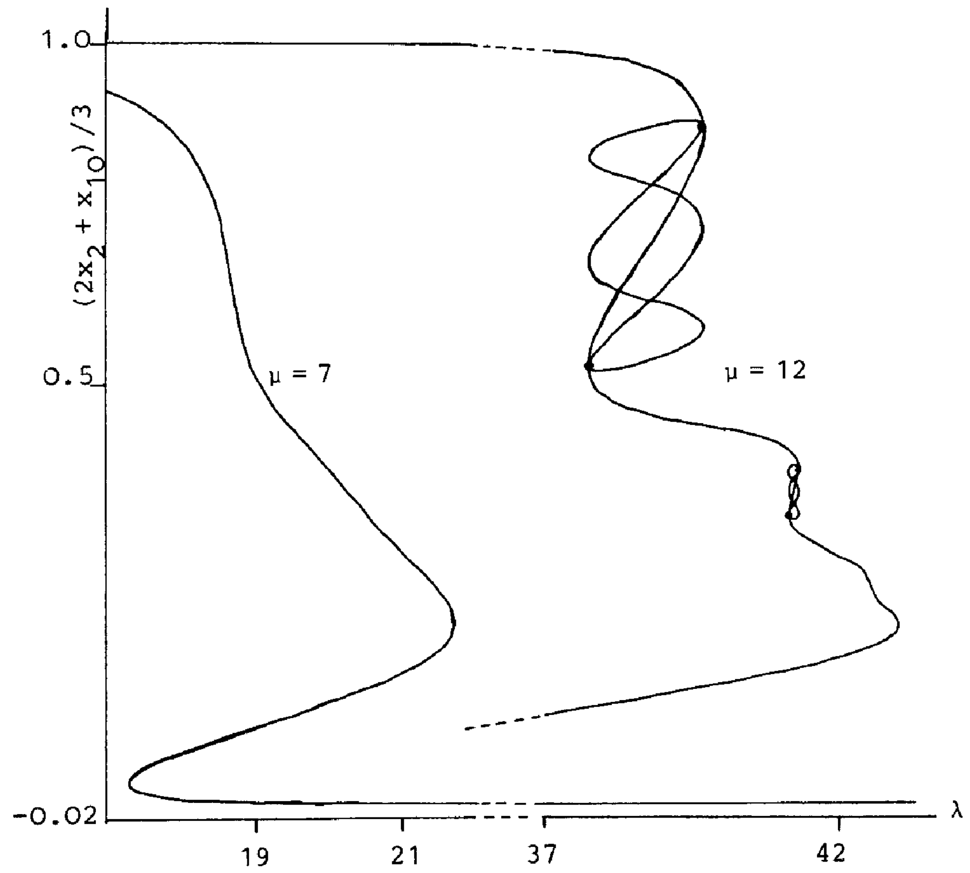

Fig. 1: solutions of (3) for $\mu = 7,12$

We are interestd in the upper configuration for $\mu = 12$ which was called a double-figure-eight in [2]. Here the main branch of symmetric solutions (i.e. $x_i = x_{N+1-i}$ $\forall i$) is intersected by a closed loop of unsymmetric solutions at two bifurcation points (marked by a dot). The topological type of these branches is more clearly seen when projecting them onto a (x_{10},x_2)-plane as is done in figure 2.

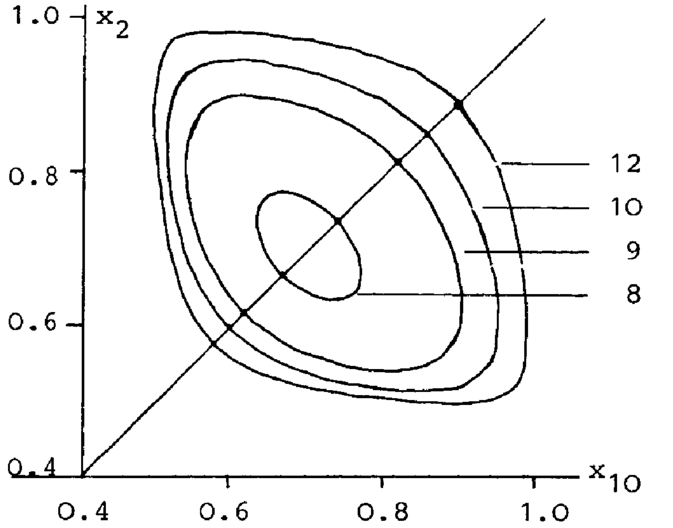

Figure 2: projection of the double-figure-eight onto (x_{10},x_2) for various values of μ.

The symmetric branch now covers the diagonal and the loops of unsymmetric solutions shrink as μ decreases. At $\mu = 7$ they have vanished.

We draw the following conclusion from these pictures. There should exist a set of parameters

$$c_o = (0,\ \mu_o,\ 1) \text{ where } 7 < \mu_o < 8$$

and a singularity z_o of (3) at $c = c_o$ such that an upward perturbation of μ instantaneously creates the bifurcation diagram of fig. 2.

In order to find the type of the singularity we use the model equations

(5) $\lambda = x^3 - ax + b,\ \lambda = y^3 - cy + d,\ a,b,c,d > 0$

which were derived in [2] from the numerical values and shown to create the double-figure-eight as well as some of its perturbations. Upon eliminating λ from (5) and setting $a = b = c = d = 0$ we end up with

(6) $f(x,y) := x^3 - y^3 = 0,$

which has $(x,y) = (0,0)$ as a singularity.

Our hypothesis is that (6) gives the correct type of the singularity z_o for the equation $T(z,c_o) = 0$. More precisely, we assume that there exists a relation

(7) $\tau(z)T(\rho(z),c_o) = (f(z_1,z_2),z_3,\ldots,z_{N+1}) \quad \forall z \in U(0) \subset \mathbb{R}^{N+1}$

where $\rho \in C^\infty(U(0), U(z_o))$ is diffeomorphic, $\rho(0) = z_o$ and $\tau(z)$ are nonsingular $N \times N$-matrices infinitely differentiable with respect to z. Here and in what follows $U(0)$, $U(z_o)$ and $U(c_o)$ denote suitable neighbourhoods not always the same at different occurrences. In terms of singularity theory, the relation (7) states the (contact-) equivalence of the germs associated with $T(\cdot,c_o)$ and $f(\cdot,\cdot) \times I_{N-1}$ where I_{N-1} denotes the identity in $\mathbb{R}^{N-1}$ (cf. the V-isomorphy in [6, Ch.II]).

Our first conclusion from (7) is a generalized relation

(8) $\tilde{\tau}(z,c)T(\tilde{\rho}(z,c),c) = (\tilde{f}(z_1,z_2,c),z_3,\ldots,z_{N+1}) \ \forall z \in U(0), c \in U(c_o)$

where $\tilde{\rho} \in C^\infty(U(0) \times U(c_o), U(z_o))$, $\rho(\cdot,c)$ are diffeomorphisms, $\tilde{\tau}(z,c)$ are nonsingular $N \times N$-matrices with C^∞-entries and $\tilde{f}$ is an unfolding of f, i.e. $\tilde{f}(z_1,z_2,c_o) = f(z_1,z_2) \ \forall z \in U(0)$. To see this, define $g \in C^\infty(U(0) \times U(c_o),\mathbb{R})$ and $\Phi \in C^\infty(U(0) \times U(c_o), \mathbb{R}^{N-1})$ by $\tau(z)T(\rho(z),c) = (g(z,c), \Phi(z,c))$ and use the implicit function theorem on

$$H(w,z,c) := (w_1-z_1,w_2-z_2,\Phi(w,c) - (z_3,\ldots,z_{N+1})) = 0$$

in order to obtain a function $w(z,c)$. Note that $H_w(0,0,c_o) = I_{N+1}$ and $H(z,z,c_o) = 0$ hold, hence $w(z,c_o) = z$ and $w(\cdot,c)$ are diffeomorphisms for $c \in U(c_o)$. Finally, let $\gamma(z,c) = g(w(z,c),c)$ and let the $N \times N$-matices $\hat{\tau}(z,c)$ be identical to I_N except for the elements

$$\hat{\tau}_{1j}(z,c) = -\int_0^1 \frac{\partial\gamma}{\partial z_{j+1}}(z_1,z_2,tz_3,\ldots,tz_{N+1},c)\,dt, \quad j = 2,\ldots,N.$$

Then a straightforward calculation yields

$\hat{\tau}(z,c)\tau(w(z,c))T(\rho(w(z,c)),c) = (g(z_1,z_2,0,\ldots,0,c),\ z_3,\ldots,z_{N+1})$

and hence (8).

From the relation (8) we obtain a local correspondence $z = \tilde{\rho}(x,y,0,\ldots,0,c)$ between the solutions z of (2) and (x,y) of

(9) $\tilde{f}(x,y,c) = 0$.

For qualitative purposes it is therefore sufficient to consider (9) instead of (2). In addition, if $f(x,y,\alpha)$ is a universal unfolding of $f(x,y)$ then to each c close to c_o there exists an α close to 0 such that the solution curves of (9) and of

(10) $f(x,y,\alpha) = 0$

are diffeomorphic (cf.[6, Ch.II]). For the particular case (6), a universal unfolding needs at least 4 parameters and one such is

(11) $f(x,y,\alpha) = x^3 - y^3 + \alpha_4 xy + \alpha_3 y + \alpha_2 y + \alpha_1, \quad \alpha = (\alpha_1,\alpha_2,\alpha_3,\alpha_4)$.

Note that (11) with $\alpha_1 = 0$ is the hyperbolic umbilic in catastrophe theory [8]. Figures 3 and 4 show two three dimensional projections of the bifurcation set

$$B = \{\alpha \in \mathbb{R}^4 : \exists x,y \in \mathbb{R} \text{ such that } f(x,y,\alpha) = f_x(x,y,\alpha) = f_y(x,y,\alpha) = 0\}$$

along with some (x,y)-solution curves of (10) associated with special values $\alpha \in B$ (indicated by arrows) and $\alpha \in \mathbb{R}^4 \setminus B$.

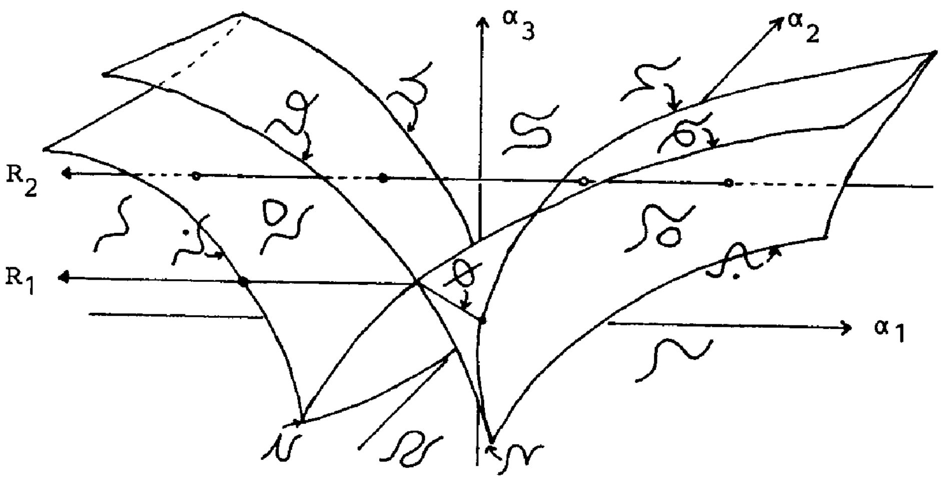

Fig. 3: Projection of B onto $\alpha_4 = 0$

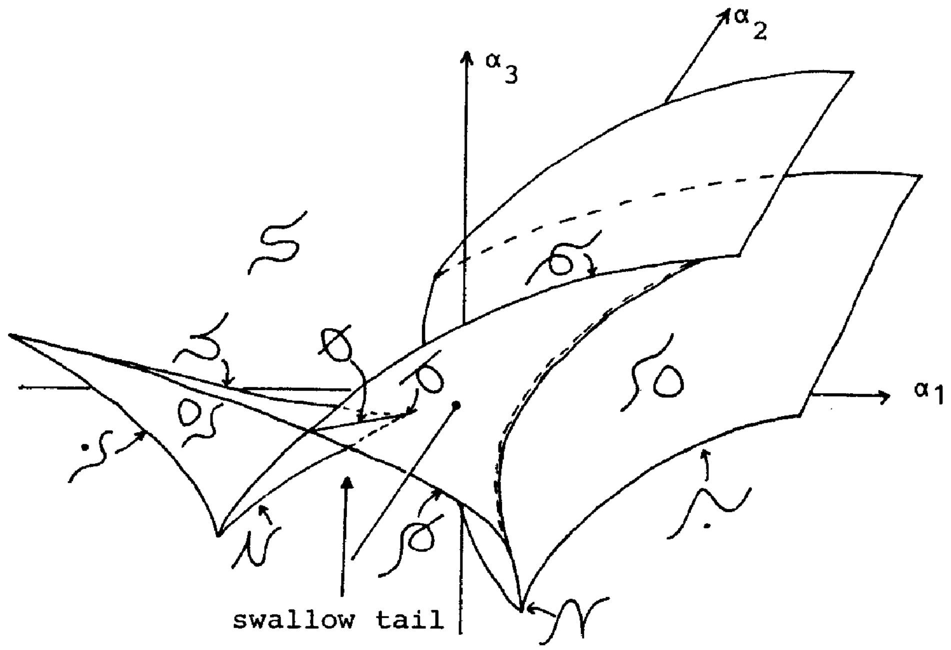

Fig. 4: Projection of B onto $\alpha_4 > 0$ fixed.

3. Testing the singularity

Let us first note that we can recover the curves of fig. 2 from fig. 3 if we let α move towards the origin on the line $\alpha_4 = 0$, $\alpha_3 = -\alpha_2 > 0$, $\alpha_1 = 0$.

Here we have $f(x,y,0,\ -\alpha_2,\alpha_2,0) = (x-y)(x^2+xy+y^2+\alpha_2)$ so that (10) describes an ellipse cut by a straight line. Our difference equations (3) correspond to this 'nongeneric' set of parameter values because of the inherent symmetry in the case $\nu = 0$ ((3) is invariant under the transformation $x_i \to x_{N+1-i}$).
If we fix $\mu = 12$ and let ν increase then this symmetry is destroyed and the curves of fig. 5 show up numerically. The perturbations of the upper configuration now correspond to parameters α moving on the ray R_1 in fig. 3.

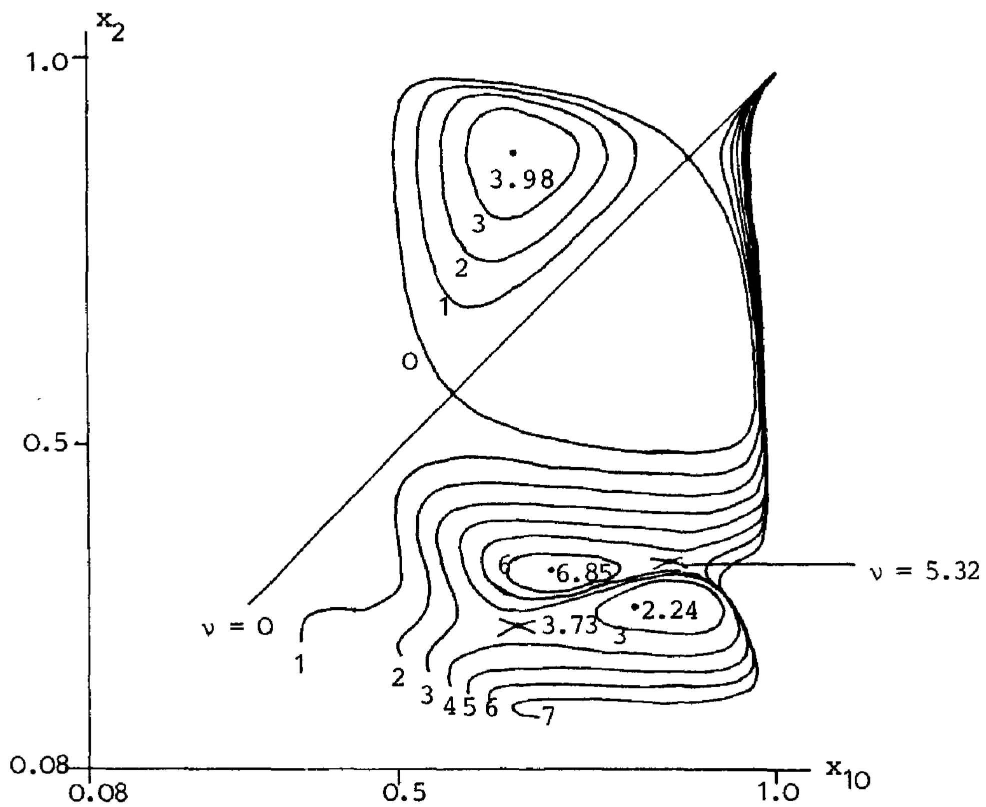

Fig. 5: solutions of (3) for $\mu = 12,\ \nu = 0,1,2,3,4,5,6,7$

Note also that the sequence of branches at the right bottom of fig. 5 is obtained when travelling on the line R_2 in fig. 3. This, however, should be the influence of a second singularity which is of the same type but located at a different point in the (z,c)-space.

A more serious test of our singularity consists in finding numerically the singular solution branches in the ν-sequence, in particular those singularities predicted by the intersections of the lines R_1 and R_2 with the bifurcation set B. The resulting isolated points and bifurcation points are shown in fig. 5. These were computed by tracing one of the curves in fig. 5 and switching to a defining equation at various points. Defining equations for bifurcation points have been set up in [7, 10] by inflating the system (2). The approach taken here rather uses a deflation of (2), which seems to be simpler conceptionally although not computationally. The numerical details and a proof of the theorem below will be contained in a forthcoming paper.

We consider an equation (2) with one parameter c(p=1) and let $T \in C^{\infty}(\mathbb{R}^{N+2}, \mathbb{R}^N)$ for simplicity. Let us decompose $\mathbb{R}^{N+1} = \Phi \oplus V$, $\mathbb{R}^N = \Psi \oplus W$ into subspaces such that $\dim\Phi = 2$, $\dim\Psi = 1$ and let $P : \mathbb{R}^N \to W$ be the projector along Ψ. Further assume that there exists a solution $(\bar{\varphi}, \bar{v}, \bar{c}) \in (\Phi \oplus V) \times \mathbb{R}$ of (2) such that $PT_v(\bar{\varphi}, \bar{v}, \bar{c}) : V \to W$ is nonsingular. Now we can define an implicit function $v(\varphi, c) \in V$ in some open neighbourhood U of $(\bar{\varphi}, \bar{c})$ by $PT(\varphi, v(\varphi,c), c) = 0$. The function $S : \Phi \times \mathbb{R} \to \Psi$, $S(\varphi,c) = (I_N - P)T(\varphi, v(\varphi,c), c)$ may then be considered as a Liapunov-Schmidt type reduction of T [9].
The defining equations for a simple bifurcation point or an isolated point of S are simply the three equations

(12) $S(\varphi,c) = 0, \quad S_\varphi(\varphi,c) = 0,$

for which we have the following result:

Theorem: $(\varphi_o, c_o) \in U$ is a regular solution of (12) if and only if $z_o = (\varphi_o, v(\varphi_o, c_o))$ is either a simple bifurcation point or an isolated point of $T(z,c_o) = 0$ (i.e. $T(z,c_o)$ is equivalent to either $z_1^2 - z_2^2$ or $z_1^2 + z_2^2$ in the sense of (7)) and $T(z,c)$ is a universal unfolding of $T(z,c_o)$.

The regularity of (φ_o, c_o) means that the system (12) has a nonsingular Jacobian at (φ_o, c_o) which implies that Newton's method is locally quadratically convergent (note however that the evaluation of S needs the solution of an implicit equation). The right-hand side of our above equivalence may be more conventionally written down in terms of the null space N_o of $T_z(z_o, c_o)$, the range W_o of $T_z(z_o, c_o)$ and the projector Q_o onto a complementary space Ψ_o of W_o: $\dim N_o = 2$, $T_c(z_o, c_o) \notin W_o$ and the quadratic form $Q_o T_{zz}(z_o, c_o) : N_o \times N_o \to \Psi_o$ is nondegenerate (i.e. there exist two nonzero eigenvalues either of the same or of the opposite sign [1,10]).

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