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# Numerical Methods for Bifurcation Problems

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# ON A GENERAL TECHNIQUE FOR FINDING DIRECTIONS PROCEEDING FROM BIFURCATION POINTS

Ralph Baker Kearfott

Various quite satisfactory analytical and numerical techniques are available for analysing bifurcation points when something about the structure is known a priori. The author previously introduced a method applicable when such information is not present, or when the arcs intersect tangentially. That method is discussed here, with particular emphasis on avenues to improvement in efficiency and reliability.

## 1. Introduction and Background

We consider the solution sets of the parametrized nonlinear system

$$H(y) = H(x, \lambda) = 0 \tag{1.1}$$

where $H : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$. Of interest are the bifurcation points $y^* = (x^*, \lambda^*)$ where rank $(DH(y^*)) < n$, and where two or more arcs in the solution set of (1.1) intersect.

Due to the ubiquitous occurrence of bifurcation in physical processes, specific techniques for finding $y^*$ and following paths away from $y^*$ are well developed. These techniques are applicable when the bifurcation point is simple (only two arcs intersect), when $y^* = (0, \lambda^*)$ (bifurcation from the "trivial" solution), when symmetry can be used, when unfoldings ([5]) are easily computed, etc. These, described in other papers in this volume and elsewhere, are usually quite efficient, and are to be preferred for the specific problems they are meant to solve.

Other methods are meant to be more general. Perhaps the two salient ones are (1) use of simplicial discretizations, possibly in conjunction with "artificial bifurcation" (cf. [16]), and (2) solution of a system of polynomial equations such that the degree of each equation equals the order

$p > 1$ of the first non-zero higher-order derivative tensor (see [12] and also [11]).

Simplicial methods are mathematically equivalent to replacing $H$ by a perturbation which has no bifurcation points, for which the paths can be followed. Typically, paths intersecting $\lambda = 0$ are followed until they diverge or intersect $\lambda = 1$, but not all paths corresponding to a bifurcation point may correspond to simplicial paths intersecting at $t = 0$; artificial bifurcation and other ad hoc techniques are used to connect these paths. Such techniques would be harder to apply when large numbers of arcs intersect.

In the Keller/Langford method ([12]), solutions of the system of polynomial equations correspond to normalized tangent vectors to arcs emanating from $y^*$. The solutions are in a one-to-one correspondence with the arcs, provided there are no multiple solutions (arcs do not intersect tangentially) and provided the solutions are isolated on the intersection of any sufficiently small sphere in $\mathbb{R}^n$ about the bifurcation point. (This follows from arguments in [12] and [11].) These equations have not been extensively employed since the coefficients depend on the p-th order partial derivatives of the components of $H$. However, if $H$ is polynomial, these derivatives can be computed analytically at compile time ([17]). In such cases, the numerical techniques described below might be successfully applied to the Keller/Langford equations (though below a different polynomial system is used).

## 2. The General Method

An implementation of the basic method is discussed in [8]. The technique depends on the fact that arcs bifurcating from $y^*$ can be approximated by arcs in the k-dimensional affine space $\Pi(y^*)$ through $y^*$ and with directions defined by the null space $\mathcal{N}(D(H)(y^*))$ of $D(H)(y^*)$. In particular, for sufficiently small $\delta$ solutions to $H(y) = 0$ on a sphere $\mathcal{S}_\delta(y^*)$ of radius $\delta$ about $y^*$ correspond to minima of $\|H\|^2$ in $\mathcal{S}_\delta(y^*) \cap \Pi(y^*)$ (throughout, $\|\cdot\|$ means Euclidean norm); a precise

one-to-one correspondence can be shown under rather general transversality conditions on the tangent and normal vectors at $y^*$ ([10]).

In [8] minima of $\|H\|$ in $\mathcal{S}_\delta(y^*) \cap \Pi(y^*)$ were found directly by using the simplex method of Nelder and Mead. Since an unspecified number of starting points was required to insure at least one such point occurred in the domain of attraction of each minimum of $\|H\|$, the procedure involved a heuristic. Also, the efficiency of the overall implementation left something to be desired.

Here, we discuss potentially more efficient procedures which in addition are less heuristic. The first of these, presented below, depends on the fact that all solutions to a polynomial system of equations can be approximated by homotopy methods. The second, explained briefly at the end of the paper, is based on a deterministically driven search similar, but not identical, to that used for computing the Brouwer degree of maps ([7]).

Let $H$ be represented by a column vector, and define $\varphi(y) = H^T(y)H(y) = \|H(y)\|^2$. Then the minimization problem is:

$$\min_{y \in \Pi(y^*)} \varphi(y) \quad \text{subject to } y \in \mathcal{S}_\delta(y^*). \tag{2.1}$$

Let $\mathcal{N}(DH(y^*)) = \operatorname{sp}\{v_1, \ldots, v_k\}$ so that $y \in \Pi(y^*) \Rightarrow y = y(a) = y(a_1, \ldots, a_k) = y^* + \sum_{\ell=1}^{k} a_\ell v_\ell$; let $\nabla_a \varphi$ represent the gradient of $\varphi$ with respect to $a$, and set $J = DH(y)$. Then:

$$\nabla_a \varphi = \begin{bmatrix} v_1^T \\ \vdots \\ v_k^T \end{bmatrix} J^T H(y). \tag{2.2}$$

Applying the Lagrange multiplier technique to (2.1), we thus conclude that all solutions of (2.1) are solutions to the system:

$$\begin{bmatrix} v_1^T \\ \vdots \\ v_k^T \end{bmatrix} J^T H(y) + \Lambda \begin{bmatrix} 2a_1 \\ \vdots \\ 2a_k \end{bmatrix} = 0, \qquad \sum_{\ell=1}^{k} a_\ell^2 - \delta^2 = 0 \tag{2.3}$$

of $k+1$ polynomial equations in the $k+1$ unknowns $a_1, \ldots, a_k, \Lambda$. Let $Y = (a_1, \ldots, a_k, \Lambda)$ and define $F : \mathbb{R}^{k+1} \to \mathbb{R}^{k+1}$ to equal the left-hand sides of (2.3). Then finding paths bifurcating from $y^*$ reduces to finding all solutions to the polynomial system $F(Y) = 0$.

Various homotopy algorithms will give, in theory with probability one, all solutions to $F(Y) = 0$ (cf. eg. [2], [3], [4], [14], [15]). We discuss these briefly in the next section; here, we use an example to observe properties of (2.3).

Consider:

$$H_1(x, \lambda) = x[x^4 - (2\lambda - 1)^2], \tag{2.4}$$

the solution set of which occurs in Fig. (2.1). Corresponding to a degenerate case exhibiting symmetry (see [6]), the bifurcation point at $(0, 1/2)$ has two branches intersecting tangentially. The arc directions are of the form $(a_1, a_2)$; the Keller/Langford equations are: $-24a_1a_2^2 = 0$; $a_1^2 + a_2^2 = \delta^2$, with simple roots $(0, \delta)$ and $(0, -\delta)$ and with double roots $(\delta, 0)$ and $(-\delta, 0)$.

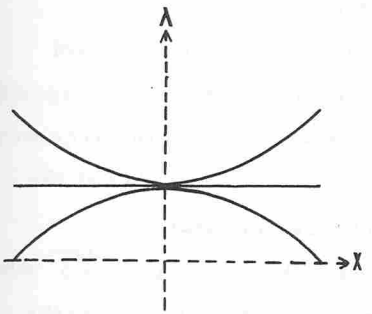


Fig. (2.1)

The system (2.3) consists of a polynomial of degree 9, a polynomial of degree 7, and a polynomial of degree 2, which in general will have 126 complex solutions, counting multiplicities. Among these solutions are distinct roots corresponding to the tangentially intersecting branches, but maxima of $\|H\|$ and non-real solutions not on $\mathcal{S}_\delta(y^*)$ also occur. Such solutions must be ignored or rejected early in the computation for (2.3) to be practical. Note, however, that in all cases only first derivatives enter into (2.3), whereas at least second order derivatives are required for the Keller/Langford equations.

## 4. A Tentative Method

Here, we consider solution algorithms for (2.3) (or for the Keller/Langford equations) involving imbeddings $\tilde{H} : \mathbb{C}^{k+1} \times [0, 1] \to \mathbb{C}^{k+1}$

of the complex extension of F, such that roots of $\tilde{H}(z, 0)$ are known and $\tilde{H}(z, 1) = F(z)$; roots of F are found by following paths from t = 0 to t = 1, ([2], [3], [4], [14], [15], etc.). In general, if the degree of the $\ell$-th component of F is $d_\ell$, there are $ns = \prod_{\ell=1}^{k+1} d_\ell$ solutions, and ns corresponding paths to be followed. Good general continuation method software (see [13], [14], [18], [19], [20], and also [1]) is available, but, due to the size of ns, naive implementations will not be reliable.

For example, the minimum distance between desired roots of F is on the order of $\sqrt[p]{\delta}$ for some p, depending on the degree of contact at $y^*$ (for (2.4), p = 2); the continuation method has been observed to jump from one path to another when the total stepsize has been allowed to exceed this value. Also, scaling problems and path-jumping will occur if the roots of H(z, 0) have norms appreciably different from $\delta$.

Additional problems occur when paths H(y) = 0 intersect $\mathscr{S}_\delta(y^*) \cap \Pi(y^*)$ and the tangents at the points of intersection are perpendicular to $\mathscr{S}_\delta(y^*)$; this would happen, e.g., if k = n + 1 and the arcs were linear rays emanating from $y^*$. In such cases, DF is singular at the solutions, and the roots are found only with reduced accuracy.

At real solutions of F(Y) = 0, $\|a\| = \delta$ and $O(\Lambda) = \sqrt[q]{\delta}$ where q is related to the degree of F. Also, for appropriate $\tilde{H}(z, 0)$, paths leading to real solutions of F will be within $\{Y : \|Y\| \leq M\sqrt[q]{\delta}\}$ for some small M. This allows early rejection of irrelevant solutions.

The method was tested using (2.4), $\delta \doteq .515388$, and using PITCON ([18], [19]). The Garcia/Zangwill homotopy ([2], [14]) was used since we had initial difficulty implementing the potentially better methods in [15]. The maximum predictor step was $.2\delta$, and path following stopped whenever $\|z\| > 5$; roots of $\tilde{H}(z, 0)$ had norms approximately 1. Computations were done on a Honeywell 68/80 using 27 bit mantissas, and $D\tilde{H}$ was computed using central differences. In Table 4.1 paths were oriented in the direction of increasing t, and the tangent-normal corrector parametrization was used. (Rheinboldt's local parametrization gave similar results with less function evaluations, also jumping paths.) The fifth

column gives the determinant of the tangent system at $F = 0$, and the sixth gives the number of evaluations of $\tilde{H}$ for that particular path. Note that root no. 2 and irrelevant roots 1 and 6 were found twice, indicating the algorithm left the path it was following. (Note also that the conjugate of irrelevant solution 3 should have been found but was not.)

Solutions

| no | x | $\lambda - \frac{1}{2}$ | $\Lambda$ | det | nf |
|---|---|---|---|---|---|
| 1 | .5 | .125 | 0 | $1 \times 2^{-2}$ | 80 |
| 2 | .5 | -.125 | 0 | $3 \times 2^{-3}$ | 88(83) |
| 3 | -.5 | .125 | 0 | $4 \times 2^{-3}$ | 83 |
| 4 | -.5 | -.125 | 0 | $3 \times 2^{-3}$ | 126 |
| 5 | 0 | .515388 | 0 | $3 \times 2^{0}$ | 95 |
| 6 | 0 | -.515388 | 0 | $3 \times 2^{0}$ | 88 |

Irrelevant Solutions

| no | x | $\lambda - \frac{1}{2}$ | $\Lambda$ | det | nf |
|---|---|---|---|---|---|
| 1 | .515388 | 0 | -.0124 | $1 \times 2^{-2}$ | 96(91) |
| 2 | 2.062i | +2.125 | 0 | $1 \times 2^{36}$ | 208 |
| 3 | 2.062i | -2.125 | 0 | $1 \times 2^{38}$ | 220 |
| 4 | -.2924 | -.4244 | -.2439 | $2 \times 2^{1}$ | 87 |
| 5 | -.2924 | .4244 | -.2439 | $1 \times 2^{1}$ | 117 |
| 6 | .2924 | -.4244 | -.2439 | $2 \times 2^{1}$ | 104(106) |
| 7 | -.515388 | 0 | -.0124 | $2 \times 2^{-3}$ | 87 |
| 8 | -2.062i | 2.125 | 0 | $3 \times 2^{37}$ | 253 |

Table 4.1

## 5. A Possible Alternative

Adjustments to the above scheme may make it more practical; it also may be practical when applied to the Keller/Langford equations instead of (2.3). However, the problem of finding all solutions to (2.3) has several characteristics which make an alternative method practical; these

are (1) the fact that $k$ is small or can be made small by use of symmetry; (2) existence of large numbers of solutions, distributed more or less uniformly over $[\Pi(y_*) \cap \mathcal{S}_\delta(y^*)] \times [-K, K]$. In this case, use of a generalized method of bisection as described in [7] and [9] becomes more attractive.

In such a generalized bisection method, simplices would not be further subdivided according to sign changes or whether a topological degree were nonzero. Instead, an analysis of the values of the components of $F$ and bounds on the norm of $D^2F$ (or more generally, Lipschitz constants for the derivatives of the components of $F$) would be used to indicate whenever a component of $F$: (i) could not vanish on a simplex, or (ii) could vanish at most once on any line in the simplex; if (i) held for one component, if (ii) held for all components, or if the diameter of the given simplex were smaller than a given tolerance, then triangulation of that simplex would stop.

Generalized bisection has been considered non-competitive in general. However, the large number of solutions and need to obtain them all makes generalized bisection appropriate for their isolation. Details and convergence proofs will be given in a later work.

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