

NUMERICAL COMPUTATION OF CUSP SINGULARITIES FOR OPERATOR EQUATIONS

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ABSTRACT. A direct method for the calculation of cubic turning points and cusps is presented. The method starts with the original system and augment it with a minimal number of equations that characterize the singularity. We will show that the resulting extended system will then be nonsingular under the canonical cusp conditions. Numerical examples will be presented to demonstrate the efficiency of the method.

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1. INTRODUCTION

Parameter dependent problems are very common in applied sciences. They attracted many authors recently. Of particular interest are critical points of various types such as bifurcation points, turning points and cusp singularities and their relation to cubic turning points. The latter case is what we will be considering here. To mention some examples from engineering and sciences, a study of the steady state solutions of flow in a stirred tank chemical reactor was given by Golubitsky and Keyfitz[5]. It was shown that the average model of such flow has exactly one cusp point. Another example arises in the study of phase behavior analysis of mixed fluids. In particular, the study of critical points where two or more phase coalesce. In this case the critical points represent degenerate minima of the difference between the energy surface and its supporting hyperplane, see Griewank and Rabier[7]. An excellent treatment of the geometry of these points is given in the book by Golubitsky and Schaeffer[6] and in Jepson and Spence[9].

The mathematical as well as the numerical treatment of cusp singularities have been analyzed by many authors. Some proposed defining systems that compute cubic turning points and cusps directly and some indirectly by adding new variables such as the null vectors to produce rather large systems, see for example Spence and Werner[18], Roose and Caulewerts [16], Zhong and Keller[20], Attili[2],

Pastor et al.[14], Lignos et al. [12], Alan[1] and Griewank and Reddien[8]. Other related work and defining systems can be found in Jepson and Spence[9, 10, 11], Seydel[17], Attili[3], Moore and Spence[13], Beyn[4] and Ren and Spence[15].

We will present a direct method to compute cubic turning points for parameter dependent problems whose projection in the parameters plane is a cusp point. The method is direct and starts with the original system and augment it with the minimal number of equations that characterizes the singularity under consideration. The resulting extended system is then solved using a Newton like method to find the cusp point which is an isolated solution to the system.

The outline of this paper will be as follows. In Section 2, we will present how to obtain the new equations needed to characterize the cusp point. Section 3 will contain the needed theory that shows that the cusp point is an isolated solution of the resulting extended system. Finally in Section 4 we present some numerical examples that shows the efficiency of the proposed system.

2. REDUCTION TO UNIVARIATE CASE AND CHARACTERIZATION OF THE SINGULARITY

Throughout this paper we will consider an operator equation of the form

$$(2.1) \quad f(x, \lambda, \mu) = 0$$

with $f : R^n \times R \times R \rightarrow R^n$. Here f can be an algebraic system or the result of discretization of a system of differential or integral equations. We will study the singularities of f as a function of x where λ and μ enter generically and without any special dependencies. We will start with simple turning point case then extend the process for cubic turning points and cusps. Our first assumption is that the matrix f_x can drop in rank by one. As a result assume at some (x_0, λ_0, μ_0) we have (with $f_x^0 \equiv f_x(x_0, \lambda_0, \mu_0)$):

Assumption (A1):

- (1) $f(x_0, \lambda_0, \mu_0) = 0$.
- (2) $N(f_x^0) = \text{span}\{\phi_0\}$.
- (3) $R(f_x^0) = \{y \in R^n; \psi_0^T y = 0\}$.
- (4) $\psi_0^T f_\lambda \neq 0$.

These conditions implies that for fixed $\mu = \mu_0$, the point (x_0, λ_0, μ_0) is a simple turning point of f with respect to the parameter λ . In order to characterize and hence to compute such points, choose $c \in R^n$ and a linear mapping $\delta : R^n \rightarrow R$ such that the matrix

$$(2.2) \quad A = \begin{bmatrix} f_x & c \\ \delta & 0 \end{bmatrix}$$

has a bounded inverse in a domain $D \subset R^n$. Such c and δ exist. For example if one chooses $c = f_\lambda$ and δ a linear functional that is linearly independent on the null space of f_x^0 then A will be nonsingular. Now consider the solution of the system

$$(2.3) \quad f = -ch; \quad \delta x = s,$$

with $s \in R$ and $h = h(s, \lambda, \mu)$ an intermediate scalar function. Differentiating (2.3) with respect to s , we obtain

$$(2.4) \quad f_x x_s = -ch_s; \quad \delta x_s = 1$$

or in matrix format

$$(2.5) \quad \begin{bmatrix} f_x & c \\ \delta & 0 \end{bmatrix} \begin{bmatrix} x_s \\ h_s \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

It can easily be seen that f_x is deficient at some s if h_s vanishes. Hence x_s will then be in the null space of f_x . The fold points of the intermediate equation for fixed $\mu = \mu_0$ are the solutions of the 2×2 system

$$(2.6) \quad \begin{aligned} h(s, \lambda, \mu_0) &= 0 \\ h_s(s, \lambda, \mu_0) &= 0. \end{aligned}$$

This means there is a 1 - 1 correspondence between respective fold points and their projections in the $\lambda\mu$ - plane. Now to characterize the cusp or the cubic turning point(explained below) one can repeat the process and do a second reduction to produce another intermediate form in a similar way. Repetition of this process will result in a 3×3 system that involves $h(s, \lambda, \mu)$ implicitly. This fact makes such process not very attractive and hence this 3×3 system will not be the one used to compute the critical point. For example instead of solving (2.6) for the simple turning point and the mentioned 3×3 system in the cusp point case. We find x_s and h_s directly as a function of (x, λ, μ) ; that is, with $x_s \equiv v \in R^n$, $h_s \equiv g \in R$ and $u^T \in R^n$ solve the systems

$$(2.7) \quad A \begin{pmatrix} v \\ g \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ and } (u^T \quad g) A = \begin{pmatrix} 0 & 1 \end{pmatrix}.$$

Considering the two parts of (2.7) and by cross multiplying we obtain

$$(2.8) \quad g = -u^T f_x v.$$

This scalar function g characterizes the singular manifold since if forced to be zero, A will drop in rank while f characterizes the solution manifold. It is their intersection which we are after. This means once g is computed we augment f with g and solve the extended system

$$(2.9) \quad \begin{aligned} f(x, \lambda, \mu) &= 0 \\ g(x, \lambda, \mu) &= 0 \end{aligned}$$

for which the critical point is an isolated solution, see Attili[2, 3]. This type of singularity is called simple (quadratic) turning point where at such point we will have $\psi_0^T f_\lambda \neq 0$ and $\psi_0^T f_{xx} \phi_0 \phi_0 \neq 0$ while at a cubic turning point with respect to λ we will have $\psi_0^T f_{xx} \phi_0 \phi_0 = 0$ and $\psi_0^T (3f_{xx}^0 \phi_0 \nu_0 + f_{xxx}^0 \phi_0 \phi_0 \phi_0) \neq 0$ where $f_x^0 \nu_0 = -f_{xx}^0 \phi_0 \phi_0$.

We will show in the next section that the cusp point with respect to λ will correspond to a simple turning point of (2.9) with respect to μ . This means if we denote (2.9) by $F(y, \mu) = 0$ where $y = (x, \lambda)$, then one can compute the cusp point as a simple turning point of $F(y, \mu)$; that is, of (2.9). This requires the computation of another $\tilde{g}(y, \mu) = \tilde{g}(x, \lambda, \mu)$ and then extend (2.9) again to produce the system

$$(2.10) \quad \begin{aligned} F(y, \mu) &= \begin{cases} f(x, \lambda, \mu) = 0 \\ g(x, \lambda, \mu) = 0 \end{cases} \\ \tilde{g}(y, \mu) &= \tilde{g}(x, \lambda, \mu) = 0 \end{aligned}$$

an $(n+2) \times (n+2)$ system which can be solved using a Newton like method.

3. CUBIC TURNING POINTS AND CUSPS

It was shown in the previous section that to compute a simple turning point of f with respect to λ and $\mu = \mu_0$ fixed we solve an extended system of the form

$$(3.11) \quad \begin{aligned} F(y, \mu) &= f(x, \lambda, \mu) = 0 \\ g(x, \lambda, \mu) &= 0 \end{aligned}$$

with $g = -u^T f_x v$ and at (x_0, λ_0, μ_0) the vectors $v_0 = \phi_0$ and $u^T = \psi_0^T$, the left and right null vectors of f_x^0 . Also if assumption (A1) is satisfied at (x_0, λ_0, μ_0) this means F_y^0 will be nonsingular at this point; that is, it satisfies $\psi_0^T f_{xx}^0 \phi_0 \phi_0 \neq 0$. As a result and by the Implicit Function Theorem, there exists an $\varepsilon > 0$ and a smooth function $y(\mu)$ such that $y(\mu_0) = y_0$ satisfies (3.1) for $|\mu - \mu_0| < \varepsilon$. Details of computation of simple turning points can be found in Attili[2, 3].

For cubic turning points and cusps we will start by the following lemma which we need later.

Lemma 3.1. *Assume that (3.1) and assumption (A1) are satisfied at (x_0, λ_0, μ_0) . Define*

$$(3.12) \quad E = \begin{bmatrix} 0 & \psi_0^T f_\lambda^0 \\ \psi_0^T f_{xx}^0 \phi_0 \phi_0 & \psi_0^T f_{x\lambda}^0 \phi_0 \end{bmatrix}$$

Then

- (1) $\dim N(F_y^0) = \dim N(E)$.
- (2) $\text{co dim } R(F_y^0) = \dim N(E)$.

Proof: To show the first part, we look for $\Phi = (p \ r) \in R^n \times R$ such that $F_y^0 \Phi = 0$. In expanded form

$$\begin{bmatrix} f_x^0 & f_\lambda^0 \\ g_x^0 & g_\lambda^0 \end{bmatrix} \begin{bmatrix} p \\ r \end{bmatrix} = 0$$

or

$$(3.13) \quad \begin{aligned} f_x^0 p + f_\lambda^0 r &= 0 \\ g_x^0 p + g_\lambda^0 r &= 0. \end{aligned}$$

The first part of (3.3) and the fact that $\psi_0^T f_\lambda^0 \neq 0$ implies that $r = 0$ and $p = \alpha_0 \phi_0$. After left multiplying by ψ_0 and taking into consideration the definition of g , the second part of equation (3.3) becomes

$$\alpha_0 \psi_0^T f_{xx}^0 \phi_0 \phi_0 = 0$$

which is equivalent to

$$E \begin{pmatrix} \alpha_0 \\ r \end{pmatrix} = 0$$

implying the first part. The second part follows in the same way by considering $\Psi_0 F_y^0 = 0$ with $\Psi_0 = (p \ r) \in R^n \times R$ and will be omitted since it will be lengthy.

As a result of this lemma, we will have $\dim(N(F_y^0)) = 1$ spanned by $\Phi_0 = \begin{pmatrix} \phi_0 \\ 0 \end{pmatrix}$ and $\dim(N(F_y^{0T})) = 1$ and is spanned by $\Psi_0 = \begin{pmatrix} \alpha \psi_0 + \beta \psi_1 \\ \beta \end{pmatrix}$ where ψ_1 is defined as

$$\text{and } \begin{aligned} \psi_1 &= 0 & \text{if } \psi_0^T f_{xx}^0 \phi_0 \phi_0 \neq 0 \\ \psi_1^T f_x^0 &= -\psi_0^T f_{xx}^0 \phi_0 & \text{if } \psi_0^T f_{xx}^0 \phi_0 \phi_0 = 0. \end{aligned}$$

We will derive conditions on f under which (x_0, λ_0, μ_0) is a simple turning point for the extended system (3.1); that is, conditions on f equivalent to saying

$$(3.14) \quad \begin{aligned} i) & F(y_0, \mu_0) = 0, \\ ii) & N(F_y^0) = \text{span}\{\Phi_0\}, \\ iii) & R(F_y^0) = \{z \in R^n; \Psi_0^T z = 0\}, \\ iv) & \Psi_0^T F_\mu^0 \neq 0, \end{aligned}$$

with Φ_0 and Ψ_0 are left and right null vectors of F_y^0 are as given earlier in this discussion.

Theorem 3.1. *Let $(y_0, \mu_0) = (x_0, \lambda_0, \mu_0)$ satisfy (3.1) and assumption (A1). Then (y_0, μ_0) is a simple turning point of (3.1) if and only if*

$$(3.15) \quad \begin{aligned} i) & \psi_0^T f_{xx}^0 \phi_0 \phi_0 = 0; \text{ rank}(E) = 1, \\ ii) & \psi_0^T f_\lambda^0 \neq 0 \quad \psi_0^T f_{xx}^0 \phi_0 \phi_2 + \psi_0^T f_{x\mu}^0 \phi_0 \neq 0 \end{aligned}$$

where $\hat{\lambda}$ and $\hat{\mu}$ are given by

$$(3.16) \quad \begin{aligned} i) & \begin{pmatrix} \hat{\lambda} \\ \hat{\mu} \end{pmatrix} = \begin{pmatrix} \alpha_1 & \alpha_2 \\ -\alpha_2 & \alpha_1 \end{pmatrix} \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \\ ii) & f_x^0 \phi_2 = -f_\mu^0, \phi_2 \in R^n; \phi_2 \notin N(f_x^0) \end{aligned}$$

with $\alpha_1 = \psi_0^T f_\lambda^0$ and $\alpha_2 = \psi_0^T f_\mu^0$.

Similar result but for different extended systems can be found in Spence and Werner[18]. This theorem gives conditions under which (x_0, λ_0, μ_0) is a simple (quadratic) turning point of the extended system (3.1) with respect to μ . Now the following theorem which we state without proof establishes that (x_0, λ_0, μ_0) will be a cubic turning point with respect to λ with $\mu = \mu_0$ fixed.

Theorem 3.2. *Let $\psi_0^T f_{xx}^0 \phi_0 \phi_0 = 0$ and $\psi_0^T (3f_{xx}^0 \phi_0 \nu_0 + f_{xxx}^0 \phi_0 \phi_0 \phi_0) \neq 0$ where $f_x^0 \nu_0 = -f_{xx}^0 \phi_0 \phi_0$. Let $\zeta_0^T f_\lambda^0 = -\psi_0^T f_{x\lambda}^0 \phi_0$, $\zeta_0^T f_x^0 = -\psi_0^T f_{xx}^0 \phi_0$ and assume $-\zeta_0^T f_\mu^0 + \psi_0^T f_{x\mu}^0 \phi_0 \neq 0$. Then a cubic turning point (x_0, λ_0, μ_0) of $f(x, \lambda, \mu) = 0$ with respect to (x, λ) and $\mu = \mu_0$ fixed corresponds to a simple turning point (x_0, λ_0, μ_0) of the extended system (3.1) with respect to (y, μ) .*

Note that the first part of the theorem; that is, $\psi_0^T f_{xx}^0 \phi_0 \phi_0 = 0$ and $\psi_0^T (3f_{xx}^0 \phi_0 \nu_0 + f_{xxx}^0 \phi_0 \phi_0 \phi_0) \neq 0$ is what characterizes a cubic turning point whose projection in the $\lambda\mu$ -plane is a cusp point. Also notice that the condition $-\zeta_0^T f_\mu^0 + \psi_0^T f_{x\mu}^0 \phi_0 \neq 0$ implies that $\Psi_0^T F_\mu^0 \neq 0$ and as a result of this theorem, we will have

$$(3.17) \quad \Psi_0^T F_{yy}^0 \Phi_0 \Phi_0 \neq 0 \text{ if and only if } \psi_0^T (3f_{xx}^0 \phi_0 \nu_0 + f_{xxx}^0 \phi_0 \phi_0 \phi_0) \neq 0$$

implying that (y, μ) is a simple turning point for (3.1). This makes the result of the theorem clearly true and again more details on similar result although for a different extended system, refer to [18].

Now as noted earlier in the previous section and to compute the simple turning point for the extended system we extend it again to obtain a new extended system of the form

$$(3.18) \quad \begin{aligned} F(y, \mu) &= \begin{cases} f(x, \lambda, \mu) = 0 \\ g(x, \lambda, \mu) = 0 \end{cases} \\ \tilde{g}(y, \mu) &= \tilde{g}(x, \lambda, \mu) = 0. \end{aligned}$$

The simple turning point of (3.1) and hence the cusp point of f with respect to λ will be an isolated solution to such system and for that purpose we will have the following theorem

Theorem 3.3. *Let (y_0, μ_0) satisfy the system (3.9) and assumption (A1). If $(y_0, \mu_0) = (x_0, \lambda_0, \mu_0)$ is a cubic turning point of $f(x, \lambda, \mu) = 0$, then the Jacobian matrix of (3.9) is nonsingular at (y_0, μ_0) .*

Proof: Since assumption (A1) is satisfied and (y_0, μ_0) is a cubic turning point of $F(y, \mu) = \begin{cases} f(x, \lambda, \mu) = 0 \\ g(x, \lambda, \mu) = 0 \end{cases}$, we will have

$$(3.19) \quad \begin{aligned} i) \quad N(F_y^0) &= \text{span}\{\Phi_0\}, \\ ii) \quad R(F_y^0) &= \{z \in R^n; \Psi_0^T z = 0\}, \\ iii) \quad \Psi_0^T F_\mu &\neq 0; F_\mu \notin R(F_y^0). \end{aligned}$$

The Jacobian of (3.9) is given by $J = \begin{bmatrix} F_y^0 & F_\mu^0 \\ \tilde{g}_y^0 & \tilde{g}_\mu^0 \end{bmatrix}$. Consider

$$(3.20) \quad \begin{bmatrix} F_y^0 & F_\mu^0 \\ \tilde{g}_y^0 & \tilde{g}_\mu^0 \end{bmatrix} \begin{bmatrix} p \\ r \end{bmatrix} = 0$$

which is equivalent to

$$(3.21) \quad \begin{aligned} i) \quad F_y^0 p + F_\mu^0 r &= 0 \\ ii) \quad \tilde{g}_y^0 p + \tilde{g}_\mu^0 r &= 0 \end{aligned}$$

From (3.12-i), we will have $r = 0$ since $F_\mu \notin R(F_y^0)$, so it will reduce to $F_y^0 p = 0$. This means $p \in N(F_y^0)$, or $p = \alpha \Phi_0$. Substituting in (3.12-ii) we obtain $\alpha \tilde{g}_y^0 \Phi_0 = 0$ and using the definition of $\tilde{g}$ we obtain $\alpha \Psi_0^T F_y^0 \Phi_0 \Phi_0 = 0$. This means α must be zero since $\Psi_0^T F_y^0 \Phi_0 \Phi_0 \neq 0$ at a cubic turning point by (3.8). This means that (3.11) has only the trivial solution. Completing the proof.

4. NUMERICAL EXAMPLES

For numerical testing, we considered two examples from applied sciences and engineering. Both are two point boundary value problems.

(1) Example 1:

We considered the problem

$$(4.22) \quad u_1'' + \lambda e^{\frac{u_1}{1+\mu u_1}} = 0; \quad u_1(0) = u_1(1) = 0$$

which describes an exothermic chemical reaction in a finite slab which was treated by Spence and Werner[18] using finite differences with a different extended system. It is known that it has a cubic turning point at $\lambda_0 = 5.229494$ and $\mu = 0.2457804$. We used simple shooting to solve (4.1) and for that reason we transformed (4.1) into a first order system and solved the initial value problem

$$(4.23) \quad \begin{aligned} u_1' &= u_2; \quad u_2' = -\lambda e^{\frac{u_1}{1+\mu u_1}} \\ u_1(0) &= 0; \quad u_2(0) = s_1 \end{aligned}$$

to get a solution at $x = 1$, namely $u_1(1)$ and $u_2(1)$ that depends on s_1 , λ and μ . Now the solution to (4.2) will now be to force $u_1(1)$ to be zero.

One equation in three unknowns s_1 , λ and μ that characterizes the solution manifold. Two more equations are then computed and added that characterizes the cusp point; that is, the $g(s_1, \lambda s_1, \mu) = 0$ and $\tilde{g}(s_1, \lambda s_1, \mu) = 0$ as explained in previous sections resulting in a rather small system of order 3×3 . The results obtained were as follows:

g	$\tilde{g}$	λ	μ
0.188914-2	-0.12698-2	5.228324	0.245856
-0.430572-3	-0.671354-4	5.229524	0.245781
-0.660599-6	-0.332915-6	5.229489	0.245780
-0.335454-9	-0.185218-9	5.229489	0.245780

As expected both g and $\tilde{g}$ are converging to zero when λ and μ are at the critical point. Newton's method was used to solve the systems involved.

(2) Example 2:

We considered Euler Buckling of a beam example, see Zeeman[19] of the form

$$(4.24) \quad \theta'' = -F \sin \theta + \varepsilon(x + \theta) \cos \theta$$

where ε is a small perturbation parameter, F is the force applied to both ends and θ is the inclination of the strut to the horizontal. To make the notation familiar, we replace F , ε and θ by μ , λ and u respectively to obtain

$$\begin{aligned} u'' &= -\mu \sin u + \lambda(x + u) \cos u, \\ u'(0) &= u'(1) = 0, \end{aligned}$$

which has a cubic turning point at $\lambda = 0$ and $\mu = \pi^2$. Again we solved the system using simple shooting and obtained the results given in the following table

g	$\tilde{g}$	λ	μ
0.372380-1	0.644706-1	-0.26145-4	9.8697242
-0.729346-4	0.382529-3	0.72659-8	9.8696042
-0.111178-6	-0.195146-6	0.85253-13	9.8696044
-0.279274-10	-0.201341-9	0.76111-13	9.8696044

The results obtained agreed very much with the expected values. Newton's method converged quadratically to the solution.

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