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Simplex Bisection and Sperner Simplices

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Abstract: An efficient numerical method for locating and computing solutions of systems of nonlinear algebraic and transcendental equations is described and the relationship between this method and the Sperner lemma is analyzed. Although our method is based on the existence of a Sperner simplex, the method avoids constructions of Sperner simplices by making sure that the existence of a Sperner simplex is retained at every iteration. Thus, a fast bisection algorithm results. Our method always converges rapidly to a solution, independently of the initial guess, and is particularly useful, since the only computable information required is the algebraic signs of the components of the function.

Keywords: Sperner simplex, Knaster–Kuratowski–Mazurkiewicz lemma, labelling lemmas, topological degree theory, generalized bisection methods, fixed points, zeros, roots, systems of nonlinear algebraic and transcendental equations.

AMS subject classifications: 47H10, 54H25, 55M20, 55M25, 58C30, 65H10.

1. Introduction

Many problems require the solution of the following equation:

$$F_n(x) = \Theta^n, \tag{1}$$

where $\Theta^n = (0,0,\ldots,0)$ is the origin of $\mathbb{R}^n$ and $F_n = (f_1, f_2, \ldots, f_n)\colon \mathcal{D} \subset \mathbb{R}^n \to \mathbb{R}^n$ is a continuous nonlinear function from a domain $\mathcal{D} \subset \mathbb{R}^n$ into $\mathbb{R}^n$. These systems of nonlinear equations arise in a large number of applications for which a solution (or sometimes all solutions) is of practical significance. Methods mainly of a contraction mapping type such as Newton's method and related classes of algorithms [28] require the starting point to be within the immediate vicinity of the eventual solution. The necessity of having a good approximation to the solution of an unknown solution is obviously a severe disadvantage. Furthermore, in many cases, these methods fail, due to the nonexistence of derivatives or poorly behaved partial derivatives.

Also, Newton's method, as well as Newton–like methods, often converge to a solution almost independently of the initial guess, while there may exist several solutions nearby, all of which are desired for the application [1]. For the fractal–like geometry of the basin of convergence of these methods see [3,4]. Because of these reasons, various approaches based upon topological degree theory and generalized bisection methods have been investigated [8, 13, 16–20, 22, 37, 39, 40, 43, 47, 50]. According to these methods one establishes the existence of at least one solution of System (1), where $F_n = (f_1, f_2, \dots, f_n) \colon \overline{\mathcal{D}} \subset \mathbb{R}^n \to \mathbb{R}^n$ is continuous on the closure $\overline{\mathcal{D}}$ of $\mathcal{D}$ and such that $F_n(x) \neq \Theta^n$ for any x on the boundary $\vartheta\mathcal{D}$ of $\mathcal{D}$, by computing the *topological degree of F_n at Θ^n relative to $\mathcal{D}$,* denoted by $\deg[F_n, \mathcal{D}, \Theta^n]$ and defined by the following sum:

$$\deg[F_n, \mathcal{D}, \Theta^n] = \sum_{x \in F_n^{-1}(\Theta^n)} \operatorname{sgn} \det J_{F_n}(x),$$

where $\det J_{F_n}$, indicates the determinant of the Jacobian matrix and sgn defines the sign function. Now, if a nonzero value of $\deg[F_n, \mathcal{D}, \Theta^n]$ is obtained then, by the Kronecker's existence theorem [28], it follows that there is at least one root in $\mathcal{D}$.

In many applications, such as numerical simulations, precise values are either impossible or time consuming to obtain [23]. These problems can be dealt with by bisection based methods that do not require precise function values [9, 12, 14, 15, 25–27, 43, 45, 46, 48–54]. The main advantage of the generalized bisection methods is that they can be applied to imprecise problems since they require only the algebraic signs of the components of the function.

In this contribution, we present a generalized bisection method applied on n–dimensional simplexes which can be used to solve large and imprecise problems.

2. Fixed point theorems and labelling lemmas

One of the most important theorems in the field of nonlinear equations is Brouwer's fixed point theorem. If we rewrite a system of nonlinear equations in fixed point form, then the theorem states that under mild assumptions we will have a fixed point, i.e. a solution. This theorem has been used for many years to prove the existence of a solution of complicated systems of nonlinear equations [10, 29, 36, 41].

Brouwer's fixed point theorem [6] states that: any continuous mapping $F_n : \sigma^n \to \sigma^n$ from an n–simplex $\sigma^n \subset \mathbb{R}^n$ into itself has at least one fixed point x^*, that is $F_n(x^*) = x^*$. A proof of Brouwer's theorem for the simplex was given by Knaster, Kuratowski and Mazurkiewicz in 1929 [21]. The Knaster, Kuratowski and Mazurkiewicz covering lemma states that: if C_i, $i \in \mathbb{N}_0 = \{0, 1, \dots, n\}$ is a family of closed subsets of σ^n satisfying the following conditions:

1. $\sigma^n = \bigcup_{i \in \mathbb{N}_0} C_i$ and
2. if $\emptyset \neq \mathcal{I} \subseteq \mathbb{N}_0$ and $\mathcal{J} = \mathbb{N}_0 - \mathcal{I}$ then $\bigcap_{i \in \mathcal{I}} \sigma^{n,i} \subseteq \bigcup_{j \in \mathcal{J}} C_j$.

Then holds that:

$$\bigcap_{i \in \mathbb{N}_0} C_i \neq \emptyset,$$

where $\sigma^{n,i} = \{v^0, v^1, \ldots, v^{i-1}, v^{i+1} \ldots, v^n\}$ determines the ith face of σ^n.

Scarf and Hansen in 1973 [30] proved a lemma similar to the above lemma. Also, an interesting generalization of the Knaster, Kuratowski and Mazurkiewicz lemma has been given by Gale [11].

The Sperner lemma is the basis for a proof of the Brouwer fixed point theorem [31, 32]. Before stating the Sperner lemma we give several concepts which are needed in the lemma.

Let $v^0, v^1, \ldots, v^n$ denote the vertices of σ^n. A k–face of σ^n determined by the vertices $v^{i_0}, v^{i_1}, \ldots, v^{i_k}$ is called the *carrier* of a point v if v lies on this k–face and not on any subface of this k–face. A function $\lambda(v)$ defined on a σ^n is called a *proper labeling function* if it satisfies the following conditions [2]:

a) $\lambda(v) \in \{0, 1, \ldots, n\}$,

b) $\{\lambda(v^0), \lambda(v^1), \ldots, \lambda(v^n)\} = \{0, 1, \ldots, n\}$,

c) If the i–face determined by the vertices $v^{k_0}, v^{k_1}, \ldots, v^{k_i}$ is the carrier of v then $\lambda\,(v) \in \{\lambda\,(v^{k_0}), \lambda\,(v^{k_1}), \ldots, \lambda\,(v^{k_i})\}$.

Let $\{\omega^0, \omega^1, \ldots, \omega^k\}$ denote the vertices of a k–simplex, $k \leq n$, of a simplicial subdivision of σ^n. This k–simplex is said to have a *complete set of labels* if the following relation holds:

$$\{\lambda(\omega^0), \lambda(\omega^1), \ldots, \lambda(\omega^k)\} = \{0, 1, \ldots, k\}.$$

The Sperner's lemma [31] states that: for any simplicial subdivision and proper labelling function of σ^n there is at least one n–simplex of the subdivision with a complete set of labels.

A Sperner simplex is this n–simplex with a complete set of labels. For well–behaved continuous functions and a fine enough simplicial subdivision, the vertices of such a simplex approximate a fixed point or a root of the mapping. One can use Sperner's lemma to give a constructive proof of Brouwer's fixed point theorem. Yoseloff in 1974 [56] proved that the Sperner's lemma can be derived from Brouwer's fixed point theorem, and therefore are equivalent. Also, a constructive proof of a permutation based generalization of Sperner's lemma has been given in [5].

Sperner in 1980 [33] gave a very general labelling lemma which states that: let the n–simplex σ^n be triangulated. Label each vertex of the simplices in the triangulation by an integer from the set $\{0, 1, \ldots, n\}$. Then the number of $(n-1)$–simplices on the boundary with labels $\{0, 1, \ldots, n-1\}$ is equal to the number of n–simplices in the interior with labels $\{0, 1, \ldots, n\}$. All simplices are counted with orientation.

3. The simplex bisection method

Bisection methods for finding solutions of systems of equations depend on a criterion which guarantees that a solution lies within a given region. Then this region is subdivided in such a way that the criterion can again be applied to the new refined one. By implementing topological degree theory we are able to give a criterion for the existence of a solution of System (1) within a given region. An existence criterion has been given in [39, 40, 50] which is based on the construction of a "characteristic polyhedron" within a scaled translation of the unit cube.

To define a Characteristic Polyhedron (CP), let B_k^n be the n-digit binary representation of the integer $(k-1)$, $1 \leq k \leq 2^n$ counting the leftmost digit first. Then the *n-binary matrix* $\mathcal{M}_n^* = [C_{ij}^*], i = 1, \ldots, 2^n$, $j = 1, \ldots, n$, is the matrix whose entry in the ith row and jth column is the jth digit of B_i^n. By replacing each zero element in the matrix $\mathcal{M}_n^*$ by -1 we get a new $2^n \times n$ matrix $\mathcal{M}_n = [C_{ij}]$, which we call an *n-complete* matrix. For example for $n = 2$ we have:

$$\begin{array}{l} B_1^2 = 00 \\ B_2^2 = 01 \\ B_3^2 = 10 \\ B_4^2 = 11 \end{array} \longrightarrow \mathcal{M}_2^* = \begin{bmatrix} B_1^2 \\ B_2^2 \\ B_3^2 \\ B_4^2 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \longrightarrow \mathcal{M}_2 = \begin{bmatrix} -1 & -1 \\ -1 & 1 \\ 1 & -1 \\ 1 & 1 \end{bmatrix}.$$

Suppose now that $\Pi^n = \langle v^1, v^2, \ldots, v^{2^n} \rangle$ is an oriented n-polyhedron in $\mathbb{R}^n$ with 2^n vertices and let $F_n = (f_1, f_2, \ldots, f_n) \colon \Pi^n \subset \mathbb{R}^n \to \mathbb{R}^n$. Then the *matrix of signs associated with F_n and Π^n*, denoted by $\mathcal{S}(F_n; \Pi^n)$, is the $2^n \times n$ matrix whose entries in the ith row are the corresponding coordinates of the vector $\operatorname{sgn} F_n(v^i) = (\operatorname{sgn} f_1(v^i), \operatorname{sgn} f_2(v^i), \ldots, \operatorname{sgn} f_n(v^i))$. An n-polyhedron Π^n is a CP if $\mathcal{S}(F_n; \Pi^n) \equiv \mathcal{M}_n$. Under some suitable assumptions on its boundary, a CP always contains at least one solution of the system $F_n(X) = \Theta^n$ (CP-criterion), since the absolute value of $\deg[F_n, \mathrm{CP}, \Theta^n]$ is equal to one [50]. In order to approximate this solution, a generalized bisection method is used, in combination with the CP-criterion outlined above, which bisects a CP in such a way that the new refined n-polyhedron is also a CP. To do this, we compute the midpoint of a "proper 1-simplex" [39] of Π^n and use it to replace that vertex of Π^n for which the vectors of their signs are identical. We call this procedure *characteristic bisection*. Finally, the number B of characteristic bisections of the edges of a Π^n required to obtain a new refined CP, $\Pi_\star^n$, whose longest edge length, $\Delta(\Pi_\star^n)$, satisfies $\Delta(\Pi_\star^n) \leq \varepsilon$, for some $\varepsilon \in (0,1)$, is given by $B = \lceil \log_2(\Delta(\Pi^n)\, \varepsilon^{-1}) \rceil$, (for details see [39, 40, 50]).

It is important to notice that the CP-criterion avoids all calculations concerning the topological degree since it requires not its exact value but only its nonzero value. Also, it is quite efficient, since the only computable information required is the algebraic signs of the components of the function. Thus, it is not affected by the function evaluations taking large or imprecise values. This method is primarily useful for small dimensions ($n \leq 10$), since the computational effort for the construction of a characteristic polyhedron [39, 40] grows exponentially with the dimension. The CP method has been applied successfully to various problems [7, 9, 42, 45, 46, 48, 49, 51–55].

By replacing the n-dimensional polyhedron by an n-dimensional simplex we obtain a generalized bisection method especially useful for large dimensions (cf. (mutatis mutandis) [24, 44]). In what follows we briefly present this method.

Consider the sets $\mathcal{V} = \{1, 2, \ldots, (n+1)\}$ and $\mathcal{C} = \{1, 2, \ldots, n\}$. Then the corresponding *n-binary matrix*, $\mathcal{M}_n^* = [C_{ij}^*], i \in \mathcal{V}, j \in \mathcal{C}$, is the $(n+1) \times n$ matrix whose entry in the ith row and jth column is the jth digit of B_m^n, where $m = 2^{n+1-i}$. Now, if we replace each zero element in the matrix $\mathcal{M}_n^*$ by -1 we shall come up with the corresponding n-*proper* matrix, $\mathcal{M}_n = [C_{ij}], \in \mathcal{V}, j \in \mathcal{C}$. For example, for $n = 1, 2, 3$ we have, respectively:

$$n=1: \quad \begin{array}{l} B_2^1 = 1 \\ B_1^1 = 0 \end{array} \longrightarrow \quad \mathcal{M}_1^* = \begin{bmatrix} B_2^1 \\ B_1^1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \longrightarrow \quad \mathcal{M}_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix};$$

$$n=2: \quad \begin{array}{l} B_4^2 = 11 \\ B_2^2 = 01 \\ B_1^2 = 00 \end{array} \longrightarrow \mathcal{M}_2^* = \begin{bmatrix} B_4^2 \\ B_2^2 \\ B_1^2 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \longrightarrow \quad \mathcal{M}_2 = \begin{bmatrix} 1 & 1 \\ -1 & 1 \\ -1 & -1 \end{bmatrix};$$

$$n=3: \quad \begin{array}{l} B_8^3 = 111 \\ B_4^3 = 011 \\ B_2^3 = 001 \\ B_1^3 = 000 \end{array} \longrightarrow \mathcal{M}_3^* = \begin{bmatrix} B_8^3 \\ B_4^3 \\ B_2^3 \\ B_1^3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \longrightarrow \mathcal{M}_3 = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & 1 \\ -1 & -1 & 1 \\ -1 & -1 & -1 \end{bmatrix}.$$

An n-*characteristic matrix* $\mathcal{X}_n = [\chi_{ij}], i \in \mathcal{V}, j \in \mathcal{C}$ is an $(n+1) \times n$ matrix which can become n-proper by permutations of its columns. An n-proper matrix is also an n-characteristic matrix. For example, the following matrices are 3-characteristic matrices:

$$\begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & 1 \\ -1 & -1 & 1 \\ -1 & -1 & -1 \end{bmatrix}, \quad \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & -1 & 1 \\ -1 & -1 & -1 \end{bmatrix}, \quad \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & -1 \\ -1 & -1 & -1 \end{bmatrix}, \quad \begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & 1 \\ -1 & 1 & -1 \\ -1 & -1 & -1 \end{bmatrix}.$$

Suppose, now that $\sigma^n = \langle v^0, v^1, \ldots, v^n \rangle$ is an oriented n-simplex in $\mathbb{R}^n$, and let $F_n = (f_1, f_2, \ldots, f_n) : \sigma^n \subset \mathbb{R}^n \to \mathbb{R}^n$ be a nonlinear function from σ^n into $\mathbb{R}^n$. Then the *matrix of signs associated with* F_n *and* σ^n, denoted by $\mathcal{S}(F_n; \sigma^n)$, is the $(n+1) \times n$ matrix whose entries in the kth row are the corresponding coordinates of the vector:

$$\operatorname{sgn} F_n(v^k) = \left(\operatorname{sgn} f_1(v^k), \operatorname{sgn} f_2(v^k), \ldots, \operatorname{sgn} f_n(v^k)\right).$$

An oriented n-simplex $\sigma^n = \langle v^0, v^1, \ldots, v^n \rangle$ in $\mathbb{R}^n$ is called a *characteristic n-simplex relative to* $F_n = (f_1, f_2, \ldots, f_n): \sigma^n \subset \mathbb{R}^n \to \mathbb{R}^n$, if the matrix of signs associated with F_n and σ^n, $\mathcal{S}(F_n; \sigma^n)$, is identical with an n-characteristic matrix $\mathcal{X}_n$.

Suppose now that σ^n is a characteristic n-simplex and that $F_n = (f_1, f_2, \ldots, f_n)$: $\sigma^n \subset \mathbb{R}^n \to \mathbb{R}^n$ is continuous. Then, under suitable assumptions, including the appropriate representation of the oriented boundary of σ^n which are similar to [16,18,34,35], $\deg[F_n, \sigma^n, \Theta^n] = \pm 1 \neq 0$, which implies the existence of a solution inside σ^n. The construction of characteristic n-simplex is similar to the construction of a characteristic polyhedron described in [39]. The characteristic simplex has common features with the Sperner simplex since by considering the following labeling function:

$$\lambda(x) = \begin{cases} i, & \text{if} \quad f_i(x) > x_i \ \text{ and } \ f_j(x) \leq x_j \quad \text{for all} \ \ j < i, \\ 0, & \text{if} \quad f_j(x) \leq x_j \ \text{ for all } \ j = 1, 2, \ldots, n, \end{cases}$$

on the vertices of a characteristic n–simplex it is easily seen that a characteristic n–simplex is a Sperner simplex.

Next, we turn to the description of a generalized bisection method, used in combination with the characteristic simplex outlined above, for computing solutions to any accuracy, subject to relative machine precision. In general a bisection procedure applied on simplexes can be determined by the following [17, 18]. Let $\sigma_0^m = \langle v^0, v^1, \ldots, v^m \rangle$ be an oriented m–simplex in $\mathbb{R}^n$, $m \le n$. Suppose that $\langle v^i, v^j \rangle$ is the longest edge of σ_0^m and let $\Upsilon = (v^i + v^j)/2$ be the midpoint of $\langle v^i, v^j \rangle$. Then the *bisection* of σ_0^m is the ordered pair of m–simplexes $\langle \sigma_{10}^m, \sigma_{11}^m \rangle$, where:

$$\sigma_{10}^m = \langle v^0, v^1, \ldots, v^{i-1}, \Upsilon, v^{i+1}, \ldots, v^j, \ldots, v^m \rangle,$$
$$\sigma_{11}^m = \langle v^0, v^1, \ldots, v^i, \ldots, v^{j-1}, \Upsilon, v^{j+1}, \ldots, v^m \rangle.$$

The m–simplexes σ_{10}^m and σ_{11}^m will be called *lower simplex* and *upper simplex*, respectively, corresponding to σ_0^m, while both σ_{10}^m and σ_{11}^m will be called *elements of the bisection* of σ_0^m. Suppose that $\sigma_0^n = \langle v^0, v^1, \ldots, v^n \rangle$ is an oriented n–simplex in $\mathbb{R}^n$ which includes at least one solution of System (1). Suppose further that $\langle \sigma_{10}^n, \sigma_{11}^n \rangle$ is the bisection of σ_0^n and that there is at least one solution of (1) in some of its elements. Then this element will be called *selected n–simplex produced after one bisection of* σ_0^n and it will be denoted by σ_1^n. Moreover, if there is at least one solution of System (1) in both elements, then the selected n–simplex will be the lower simplex corresponding to σ_0^n. Suppose now that the bisection is applied with σ_1^n replacing σ_0^n and thus obtaining σ_2^n. Suppose further that this process continues for p iterations. Then we call σ_p^n *the selected n–simplex produced after p iterations of the bisection of* σ_0^n.

In our case the selected n–simplex is obtained by bisecting the characteristic n–simplex σ^n in such a way that the new refined n–simplex is also a characteristic one. To do this the method computes the midpoint $\Upsilon = (v^i + v^j)/2$ of an edge of σ_p^n and uses it to replace that vertex of this edge for which the vectors of their signs are identical. If the vector of signs of Υ is identical with another vertex of σ^n, for example v^k, then σ_p^n is transformed by replacing v^k with the point $\mathrm{ref}v^k = 2K_k - v^k$ which is called the *reflection* of v^k across the barycenter K_k of the k–th face of σ_p^n. Of course, if the boundary of the simplex obeys the assumptions of the Knaster, Kuratowski and Mazurkiewicz covering lemma then the reflection step is not necessary. These assumptions are not explicitly checked, and the method thus uses heuristics in locating the root. Also, when the thickness of the simplex [38] becomes small (the simplex is long and thin) the method expands it properly.

For an error analysis, suppose that σ_p^n is the selected n–simplex produced after p bisections of the starting n–simplex σ_0^n; then we use the barycenter K_p^n of σ_p^n to approximate the solution r of System (1) which is included in σ_p^n. The diameter δ_p of σ_p^n, i.e. the length of the largest edge of σ_p^n, can be bounded by [17]:

$$\delta_p \le \left(\sqrt{3}/2\right)^{\lfloor p/n \rfloor} \delta_0,$$

where δ_0 is the diameter of σ_0^n and the notation $\lfloor \cdot \rfloor$ refers to the largest integer which is less than or equal to the real number quoted. Now, for any point T in σ_p^n the following relationship is valid [37]:

$$\|T - K_p^n\| \leq \frac{n}{n+1} \left(\sqrt{3}/2\right)^{\lfloor p/n \rfloor} \delta_0.$$

An *error estimate* ε_p for K_p^n can be defined by the following quantity [37]:

$$\varepsilon_p = \frac{n}{n+1} \left(\delta_p^2 - \frac{n-1}{2n} \mu_p^2\right)^{1/2},$$

where μ_p is the microdiameter of σ_p^n, i.e. the length of the smallest edge of σ_p^n. Then the following relations hold [37]:

a) $\varepsilon_p \leq \frac{n}{n+1} \left(\sqrt{3}/2\right)^{\lfloor p/n \rfloor} \delta_0,$

b) $\varepsilon_p \leq \left(\sqrt{3}/2\right)^{\lfloor p/n \rfloor} \varepsilon_0,$

c) $\lim_{p \to \infty} \varepsilon_p = 0,$

d) $\lim_{p \to \infty} K_p^n = r.$

The above described characteristic bisection method applied on simplexes was implemented using a new Fortran program. This has been applied to several test functions and our experience is that the method behaves predictably and reliably even for problems with very high dimensions.

Also, we have applied our method to problems which are very difficult to solve using traditional methods. In particular, we have applied it to the numerical computation of the periodic orbits of nonlinear mappings and we have succeeded to compute periodic orbits of periods which reach up to hundred of thousands. The results obtained by the new method are similar to those obtained by the CP method for small dimensions exhibited in [7,42,48,51,54,55].

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