Turning Points and Bifurcations for Homotopies of Analytic Maps

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Introduction

- Numerical continuation methods have found successful use in the approximation of solution curves of ordinary and partial differential equations involving a bifurcation parameter. In this setting, a single connected component is traced and points of special interest, such as turning points and bifurcation points may be sought.
- Another frequent application of numerical continuation involves the approximation of all of the complex solutions of systems of n complex polynomials in n complex variables.
- A considerable amount of effort has gone into formulating efficient homotopies so that all of the complex solutions of a polynomial system may be found by tracing homotopy paths, see for example, the reviews by T.-Y.Li, and the book by Sommese and Wampler.

Application to nonlinear BVPs

- Finding all solutions to polynomial systems has led to attempts to approximate all of the solutions to certain types of boundary value problems by means of putting finite difference approximations into a complex setting, and applying the homotopy method to the resulting system, see Allgower, Bates,Sommese and Wampler, and Allgower, Cruceanu and Tavener.
- One of the challenges to this approach is that the number of solutions to the system generally becomes very large if the number of mesh points becomes large. Yet on the other hand, only the (usually much smaller) number of purely real solutions is of interest.
- The remedy has been to start with a very coarse finite difference mesh and to refine it by introducing a *single* new mesh point in a continuous way. After the homotopy paths have been traced to conclusion the process may be repeated.

Analytic Maps

- For analytic maps, numerical experience with the above approach has revealed that very often the homotopy paths have turning points where the derivative of the homotopy parameter changes sign. For polynomial maps, this phenomenon can be prevented by making a random type of perturbation, such as the "γ-trick", in the homotopy used by Sommese and Wampler.
- We use arclength continuation (rather than continuation in the homotopy parameter) to round turning points. We show that simple turning points of homotopy paths of complex analytic maps are necessarily also bifurcation points.
- By further showing that the curvatures of the bifurcating curves are of opposite sign, (but of equal magnitude) and also that the tangents have a special orthogonal relationship, we can construct an algorithm to trace complex homotopy paths monotonically.

Definitions and Preliminary Results

We first consider matters in the real context and assume (homotopy) paths to be parametrized with respect to arclength, s. Let $H : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R}^n$. We will be concerned with tracking solutions to $H(t, x) = 0$ from $t = 1$ to $t = 0$ via arclength continuation.

Definition 1 *Let $H : \mathbb{R}^{n+1} \rightarrow \mathbb{R}^n$ be sufficiently smooth. Suppose that $c : J \rightarrow \mathbb{R}^{n+1}$, $c(s) = (t(s), u(s))$ is a smooth curve, defined on an open interval J, and parametrized with respect to arclength such that $H(c(s)) = 0$ for $s \in J$. The vectors $\pm(\dot{t}, \dot{u})$ are unit tangent vectors to c. The point $c(\bar{s})$ is said to be a* **simple turning point** *of the solution curve c if $\dot{t}(\bar{s}) = 0$, $\ddot{t}(\bar{s}) \neq 0$ and the* augmented Jacobian

$$\begin{pmatrix} \dot{t} & \dot{u}^\top \\ H_t & H_u \end{pmatrix}$$

is non-singular at $s = \bar{s}$.

Bifurcation Point

Definition 2 *Let* $H : \mathbb{R}^{n+1} \longrightarrow \mathbb{R}^n$ *be sufficiently smooth. Suppose that* $c : J \longrightarrow \mathbb{R}^{n+1}$ *is a smooth curve, defined on an open interval* J*, and parametrized with respect to arclength such that* $H(c(s)) = 0$ *for* $s \in J$*. The point* $c(\bar{s})$ *is called a* **bifurcation point** *of the equation* $H = 0$ *if there is an* $\epsilon > 0$ *such that every neighborhood of* $c(\bar{s})$ *contains zero-points of* H *which are not on* $c\left((\bar{s} - \epsilon, \bar{s} + \epsilon)\right)$*.*

An immediate consequence of this definition is that a bifurcation point $c(\bar{s})$ of $H = 0$ must be a singular point of H. Hence, the Jacobian $H'(c(\bar{s}))$ must have a kernel of dimension at least two.

Simple Bifurcation Point

Definition 3 *Let* $H : \mathbb{R}^{n+1} \to \mathbb{R}^n$ *be sufficiently smooth. A point* $\bar{u} \in \mathbb{R}^{n+1}$ *is called a* **simple bifurcation point** *of the equation* $H = 0$ *if the following conditions hold:*

(1) $H(\bar{u}) = 0$*;*

(2) $\dim \ker H'(\bar{u}) = 2$*;*

(3) $e^\top H''(\bar{u})[\phi, \psi]$ *has one positive and one negative eigenvalue, where* e *spans* $\ker H'(\bar{u})^\top$ *and* ϕ *and* ψ *together span* $\ker H'(\bar{u})$*.*

Characterizing Simple Bifurcation Points

The following results furnish a criterion for detecting a simple bifurcation point when traversing a curve $c(s)$.

Theorem 1 *Let* $H : \mathbb{R}^{n+1} \to \mathbb{R}^n$ *be sufficiently smooth and* $\bar{u} \in \mathbb{R}^{n+1}$ *a simple bifurcation point of the equation* $H = 0$*. Then there exist two smooth curves* $c_1(s), c_2(s) \in \mathbb{R}^{n+1}$*, parametrized with respect to the arclength* s*, defined for* $s \in (\bar{s} - \epsilon, \bar{s} + \epsilon)$ *and* $\epsilon > 0$ *sufficiently small, such that the following holds*

(1) $H(c_i(s)) = 0, i \in \{1, 2\}, s \in (\bar{s} - \epsilon, \bar{s} + \epsilon)$;

(2) $c_i(\bar{s}) = \bar{u}, i \in \{1, 2\}$;

(3) $\dot{c}_1(\bar{s}), \dot{c}_2(\bar{s})$ *are linearly independent;*

(4) $H^{-1}(0)$ *coincides locally with* $\mathrm{range}(c_1) \cup \mathrm{range}(c_2)$.

Sign Criterion

Theorem 2 *Let $\bar{u} \in \mathbb{R}^{n+1}$ be a simple bifurcation point of the equation $H = 0$. Using the notation of Definition 3 and Theorem 1, the determinant of the augmented Jacobian*

$$\det \begin{pmatrix} H'(c_i(s)) \\ \dot{c}_i(s)^\top \end{pmatrix}$$

changes sign at $s = \bar{s}$ for $i \in \{1, 2\}$.

Continuation for Complex Analytic Maps

Let $H : \mathbb{R} \times \mathbb{C}^n \to \mathbb{C}^n$, be a smooth homotopy and assume that $H(t, w)$ is analytic in the variables w. Further, let $w = u + iv$ for $w \in \mathbb{C}^n$, where $u, v \in \mathbb{R}^n$ denote the real and the imaginary parts of w respectively.

We define $H^r, H^i : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ by

$$\begin{aligned} H^r(t, u, v) &:= \tfrac{1}{2} \left(H(t, w) + H(t, \overline{w}) \right), \\ H^i(t, u, v) &:= \tfrac{-i}{2} \left(H(t, w) - H(t, \overline{w}) \right), \end{aligned} \tag{1}$$

and the map $\hat{H} : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^{2n}$ by

$$\hat{H}(t, u, v) := \begin{pmatrix} H^r(t, u, v) \\ -H^i(t, u, v) \end{pmatrix}. \tag{2}$$

Complex Tracing

We wish to trace a smooth curve $\hat{c} : s \mapsto (t(s), u(s), v(s))$ in $\hat{H}^{-1}(0)$, where s is an arclength parameter. Let $\hat{c}(s)$ be a column vector, i.e.,

$$\hat{c}(s) = \begin{pmatrix} t(s) \\ u(s) \\ v(s) \end{pmatrix} .$$

Differentiating $\hat{H}(t(s), u(s), v(s))$ with respect to s yields

$$\begin{pmatrix} H_t^r & H_u^r & H_v^r \\ -H_t^i & -H_u^i & -H_v^i \end{pmatrix} \begin{pmatrix} \dot{t} \\ \dot{u} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} . \tag{3}$$

An Eigenvalue Result

From (1) we obtain the Cauchy-Riemann equations

$$H_v^r = -H_u^i \quad \text{and} \quad H_v^i = H_u^r. \tag{4}$$

and therefore

$$\hat{H}_{(u,v)} = \begin{pmatrix} H_u^r & -H_u^i \\ -H_u^i & -H_u^r \end{pmatrix}$$

is block symmetric.

Furthermore, if μ is an eigenvalue of $\hat{H}_{(u,v)}$ with corresponding eigenvector $\binom{\tilde{u}}{\tilde{v}}$, then $-\mu$ is also an eigenvalue with corresponding eigenvector $\binom{\tilde{v}}{-\tilde{u}}$. Eigenvalues of $\hat{H}_{(u,v)}$ therefore occur in symmetric pairs about zero and $\det \hat{H}_{(u,v)}$ never changes sign.

Sign Change Result for Analytic Maps

Applying the Cauchy-Riemann equations (4) and augmenting (3) with a normalized tangent vector corresponding to arclength parametrization, we obtain

$$\begin{pmatrix} \dot{t} & \dot{u}^\top & \dot{v}^\top \\ H_t^r & H_u^r & H_v^r \\ -H_t^i & -H_u^i & -H_v^i \end{pmatrix} \begin{pmatrix} \dot{t} & 0^\top & 0^\top \\ \dot{u} & \mathsf{Id} & 0 \\ \dot{v} & 0 & \mathsf{Id} \end{pmatrix} = \begin{pmatrix} 1 & \dot{u}^\top & \dot{v}^\top \\ 0 & H_u^r & -H_u^i \\ 0 & -H_u^i & -H_u^r \end{pmatrix} \tag{5}$$

and therefore

$$\dot{t} \det \begin{pmatrix} \dot{t} & \dot{u}^\top & \dot{v}^\top \\ H_t^r & H_u^r & H_v^r \\ -H_t^i & -H_u^i & -H_v^i \end{pmatrix} = \det \begin{pmatrix} H_u^r & -H_u^i \\ -H_u^i & -H_u^r \end{pmatrix} = \det \hat{H}_{(u,v)}. \tag{6}$$

Since the sign of $\det \hat{H}_{(u,v)}$ remains constant, if U is a neighborhood of a parameter value $\bar{s}$ such that $\hat{c}(s)$ are regular points of $\hat{H}$ for $s \in U \setminus \{\bar{s}\}$, equation (6) implies that $\dot{t}(\hat{c}(s))$ can change sign at $s = \bar{s}$ if and only if

$$\det \begin{pmatrix} \dot{t} & \dot{u}^\top & \dot{v}^\top \\ H_t^r & H_u^r & H_v^r \\ -H_t^i & -H_u^i & -H_v^i \end{pmatrix} \tag{7}$$

evaluated at $\hat{c}(s)$ changes sign.

Turn-Bif. Theorem

Theorem 3 *Let* $\hat{c}(s) = (t(s), u(s), v(s))$ *be a solution curve in* $\hat{H}^{-1}(0)$ *and let* $\hat{c}(\bar{s})$ *be a simple turning point of the curve* $\hat{c}$ *with* $\dot{t}(\bar{s}) = 0$ *with tangent vector* $(0, \dot{u}(\bar{s})^T, \dot{v}(\bar{s})^T)$*. Then the vector* $(0, \dot{v}(\bar{s})^T, -\dot{u}(\bar{s})^T)$ *lies in the kernel of the augmented matrix, and if the rank is maximal, then* $\hat{c}(\bar{s})$ *is a simple bifurcation point of the equation* $\hat{H} = 0$*.*

Proof – application of Cauchy Riemann equations and verify the results for the real case.

Curvature Result

Theorem 4 *Under the assumptions of Theorem 3, let us now denote the two bifurcating solution curves of* $\hat{H}^{-1}(0)$ *by* $\hat{c}_i(s) := (t_i(s), u_i(s), v_i(s))$, $i \in \{1, 2\}$. *The curves are defined for* s *near* $\bar{s}$ *and* $\tilde{c} := \hat{c}_1(\bar{s}) = \hat{c}_2(\bar{s})$ *is the bifurcation point. Then*

(i) $(0, \dot{u}_1(\bar{s}), \dot{v}_1(\bar{s}))$ *and* $(0, -\dot{v}_1(\bar{s}), \dot{u}_1(\bar{s}))$ *are orthogonal unit tangents to* $\hat{c}_1(s)$ *and* $\hat{c}_2(s)$ *at* $s = \bar{s}$, *respectively;*

(ii) $\ddot{t}_1(\bar{s}) = -\ddot{t}_2(\bar{s})$.

Monotonicity

- Most numerical implementations of continuation methods construct tangent “predictor” vectors as points along the branch are calculated. Turning points are easily detected by, for example, monitoring whether the inner product of successive unit tangent vectors becomes negative.
- At a turning point, the tangent to the path has the form $(0, \dot{u}(\bar{s}), \dot{v}(\bar{s}))$. One can now easily switch the branches by choosing as a predictor the tangent $(0, \dot{v}(\bar{s}), -\dot{u}(\bar{s}))$ of the bifurcating branch.
- The new path bifurcating from the turning point may have additional turning points, but these can be handled in the same manner. Therefore, one will be able to continue to track the solution path monotonically as t decreases towards 0.

BVP Application

- We have applied numerical continuation for solving the problem of approximating *all* the solutions of a class of nonlinear second order semilinear elliptic boundary value problems with Dirichlet boundary conditions on a rectangular domain.
- It has been noted, e.g., by Breuer-McKenna-Plum, that there are very few theoretical results concerning how many solutions such a problem may have, or indeed, if there are any solutions at all.
- This state of affairs is somewhat better in the corresponding case of second order ordinary differential equations, where a number of existence and multiplicity results are available in several papers and books.

ODE

The example considered by Allgower,Bates, Sommese and Wampler was

$$u'' = f(x, u, u')$$

with general linear boundary conditions and f assumed to be a polynomial map.

For this case, the totality of solutions of the polynomial systems of equations was found by embedding the systems in a complex setting and applying a numerical homotopy continuation method to compute all of the complex solutions of the polynomial system.

Issues

- One issue is that the requirement for an accurate approximation can result in a very large polynomial system and therefore an enormous number of complex solutions, among which are only a few real solutions that are actually of interest. For example, N quadratic equations would generally have 2^N solutions in $\mathbb{C}^N$. Furthermore, even among the real solutions, there may be spurious solutions which arise as numerical artifacts and do not converge to solutions of the boundary value problem.
- The above issues in the case of two point boundary value problems by means of two remedial steps.

Mesh Deformation

- We discard the obviously irrelevant solutions, including the real solutions which do not exhibit properties which theoretical results indicate must hold, for example, symmetry properties.
- We start with a crude mesh (and hence a low dimensional system) and then introduce a new mesh point via a continuous deformation of the mesh.
    - Assuming that the solutions have been obtained for a uniform mesh with, say N points, a new point is introduced, for example, at the right boundary and this point is then allowed to be continuously moved leftward until a uniform mesh with $(N+1)$ points is achieved.
    - This uses numerical continuation in yet another way, since the homotopy parameter now is used to continuously deform the mesh in the difference equations.
    - Starting points for solutions when the new point is introduced are simply the zero points of a single polynomial equation, which are generally easy to find. For general analytic maps, all starting solutions within chosen bounds can be found by a cellular exclusion algorithm.

ODE Deformation

Consider the second order boundary value problem on the interval $[a, b] \subset \mathbb{R}$

$$u'' = f(x, u),\ u(a) = \alpha \text{ and } u(b) = \beta \tag{8}$$

Using a central difference approximation with a uniform mesh for example, we can approximate a solution $u(x)$ of (8) by an N-tuple of numbers $(u_1, u_2, \ldots, u_N)^T$ such that $u_i \approx u(x_i)$, $\forall i = 1, \ldots, N$, where we set $h := \frac{b-a}{N+1}$, $x_i := a + ih, \forall i = 0, \ldots, N+1$, $u_0 = \alpha$, and $u_{N+1} = \beta$.

The discretization of (8) takes the form of the following system,

$$\mathcal{D}_N \left\{ \begin{array}{ccccccc} u_0 & - & 2u_1 & + & u_2 & = & h^2 f(x_1, u_1), \\ \vdots & & \vdots & & \vdots & = & \vdots \\ u_{N-1} & - & 2u_N & + & u_{N+1} & = & h^2 f(x_N, u_N). \end{array} \right.$$

Steps of Solving

The process of finding the solutions can be sketched in four steps.

1. Find all the solutions of the discretization $\mathcal{D}_N$ for some small N.
2. Discard all unreasonable solutions and denote by $\mathcal{S}_N$ the set of the solutions which are kept.
3. If the mesh size is not sufficiently small or the cardinality of $\mathcal{S}_N$ has not yet stabilized, then add a mesh point to obtain the discretization $\mathcal{D}_{N+1}$. Use the solutions in $\mathcal{S}_N$ to generate solutions of $\mathcal{D}_{N+1}$ and then return to Step 2 to generate $\mathcal{S}_{N+1}$.
4. Once the mesh size is sufficiently small and the cardinality of $\mathcal{S}_N$ becomes stable, refine the solutions to a more consistent grid with a fast nonlinear solver.

Deformation Map

Let $H_{N+1}(t, u_1, u_2, \ldots, u_{N+1}) =$

$$\begin{pmatrix} u_0 - 2u_1 + u_2 & - & h(t)^2 f(x_1(t), u_1) \\ & \vdots & \\ u_{N-2} - 2u_{N-1} + u_N & - & h(t)^2 f(x_{N-1}(t), u_{N-1}) \\ u_{N-1} - 2u_N + U_{N+1}(t) & - & h(t)^2 f(x_N(t), u_N) \\ u_N - 2u_{N+1} + U_{N+2}(t) & - & h(t)^2 f(x_{N+1}(t), u_{N+1}) \end{pmatrix},$$

where

$$\begin{cases} x_i(t) = a + ih(t), \qquad \forall i = 1, \ldots, N+1 \\ u_0 = \alpha \\ h(t) = t\left(\frac{b-a}{N+1}\right) + (1-t)\left(\frac{b-a}{N+2}\right) \\ U_{N+1}(t) = (1-t)u_{N+1} + \beta t \\ U_{N+2}(t) = \beta(1-t). \end{cases}$$

Explanation

(a) At $t = 0$, H_{N+1} represents the system $\mathcal{D}_{N+1}$.

(b) At $t = 1$, H_{N+1} can be interpreted as the system $\mathcal{D}_N$ with a new mesh point having the value u_{N+1} at $x_{N+1} = b$ and a new right-hand boundary having the value $U_{N+2}(1) = 0$ at $x_{N+2} = b + h(1)$.

(c) As t goes from 1 to 0, the mesh points are squeezed back inside of $[a, b]$ and right hand boundary condition $u(b) = \beta$ is transferred from U_{N+1} to U_{N+2} as U_{N+1} is enforced to equal u_{N+1}, i.e.,

$$U_{N+2}(0) = \beta \text{ and } U_{N+1}(0) = u_{N+1}.$$

Solving the new System

To find all the solutions of $\mathcal{D}_{N+1}$, we will use numerical continuation to track the zeros of H_{N+1} as t goes from 1 to 0. At $t = 1$, we have a list $\mathcal{S}_N$ of solutions $(u_1, u_2, \ldots, u_N)^T$ satisfying the first N equations of H_{N+1}, while the final equation is

$$u_N - 2u_{N+1} = h(1)^2 f\left(b, u_{N+1}\right), \tag{9}$$

which is the **only** place where u_{N+1} appears.

For each solution $(u_1, u_2, \ldots, u_N)^T$ in $\mathcal{S}_N$, we use this equation to find the corresponding values of u_{N+1}. These are the starting points of continuation paths leading to the solutions of $\mathcal{D}_{N+1}$.

In the case of polynomial nonlinearity when $f(x,u)$ from (8) is a real polynomial $p(u)$, we can conveniently obtain the starting points for $H_{N+1}(1, u_1, u_2, \ldots, u_{N+1}) = 0$ by solving the single polynomial equation

$$u_N - 2u_{N+1} + U_{N+2}(1) - \left(\frac{b-a}{N+1}\right)^2 p(u_{N+1}) = 0, \tag{10}$$

for u_{N+1} given u_N from the solutions in $\mathcal{S}_N$. All the solutions (real and complex) of (10) can be found using standard available software.

2D Problem

- The method of finding all the solutions of second order ordinary differential equations may be generalized to a class of nonlinear second order semilinear elliptic boundary value problems with Dirichlet boundary conditions on a rectangular domain, and with polynomial nonlinearities.
- Most of the difficulties met for the one dimensional case are also encountered again.
- Further difficulties that appear due to the generalization to a higher dimension involve how to introduce only a *single* new mesh point for a continuous mesh deformation. We build a homotopy function associated with a central difference discretization of the Laplace operator as a combination of some sparse matrices and vectors and introduce mesh points in to rows and columns alternately.

Nonlinear Elliptic Problem

We consider the problem of finding *all* the solutions for a nonlinear bifurcation problem of the form

$$\Delta u = f(\lambda, x, y, u, u_x, u_y) \qquad \text{on} \quad \Omega \subset \mathbb{R}^2$$
$$u|_{\partial\Omega} = g.$$

where Ω is a rectangular domain.

The difficulties which arise in the one dimensional case also occur here.

In addition, the analogous discretizations after complexification, frequently lead to homotopy paths with turning points, i.e., bifurcation points. These may now be handled by the means we have described.

Numerical Example

Consider the following partial differential equation in two dimensions,

$$\Delta u = -(1+u^2) \quad \text{on } \Omega = [0,1]\times[0,1], \tag{11}$$

$$u = 0 \quad \text{on } \partial\Omega. \tag{12}$$

Using a tracking method based on arclength continuation and the techniques presented above, we obtained the results in the following Table. In particular, we switched branches at turning points as discussed in above.

Number of solutions vs N

N	No. solns	No. real solns	N	No. solns	No. real solns
1	2	2	9	512	2
2	4	2	10	1024	2
3	8	2	11	2048	2
4	16	2	12	4096	2
5	32	6	13	8192	2
6	64	4	14	16384	2
7	128	4	15	32768	2
8	256	4	16	65536	2

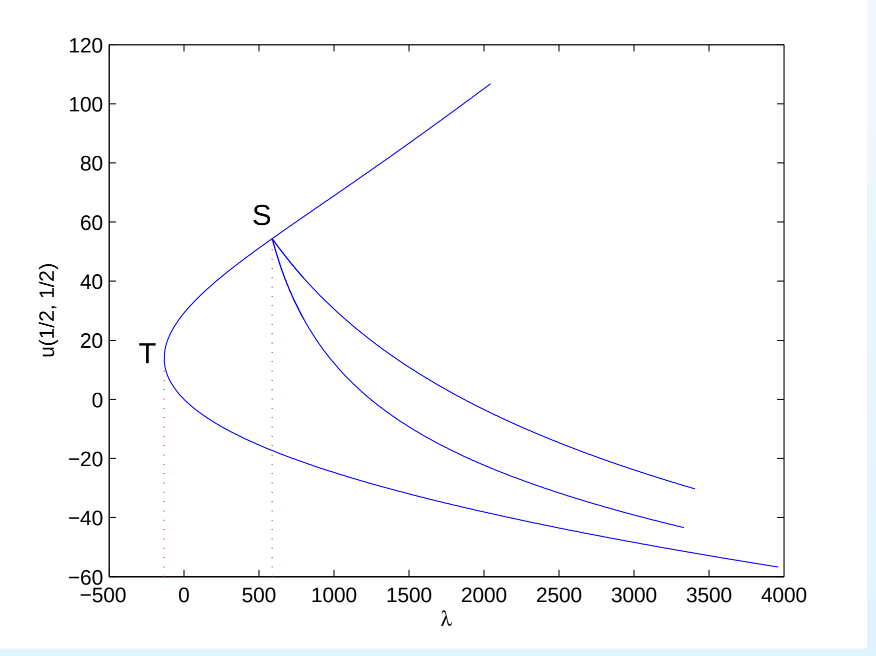
The number of solutions for $\Delta u = -(1 + u^2)$ on $\Omega = [0, 1] \times [0, 1]$ with zero Dirichlet boundary conditions.

Breuer, McKenna and Plum

Consider the bifurcation problem

$$\Delta u + u^2 = \lambda \sin \pi x \sin \pi y \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega. \qquad (13)$$

Starting with the 4 solutions found for $\lambda = 800$ on a mesh with 31×31 interior points, we used arclength numerical continuation to construct the bifurcation diagram below.



Observations

- We found a turning point T at $\lambda_T \approx -133.3$ at which one eigenvalue of the Jacobian changes sign. The Jacobian is in fact $A + 2\,\mathrm{diag}(\vec{u})$, where A is the stiffness matrix.
- We also found a symmetry breaking bifurcation S at $\lambda_S \approx 587.7$ at which a pair of other eigenvalues of the Jacobian (a double eigenvalue) changes sign.
- We performed continuation for values of λ up to 8000 and saw no indication that another eigenvalue will approach zero as λ increases.
- We performed homotopy continuation for a few different values of λ and confirmed that there are no real solutions for $\lambda < \lambda_T$, two real solutions if $\lambda_T < \lambda < \lambda_S$, and four real solutions if $\lambda > \lambda_S$.
- There do not seem to be disjoint real branches in this bifurcation diagram.

Summary

- We have studied homotopy paths for analytic maps under arclength parametrization. Simple turning points have been shown to be simple bifurcation points.
- At the bifurcation point the curves have orthogonal tangents and the same absolute curvature but of opposite sign. This facilitates predictor-corrector continuation by switching branches at turning points the homotopy paths can be monotonically traced.
- Applications have been made to nonlinear boundary value problems.