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On the numerical detection of a bifurcation simplex in a curve

Abstract We present a numerical method which detects the presence and position of a *bifurcation simplex*, a regular (k + 1)-dimensional simplex, which may be considered as a "fat bifurcation point", in the curve of zeroes of the C^1 map $f : \mathbb{R}^{k+1} \to \mathbb{R}^k$. On the other hand, a bifurcation simplex appears in the neighbourhood of the bifurcation point, meaning that we have a method to approximately locate the bifurcation point as well. The method does not require any estimation of the derivative of the function f and refers to the values of the map f only through the vertices of certain triangulation. The bifurcation simplex is detected by a change in the value of the Brouwer degree of the restriction of the map f to the appropriate k-simplex.

2010 Mathematics Subject Classification: 65H10, 65H20.

 $Key\ words\ and\ phrases:$ path following algorithm, bifurcation point, bifurcation simplex.

1. Introduction. Let $f : \mathbb{R}^{k+1} \to \mathbb{R}^k$ be a C^1 map and the C^1 curve $\gamma : (a, b) \to \mathbb{R}^{k+1}$ consist of the zeroes of the map f, i.e. for each $t \in (a, b)$ the equality $f(\gamma(t)) = 0$ holds. We will consider here an algorithm tracing the curve γ numerically. Algorithms of this class have been developed since the 1960s and, for an extensive review of different concepts, we would like to direct the reader to the monography [1] and a shorter review article by the same authors [2]. Now we would like to mention that there are two main classes of algorithms: piecewise-linear methods (PL-methods) and predictor-corrector methods (PC-methods), and briefly describe both of them.

PL-methods start with a triangulation \mathbb{T} of the domain and approximation of the map f using a piecewise affine function $f_{\mathbb{T}}$, extending f from its values at the vertices of the triangulation. Then the set of zeroes of the map $f_{\mathbb{T}}$ is identified, starting from a simplex known to contain a zero of the function f.

The class of PC-methods starts with another idea. For a smooth map f, if we assume that the solution set is, locally, a simple C^1 curve, we can

 $^{^{*}}$ This publication is co-financed by the European Union as part of the European Social Fund within the project Center for Applications of Mathematics (project no. UDA–POKL.04.02.00–00–108/11–00)

estimate the next point in the curve by estimating the value of the derivative of the curve's parametrization. This leads directly to a certain initial value problem for a first order ordinary differential equation, which may be solved numerically. It is generally observed that both methods work very well when the set of zeroes is a simple curve - i.e. is locally homeomorphic to the interval. Problems appear when there is a *bifurcation point* in the curve.

The concept of a bifurcation point is defined in a very general way (see the classic book [3]), but here we will follow Definition 8.1.1. from [1]. This approach better matches the finite-dimensional case. Moreover, in the considered case, we do not have a natural parameter in our problem: the parameter λ may be chosen as one that parametrizes the curve γ of the zeroes of the map f, but this is not the kind of input data which is naturally related to the map f.

DEFINITION 1.1 Let us assume that $f : \mathbb{R}^{k+1} \to \mathbb{R}^k$ is a continuous map and that we have such an injective C^1 curve $\gamma : (a, b) \to \mathbb{R}^{k+1}$ that $f(\gamma(t)) = 0$. The point $\gamma(t_0)$, where $t_0 \in (a, b)$, is called a bifurcation point of the map f, if there exists such an $\varepsilon > 0$ that each open neighbourhood $U \subset \mathbb{R}^{k+1}$ of $\gamma(t_0)$ contains zeroes of f which do not belong to $\gamma(t_0 - \varepsilon, t_0 + \varepsilon)$.

According to this definition, a bifurcation point is always one of the points in the known curve of the zeroes of the map f. We will call this curve the *trivial solutions* curve. Of course the implicit function theorem is of great help here, as it provides a necessary condition for a bifurcation point to exist.

COROLLARY 1.2 If $\gamma(t_0)$ is the bifurcation point of the C^1 map $f : \mathbb{R}^{k+1} \to \mathbb{R}^k$, then the rank of the derivative $Df(\gamma(t_0))$ is not maximal (i.e. it is less than k).

These ideas have been extensively studied by many authors (initially [4], [5], more recently in [10]) in the context of maps $f : \mathbb{R} \times E \to E$, where E is a Banach space and $f(\lambda, 0) = 0$, thus having a trivial line of solutions identified as $\gamma(\lambda) = (\lambda, 0)$ for $\lambda \in \mathbb{R}$. In this context, a bifurcation point is one which contains, in any open neighbourhood, nontrivial solutions, i.e. such zeroes (λ, x) of f, that $x \neq 0$. Sufficient conditions for the existence of a bifurcation point are given in terms of the properties of the derivative of the map f at a given trivial solution $(\lambda_0, 0)$. On the other hand, sufficient conditions for the existence of bifurcation points may be expressed in terms of some topological invariants. These two approaches are clearly related, with the topological approach being more general, because it may be considered in the context of maps f, which are not necessarily smooth. We should mention here in particular the theorem of Krasnoselski (see the classic book [9], also [7] where some more recent results are presented); which has many known generalizations. These generalizations lead to the conclusion that a change in the topological (Leray-Schauder) degree is a sufficient condition for a bifurcation point to appear (see e.g. Theorem 2.5 from [8] – the theorem given below is actually a weaker form of this global bifurcation theorem).

Theorem ([8], Theorem 2.5). Let $F : \mathbb{R} \times E \to E$ be completely continuous such that $F(\lambda, 0) = 0$ for $\lambda \in \mathbb{R}$. Let $a, b \in \mathbb{R}$ (a < b) be such that u = 0 is an isolated solution of the equation,

$$u - F(\lambda, u) = 0, \qquad u \in E,$$

for $\lambda = a$ and $\lambda = b$, where (a, 0), (b, 0) are not bifurcation points of $u - F(\lambda, u)$. Furthermore, assume that

$$\deg(I - F(a, \cdot), B(0, r)) \neq \deg(I - F(b, \cdot), B(0, r)),$$

where B(0,r) is an isolating neighbourhood of the trivial solution. Then there exists such a bifurcation point $(\lambda, 0)$ of the map $u - F(\lambda, u)$ that $\lambda \in (a, b)$.

This idea has inspired numerous results (for a review of the concept and different results we again refer the reader to [9] and [7] mentioned earlier). In this paper we will also follow this concept, indicating how a change in topological degree (the Brouwer degree in a finite dimensional case) may be used to show numerically the existence and location of a bifurcation point in the curve of zeroes of the map f being traced.

Both the PL and PC methods experience problems in the neighbourhood of bifurcation points. The most important problem for both methods is that, at each step of the algorithm, at most one new point is indicated on the curve (door-in-door-out property). Hence, in the case of bifurcation points, we may choose at most one of the possible branches. On the other hand, we should also mention here that the problem of locating bifurcation points on a curve has been extensively studied and there are known methods which enable detection of the bifurcation points appearing within a single predictor-corrector step (see Chapter 8 of [1], particularly Theorem 8.1.14). This theorem states that when the C^1 curve γ crosses a simple bifurcation point at some point t_0 , then the determinant of the matrix, whose first columns are formed by $Df(\gamma(t))$ and last column by $\gamma'(t)$, changes its sign. It is worth observing that the assumption

$$\det \left[Df(\gamma(t)), \gamma'(t) \right] > 0$$

defines the orientation that is followed by the regular Euler prediction method. A single Euler prediction step (as described in [1], algorithm 3.3.7) is given by

$$u_{i+1} = u_i + h\mathcal{T}(Df(\gamma(t))),$$

where $\mathcal{T}(Df(\gamma(t)))$ is the tangent vector induced by the matrix $Df(\gamma(t))$ (see [1], Definition 2.1.7). When the bifurcation point is crossed, the orientation of the vector $\mathcal{T}(Df(\gamma(t)))$ changes and the method starts to move backwards.

In order to compensate for this effect we should update the previous formula to

$$u_{i+1} = u_i + wh\mathcal{T}(Df(\gamma(t))),$$

where $w \in \{-1, +1\}$ is switched to the opposite value each time a bifurcation point is detected (see Algorithm 8.1.17 in [1] for details).

Recently, in [6] a new approach to path following was presented. It is referred to as FSC (Follow Sign Changes) algorithm. At each step, the method builds a regular (k + 1)-simplex¹ and based on the signs of the coordinate functions of the map f at the simplex vertices, some of the faces of the simplex are suggested as those which should be followed. Therefore, if there is a bifurcation point inside the simplex, the algorithm may trace all the branches which start there. Numerical experiments presented in [6] show that the algorithm works well in a situation where 8 branches emanate from a bifurcation point.

The algorithm selects the face F_i of the simplex only when each coordinate function of the map f changes sign at the vertices belonging to the face F_i . The topological argument here is that the face showing the sign changes may have a nonzero topological (Brouwer) degree for a map f restricted to the face F_i . Actually, it is shown that when there exists a coordinate with a constant sign, then the Brouwer degree equals zero. We will examine this issue more deeply in the next section.

Below, we are going to suggest a modification of the FSC algorithm, which allows us to detect whether a bifurcation has appeared at a given step of the algorithm or not. We are generally following the idea given in Chapter 8 of [1]. However, we do not refer to the derivative Df(x), but instead suggest a certain affine map, which may be used to detect a change in the Brouwer degree.

We must take into account the fact that any numerical method looking at Euclidean space with a certain resolution may face natural difficulties in precisely locating a bifurcation point. Hence, it might be a good idea to introduce the more suitable concept of *the bifurcation simplex* instead. So, when we look at simplices as "fat points", it is reasonable to suggest the following definition.

DEFINITION 1.3 We call the (k+1)-simplex $\sigma \subset \mathbb{R}^{k+1}$ a bifurcation simplex of the map f if there exist at least 3 different faces of the simplex containing the zeroes of the map f, and the set $f^{-1}(0) \cap \partial \sigma$ is not contained in any sum of two faces of σ .

This definition may seem slightly technical, but we need to exclude the situation when there is a single zero of f in $\partial \sigma$ lying at a vertex of σ , or two zeroes belonging to different edges. Obviously, if the bifurcation simplex

¹We call a simplex regular if all its edges have the same length.

 σ is identified, it does not necessarily mean that there exists a bifurcation point in the curve γ inside the simplex σ . Both the situation of two curves intersecting at a bifurcation point, and two curves passing close to each other inside the simplex σ may make the simplex σ a bifurcation simplex. This just means that, at the resolution given by the simplex edge, we are not able to distinguish between these two situations.

Moreover, a simplex containing a bifurcation point is not necessarily a bifurcation simplex. A bifurcation simplex may even appear relatively far from the corresponding bifurcation point, but this happens when two curves are so close to each other that we cannot distinguish them at the resolution imposed by the simplex edge (see Figure 1).



a) a bifurcation simplex close to the bifurcation point b) a bifurcation simplex far from the bifurcation point

Figure 1: With a fixed resolution (simplex edge length) the bifurcation point not necessarily belongs to the bifurcation simplex. Bifurcation simplices are shaded.

Although there does not exist any universal relation between a bifurcation point and the corresponding bifurcation simplex, we can see that a bifurcation simplex is a practical approximation of a bifurcation point at a fixed resolution.

At the end of the paper we specify some rigorous conditions (see Lemma 3.5) that allow us to identify a bifurcation simplex. Unfortunately, the conditions are not easy to verify effectively. Hence, we give some heuristic methods and arguments aimed at developing a practical implementation.

2. Degree with respect to a k-simplex. In this section we will look more closely at the local Brouwer degree of the map investigated in [6].

We are going to check not only whether the degree is nonzero or not, but also whether it equals +1 or -1. Also, we will show that this leads to a sufficient condition (of Krasnoselski type) for the existence of a bifurcation point. Moreover, it will be easy to check this condition numerically.

Let us start with the basic notation which will be used below. Let $e_i \in \mathbb{R}^k$ be the *i*-th vector of the standard basis i.e. $e_i = (0, ..., 0, 1, 0, ..., 0)$, where the only nonzero value is the *i*-th coordinate. For consistency, let us denote $e_0 = 0$. Then $\Delta \subset \mathbb{R}^k$ equals $\Delta = \operatorname{conv}\{e_0, e_1, ..., e_k\}$, i.e. it is the (closed) simplex spanned by $e_0, e_1, ..., e_k \in \mathbb{R}^k$. Here, by convA we mean the convex hull of the set A. Let Δ_0 denote the set of interior points of Δ . We will later refer to the concept of the k-simplex V as a convex hull of the set of k + 1points $v^0, v^1, ..., v^k \in \mathbb{R}^{k+1}$, but additionally we assume it is homeomorphic to the standard simplex Δ . Equivalently, we may require that the vectors $v^i - v^0$ for i = 1, ..., k are linearly independent (following [1] we call such points affine independent). When we define the order of the vertices of V(we may think of this as setting the orientation in V), we have exactly one affine map $j_V : \Delta \to \mathbb{R}^{k+1}$ given by

$$j_V(e_i) = v^i, \qquad i = 0, 1, ..., k.$$

For this map we can see that $j_V(\Delta) = V$.

In the remainder of this section we assume that $\gamma : (a, b) \to \mathbb{R}$ is the C^1 curve of the zeroes of the map f, i.e. $f(\gamma(t)) = 0$ for $t \in (a, b)$.

LEMMA 2.1 Let us assume that such a k-simplex $V \subset \mathbb{R}^{k+1}$ is given that

$$j_V(\Delta) \cap f^{-1}(0) = j_V(\Delta_0) \cap f^{-1}(0) = \{\gamma(t_0)\}$$

and $\gamma(t_0)$ is a regular zero of the map f. Moreover, let us assume that the curve γ passes transversally through the simplex V. This may be described by the following condition:

(B) the vectors $v^1 - v^0, v^2 - v^0, ..., v^k - v^0, \gamma'(t_0)$ are linearly independent (i.e. form the basis of \mathbb{R}^{k+1}).

Then the Brouwer degree $\deg(f \circ j_V, \Delta_0)$ is well defined and equals ± 1 .

PROOF By the assumptions of the Lemma, the map $f \circ j_V$ has exactly one zero $x_0 \in \Delta$ and $x_0 = j_V^{-1}(\gamma(t_0)) \in \Delta_0$. It is enough to show that this is a regular zero of the map $f \circ j_V$. As we can see, the derivative Dj_V is the matrix whose *i*-th column equals $v^i - v^0$ for i = 1, ..., k.

Now we are going to show that the only zero of the linear map $Df(x_0) \circ Dj_V$ equals 0. So let $h \in \mathbb{R}^k$ be such that

$$Df(j_V(x_0))(Dj_Vh) = 0.$$

Hence, $Dj_V h \in KerDf(j_V(x_0))$. The kernel of the linear map $Df(j_V(x_0))$ is a subspace of dimension 1 and is spanned by $\gamma'(t_0)$. On the other hand,

the vector $Dj_V h$ is spanned by $v^1 - v^0, v^2 - v^0, ..., v^k - v^0$. By assumption (B) we can see that h = 0.

Let us call the value

 $\deg(f \circ j_V, \Delta_0)$

the degree of the map f with respect to the k-simplex V. Below, we are going to present two properties of this degree.

First, we will show that the degree with respect to the k-simplex depends continuously on V(t) for $t \in (\alpha, \beta)$. We can think of this as a simplex V(t)sliding along the curve γ .

LEMMA 2.2 Let us assume that the family of k-simplices $V(t) \subset \mathbb{R}^{k+1}$, $V(t) = \operatorname{conv}\{v^0(t), v^1(t), ..., v^k(t)\}$ satisfies

$$j_{V(t)}(\Delta) \cap f^{-1}(0) = j_{V(t)}(\Delta_0) \cap f^{-1}(0)$$

for $t \in (\alpha, \beta)$. Moreover, let us assume that the vertices $v^i(t)$, (i = 0, 1, ..., k) change continuously. Then the degree

$$\deg(f \circ j_{V(t)}, \Delta_0)$$

is constant.

PROOF This observation is the direct consequence of the homotopy property of the Brouwer degree. Let us fix two values $t_1, t_2 \in (\alpha, \beta)$ and the homotopy $h: [0, 1] \times \Delta \to \mathbb{R}^k$ given by

$$h(\tau, x) = f(j_{V(\tau t_1 + (1 - \tau)t_2)}(x)).$$

Our assumptions guarantee that this homotopy does not have a zero on the boundary $\partial \Delta$, hence

$$\deg(f \circ j_{V(t_1)}, \Delta_0) = \deg(f \circ j_{V(t_2)}, \Delta_0).$$

Now we are going to show that given a k-simplex $V \subset \mathbb{R}^{k+1}$ satisfying the assumptions of Lemma 2.1 with $\gamma(t_0)$ being a regular zero of the map f, we may change it slightly, while ensuring that the condition (B) remains satisfied.

LEMMA 2.3 Let the k-simplex $V_0 \subset \mathbb{R}^{k+1}$, $V_0 = \operatorname{conv}\{v_0^0, v_0^1, ..., v_0^k\}$ satisfy $j_{V_0}(\Delta) \cap f^{-1}(0) = j_{V_0}(\Delta_0) \cap f^{-1}(0) = \{\gamma(t_0)\},$

where $\gamma(t_0)$ is a regular zero of f. Moreover, let us assume that condition (B) is satisfied. Then there exists such an $\varepsilon > 0$ that for all V = $\operatorname{conv}\{v^0, v^1, ..., v^k\}$ satisfying $|v^i - v_0^i| < \varepsilon$, the k-simplex V satisfies

(i) $j_V(\Delta) \cap f^{-1}(0) = j_V(\Delta_0) \cap f^{-1}(0) = \{\gamma(t_V)\}, \text{ for some } t_V;$

(ii) the vectors $v^1 - v^0, v^2 - v^0, ..., v^k - v^0, \gamma'(t_V)$ are linearly independent (i.e. condition (B) is satisfied for the simplex V).

PROOF Because $0 \notin (f \circ j_{V_0})(\partial \Delta)$ and because of the continuous dependence of $f \circ j_V$ on V, we can see that, for some positive $\varepsilon > 0$, for all $V = \operatorname{conv}\{v^0, v^1, ..., v^k\}$ satisfying $|v^i - v_0^i| < \varepsilon$ we have $0 \notin (f \circ j_V)(\partial \Delta)$. This implies that all the maps $f \circ j_V$ may be joined by homotopy to $f \circ j_{V_0}$, hence the value of the Brouwer degree $\operatorname{deg}(f \circ j_V, \Delta_0)$ remains constant (i.e. nonzero). Consequently, the set $j_V(\Delta_0) \cap f^{-1}(0)$ is a nonempty one.

Now let us check if it is possible for the set $j_V(\Delta_0) \cap f^{-1}(0)$ to contain two points for V being arbitrarily close to V_0 . Let $x_n, y_n \in V_n, x_n \neq y_n$, where $V_n \to V_0$ and $f(x_n) = f(y_n) = 0$. Taking appropriate subsequences, we may assume that all the sequences $\{x_n\}, \{y_n\}$ and $\{(x_n - y_n)/|x_n - y_n|\}$ are convergent. Since x_n and y_n converge to a zero of the map f belonging to V_0 , their common limit must be x_0 . Let us assume that

$$\frac{x_n - y_n}{|x_n - y_n|} \to p_0 \in \mathbb{R}^{k+1}.$$

As we can observe, p_0 is a nonzero vector spanned by $\{v_0^i - v_0^0 : i = 1, 2..., k\}$. However, $f(x_n) = f(y_n) = 0$ implies that the point p_0 belongs to the kernel of $Df(x_0)$. The kernel is one-dimensional, spanned by $\gamma'(t_0)$, which is not linearly dependent on $\{v_0^i - v_0^0 : i = 1, 2..., k\}$. This creates a contradiction and shows that, for V close to V_0 , the set of zeroes contains at most one element.

Therefore, we may conclude that, for V close enough to V_0 , there exists exactly one zero of f in V. Because the zeroes converge to x_0 as V converges to V_0 , by the implicit function theorem they must belong to the curve γ . This completes the proof.

3. Algorithm for identifying degree changes. We are now going to refer the observations presented in the previous section to the algorithm presented in the paper [6]. Let us now briefly describe the FSC algorithm presented in the above-mentioned paper.

- 1. The algorithm starts from an initial zero of the map f and an initial (k+1)-simplex σ_0 surrounding this zero.
- 2. For a given simplex σ_i , we identify its k-dimensional faces, satisfying the condition

(C1) for a k-dimensional face V there exists such a coordinate function $f_j, j \in \{1, ..., k\}$ that the function f_j has constant sign for all the points c in the face V boundary.

These faces will be excluded from further processing. In practical implementation, the sign of the coordinate functions f_j is checked only at vertices of face V.

3. For each k-dimensional face of σ_i , which was not discarded in the previous step, a pivoting step is performed and a regular (k + 1)-simplex σ'_i , different from σ_i is found. Within the pivoting step, for a given k-dimensional face V of σ_i , we look for two such vertices v_i and v'_i , that $\operatorname{conv}(V, w)$, for $w \in \{v_i, v'_i\}$, forms a regular simplex. Of course one of these simplices is σ_i and the other is σ'_i .

Then it is checked whether σ'_i was processed before. If not, then σ'_i is placed into a stack for further processing.

- 4. Take the next (k + 1)-dimensional simplex from the stack and return to step 2.
- 5. The algorithm requires a stop condition, e.g. we exclude all the faces which contain at least one vertex outside a predefined cube.

The center of each (k + 1)-simplex placed on the stack is considered to be an approximation of a zero of f.

The idea is presented in Figure 2 in the 2-dimensional case. This picture should only be seen as a presentation, as it clearly shows the geometrical intuitions behind the method. Still, the 2-dimensional case is rather trivial, and to justify it, one does not need any arguments regarding topological degree.



Figure 2: Tracing a curve in \mathbb{R}^2 .

Let us note that, instead of taking the centre of a simplex as an approximation of a zero of the map f, we may treat the entire simplex as a "fat point", which definitely contains the zero of the map f, and the polyhedron built of the identified simplices as an approximation of the curve.

We are now going to focus on the special case of a curve which consists only of regular zeroes of the map f, implying that the curve does not have any bifurcation points. LEMMA 3.1 Let us assume that the curve γ of zeroes of the map f passes through the (k + 1)-simplex $\sigma \subset \mathbb{R}^{k+1}$ in such a way that $f^{-1}(0) \cap \partial \sigma =$ $\{\gamma(\alpha), \gamma(\beta)\}$ and $\gamma(\alpha) \in j_V(\Delta_0), \ \gamma(\beta) \in j_W(\Delta_0), \ where V \ and W \ are$ $different faces of the simplex <math>\sigma$ such that $V = \operatorname{conv}\{v^0, v^1, ..., v^k\}, \ W =$ $\operatorname{conv}\{w^0, v^1, ..., v^k\}$. Then

$$\deg(f \circ j_V, \Delta_0) = \deg(f \circ j_W, \Delta_0).$$

PROOF A sample situation described in the assumptions above (in the 3dimensional case, i.e. for k = 2) is presented in Figure 3.



Figure 3: Curve passing through a 3-simplex.

We will refer to Lemma 2.2. First, we will define the family of k-simplices joining V and W by

$$V(\tau) = \operatorname{conv}\{(1-\tau)v^0 + \tau w^0, v^1, ..., v^k\}, \qquad \tau \in [0, 1].$$

Let us take any $x \in \partial \Delta$, with $x = (x_1, ..., x_k)$ and denote $x_0 = 1 - (x_1 + ... + x_k)$. This means that $(x_0, x_1, ..., x_k)$ may be interpreted as the barycentric coordinates of the point $x \in \Delta$. If $x \in \partial \Delta$, then at least one of its barycentric coordinates must equal 0. Let us observe that

$$j_{V(\tau)}(x) = \tau x_0 w^0 + (1 - \tau) x_0 v^0 + x_1 v^1 + \dots x_k v^k \in \sigma,$$

and the values τx_0 , $(1-\tau)x_0$, $x_1, ..., x_k$ are the barycentric coordinates of the point $j_{V(\tau)}(x)$ in the (k+1)-simplex σ . When $x_i = 0$ for some i = 0, 1, ..., k, then this point belongs to the boundary $\partial \sigma$. Also, the only zeroes of f which belong to $\partial \sigma$ are $\gamma(\alpha)$ and $\gamma(\beta)$, but their barycentric coordinates in σ require that $\tau = 0$ or $\tau = 1$, as appropriate. This implies that $x \in \Delta_0$, so it cannot belong to $\partial \Delta$.

This means that

$$j_{V(t)}(\partial \Delta) \cap f^{-1}(0) = \emptyset$$

so the assumptions of Lemma 2.2 are satisfied and the degree must be constant

$$\deg(f \circ j_V, \Delta_0) = \deg(f \circ j_W, \Delta_0).$$

REMARK 3.2 As we can see, it does not matter how the vertices are labeled, so we have the same conclusion for any two faces with $v^i \neq w^i$ (not necessarily for i = 0).

Now, as a simple consequence of Lemma 3.1, we may give a sufficient condition for the existence of a bifurcation simplex.

THEOREM 3.3 Let us assume that there exist two faces $V = \operatorname{conv}\{v^0, v^1, ..., v^k\}$ and $W = \operatorname{conv}\{w^0, v^1, ..., v^k\}$ of the (k+1)-simplex $\sigma \in \mathbb{R}^{k+1}$, such that

 $\deg(f \circ j_V, \Delta_0) \neq \deg(f \circ j_W, \Delta_0),$

and that both values are nonzero. Then there exists a face \hat{V} of σ , different from V and W, which contains a zero of f, so σ is a bifurcation simplex.

PROOF From the assumptions of the present theorem, we know that there is no zero of the map f on the boundary of the faces V and W. Let us assume now that there is no zero of the map f belonging to some other face of σ , i.e.

$$f^{-1}(0) \cap (\partial \sigma \setminus (V \cup W)) = \emptyset.$$

In this case, we may again apply Lemma 2.2 as we did in the proof of Lemma 3.1, and see that

$$\deg(f \circ j_V, \Delta_0) = \deg(f \circ j_W, \Delta_0),$$

which contradicts our assumption.

Hence, there must exist a zero of the map f belonging to $\partial \sigma \setminus (V \cup W)$. However, because the degrees deg $(f \circ j_V, \Delta_0)$ and deg $(f \circ j_W, \Delta_0)$ are nonzero, we are certain that there are zeroes of f belonging to V and W, so the set $f^{-1}(0) \cap \partial \sigma$ cannot be covered by two faces of the simplex σ .

REMARK 3.4 One could ask how it may be guaranteed that both degrees are nonzero. We can see that by Lemma 2.1 it is sufficient that simplex $\sigma \subset \mathbb{R}^{k+1}$ has two faces satisfying condition (B). This happens, for example, when the face V is orthogonal to $\gamma'(t_0)$. Moreover, Lemma 2.3 shows that when we disturb such an orthogonal simplex a little bit, it still satisfies the assumptions of Lemma 2.1.

In order to apply Theorem 3.3, we will need a method to verify whether there is a change in the Brouwer degree between two faces of the simplex σ . A sufficient condition and its practical approximation will be presented below.

Let us now concentrate on the k-simplex $V \subset \mathbb{R}^{k+1}, V = \operatorname{conv}\{v^0, v^1, ..., v^k\}$ and the values of the map f at the vertices of V. We will try to replace the map $f \circ j_V : \Delta \to \mathbb{R}^k$ with such an affine map $g_V : \Delta \to \mathbb{R}^k$ that $g_V(e_i) = f(v^i)$. We will indicate sufficient conditions for the maps $f \circ j_V$ and g_V to be joined by homotopy, and we will keep the value of the Brouwer degree constant. Then we may observe that it is easy to calculate the value of the degree of the map g_V .

Let us assume now that

$$f^{-1}(0) \cap j_V(\Delta) = f^{-1}(0) \cap j_V(\Delta_0).$$

We are particularly interested in the situation when the set of zeroes $f^{-1}(0) \cap j_V(\Delta)$ may be linearly separated from the image of each face of the simplex Δ . This will be specified much more precisely in the assumptions of the next lemma.

LEMMA 3.5 Let us assume that

(LS) for each i = 0, 1, ..., k there exists such a linear functional $\varphi_i : \mathbb{R}^k \to \mathbb{R}$ that

$$\varphi_i(f(j_V(x))) > 0,$$

for all $x \in \Delta_i$, where $\Delta_i = \operatorname{conv}\{e_j : j \neq i\}$ is the (k-1)-dimensional face of Δ , not containing e_i .

Then the map $f \circ j_V$ may be joined by homotopy to the affine map $g_V : \Delta \to \mathbb{R}^k$ given by $g_V(e_i) = f(j_V(e_i))$.

PROOF We can see that

$$g_V(x_0, x_1, \dots, x_k) = f(v^0)x_0 + f(v^1)x_1 + \dots + f(v^k)x_k,$$

where $(x_0, x_1, ..., x_k)$ are the barycentric coordinates of the point $x \in \Delta$.

Then, for any $x \in \partial \Delta$, we have $x \in \Delta_i$ for some $i \in \{0, 1, ..., k\}$, and hence the *i*-th barycentric coordinate $x_i = 0$. Thus $\varphi_i(f(v^j)) > 0$ for $j \neq i$, and hence $\varphi_i(g_V(x)) > 0$ and $\varphi_i(f(j_V(x))) > 0$ for all $x \in \Delta_i$. It follows that, for any $\tau \in [0, 1]$ and $x \in \Delta_i$

$$\varphi_i(\tau f(j_V(x)) + (1-\tau)g_V(x)) > 0.$$

Hence, the homotopy $h(\tau, x) = \tau f(j_V(x)) + (1 - \tau)g_V(x)$ is well defined and this completes the proof.

REMARK 3.6 If, for a given face Δ_i of Δ , there exists a coordinate function $f_j \circ j_V$ which has a constant sign on Δ_i , then the linear functional φ_i may be chosen to be a projection (maybe with the reversed sign) onto the j-th coordinate vector. However, as we can easily see, if condition (C1) is satisfied, then it is not possible that such a coordinate function exists for all faces Δ_i . In other words, there must exist at least one face Δ_i such that each coordinate of the function f changes its sign at the vertices of the face Δ_i . In this situation, we must look for a function φ_i which is not a projection onto some coordinate vector.

The main intuition behind the (LS) condition is that we can approximate the image of the k-simplex V by the simplex spanned by the image of the vertices of the simplex, i.e.

$$f(\mathrm{conv}\{v^0,v^1,...,v^k\})\approx\mathrm{conv}\{f(v^0),f(v^1),...,f(v^k)\}.$$

The main motivation here is that

$$f(\operatorname{conv}\{v^0, v^1, ..., v^k\}) \subset N_{\omega_f(h)}(\operatorname{conv}\{f(v^0), f(v^1), ..., f(v^k)\}),$$

where ω_f is the modulus of continuity of the function f, h is the length of the simplex's edges and

$$N_{\varepsilon}(A) = \{y : \exists_{x \in A} | y - x| \le \varepsilon\}$$

denotes the closed ε -neighbourhood of the compact set A. To show this, let us take $y \in f(\operatorname{conv}\{v^0, v^1, ..., v^k\})$, meaning that y = f(x) for some $x \in \operatorname{conv}\{v^0, v^1, ..., v^k\}$. Then $|x - v^i| \leq h$ for some vertex v^i implying that $|f(x) - f(v^i)| \leq \omega_f(h)$.

For a fixed $i \in \{0, 1, ..., k\}$ and the (k - 1)-simplex

$$V^f_i = \operatorname{conv}\{f(v^0), f(v^1), ..., f(v^{i-1}), f(v^{i+1}), ..., f(v^k)\},$$

there exists such a linear functional $\varphi_i : \mathbb{R}^k \to \mathbb{R}$ that $\varphi_i(y) = c > 0$ is constant for all $y \in V_i^f$.

Assuming $f(V_i) = f(j_V(\Delta_i))$ is close to V_i^f , we can expect that

$$\varphi_i(f(j_V(\Delta_i))) > 0,$$

i.e. the (LS) condition is satisfied. Figure 4 shows examples of a situation in which (LS) is satisfied and one in each (LS) is not satisfied.

Following this intuition we may, from now on, assume that the (LS) condition is satisfied by each k-simplex considered. In this case, it is easy to calculate the value of the Brouwer degree deg (g_V, Δ_0) , as it is the sign of the determinant of the matrix with *i*-th column equal to $f(v^i)$ (naturally, when $g_V^{-1}(0) \in \Delta_0$).

Therefore, we can now see that by keeping the vertices of the k-simplices V ordered and keeping the order unchanged, we may detect when the degree $\deg(f \circ j_V, \Delta_0)$ changes. In order to do so, we just need to slightly modify the FSC algorithm as follows:

(a) at each step the k-simplex V (i.e. each face of the (k + 1)-dimensional simplex σ) is described by an *ordered* sequence of vertices

$$V = \operatorname{conv}\{v^0, v^1, ..., v^k\}$$



Figure 4: Examples of when the LS condition is satisfied (a) and is not satisfied (b). The shaded area is the simplex spanned by $f(v_1)$, $f(v_2)$ and $f(v_3)$. The bigger area is the image of the simplex spanned by v_1 , v_2 and v_3 .

Another k-dimensional face W of the simplex σ has one of the vertices v^i replaced by another vertex w of the simplex σ . Then the face W should be identified as the ordered set of vertices

$$W = \operatorname{conv}\{v^0, ..., v^{i-1}, w, v^{i+1}, ..., v^k\};$$

(b) in the case when $\deg(f \circ j_V, \Delta_0) \neq \deg(f \circ j_W, \Delta_0)$ i.e.

$$\begin{split} & \operatorname{sign} \det[f(v^1), ..., f(v^{i-1}), f(v^i), f(v^{i+1}), ..., f(v^k)] \neq \\ & \operatorname{sign} \det[f(v^1), ..., f(v^{i-1}), f(w), f(v^{i+1}), ..., f(v^k)]; \end{split}$$

we know that σ is a bifurcation simplex for the map f.

The modification presented above allows us to detect whether the simplex σ is a bifurcation simplex. We should note that the FSC algorithm may indicate more than two simplex faces by itself, but this does not mean that the investigated simplex is a bifurcation simplex. It may happen that some faces indicated by the FSC algorithm only contain *spurious solutions*. The FSC algorithm by itself may follow multiple bifurcation branches, as well as the branches of spurious solutions, but we never know which case holds. Using the change suggested above we can say whether the investigated simplex *really is* a bifurcation simplex, thus improving the pure FSC algorithm.

Additionally, it may prove very interesting if we can detect whether there exists a bifurcation simplex *somewhere* on the curve γ . We have two ksimplices V and W intersected by the curve $\gamma(t)$ and want to see whether the value of deg $(f \circ j_V, \Delta_0)$ equals deg $(f \circ j_W, \Delta_0)$ or not. We would like to be able to draw the conclusion that if deg $(f \circ j_V, \Delta_0) \neq \text{deg}(f \circ j_W, \Delta_0)$, then there exists a bifurcation simplex on the curve γ somewhere between the faces V and W. It is quite obvious that, when we can join the face V to the face W by a sequence of (k + 1)-simplices, maintaining the orientation of the simplices, and keeping the curve γ in the interior of the sum of the simplices (just like the FSC algorithm does), then a change in the degree implies the existence of a bifurcation simplex.

Acknowledgement. This publication is co-financed by the European Union as part of the European Social Fund within the project Center for Applications of Mathematics. I would also like to thank the anonymous referee for all comments and remarks that considerably improved the paper. I would also like to thank editors of Mathematica Applicanda for numerous comments improving the language of this paper.

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Metoda wykrywania sympleksów bifurkacji na krzywej Jacek Gulgowski

Streszczenie W pracy podany jest opis metody numerycznej wykrywającej sympleksy bifurkacji, foremne (k + 1)-wymiarowe sympleksy, które można uważać za "pogrubione punkty bifurkacji", leżące na krzywej zawierającej zera odwzorowania klasy $C^1 f: \mathbb{R}^{k+1} \to \mathbb{R}^k$. Sympleksy bifurkacji znajdują się (zwykle) w pobliżu punktów bifurkacji, co oznacza, że podana metoda pozwala zlokalizować przybliżone położenie punktów bifurkacji leżących na krzywej w zbiorze zer odwzorowania f. Podana metoda nie wymaga żadnych oszacowań na pochodną odwzorowania f– odwołuje się jedynie do wartości odwzorowania f w wierzchołkach sympleksów pewnej triangulacji przestrzeni \mathbb{R}^{k+1} . Sympleks bifurkacji wykrywany jest poprzez zmianę wartości stopnia topologicznego (stopnia Brouwera) na odpowiednich obcięciach f do k-wymiarowych sympleksów zawartych w przestrzeni \mathbb{R}^{k+1} .

2010 Klasyfikacja tematyczna AMS (2010): 65H10, 65H20.

Słowa kluczowe: algorytmy śledzenia krzywych, punkt bifurkacji, sympleks bifurkacji.



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Communicated by: Henryk Woźniakowski

(Received: 11th of January 2015; revised: 5th of June 2015)