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On the complexity of isolating real roots and computing with certainty the topological degree

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Abstract

In this contribution the isolation of real roots and the computation of the topological degree in two dimensions are considered and their complexity is analyzed. In particular, we apply Stenger's degree computational method by splitting properly the boundary of the given region to obtain a sequence of subintervals along the boundary that forms a sufficient refinement. To this end, we properly approximate the function using univariate polynomials. Then we isolate each one of the zeros of these polynomials on the boundary of the given region in various subintervals so that these subintervals form a sufficiently refined boundary.

Key words and phrases: topological degree, B–splines, Bézier curves, zero isolation, locating and computing roots, sign determination, generalized bisection, characteristic bisection.

1 Introduction

Many problems in different areas of science and technology can be reduced to a study of a set of solutions of an equation of the form $F(x) = p$ in an appropriate space. Topological degree theory has been developed as means of examining this solution set and obtaining information on the existence of solutions, their number and their nature. This theory is widely used in the study of nonlinear differential (ordinary and partial) equations. It is useful, for example, in bifurcation theory and in providing information about the existence and stability of periodic solutions of ordinary differential equations as well as the existence of solutions of certain partial differential equations. Several of these applications involve the use of various fixed point theorems which can be provided by means of topological degree [11, 35, 64, 65, 66, 69].

Since Stenger's remarkable and pioneering work [53], many approaches have been developed and studied to compute the topological degree of a function (see e.g., [1, 6, 7, 24, 25, 29, 54, 55, 56, 57, 68, 72, 74]). Stenger's method expresses the topological degree of a continuous mapping $F_n = (f_1, \dots, f_n)\colon \overline{\mathcal{D}}_n \subset \mathbb{R}^n \to \mathbb{R}^n$ defined on a bounded domain $\mathcal{D}_n$ in $\mathbb{R}^n$ as a constant times a sum of determinants of various $n \times n$ matrices. The value of the topological degree gives information about the existence of a solution of the equation $F_n(x) = \Theta_n$, (where $\Theta_n = (0, \dots, 0)$ denotes the origin in $\mathbb{R}^n$) within $\mathcal{D}_n$. In particular, Kronecker's theorem [3, 11, 41] states that the equation $F_n(x) = \Theta_n$ has at least one zero in $\mathcal{D}_n$ if the degree is not zero relative to $\mathcal{D}_n$.

Although, the value of the topological degree gives qualitative information about the existence of solutions, it does not give quantitative information about the solution values. On the other hand, using the nonzero value of topological degree we are able to obtain upper and lower bounds for solution values. To this end, by computing a sequence of bounded domains with nonzero values of topological degree and decreasing diameters, we are able to obtain a region with arbitrarily small diameter that contains at least one solution of the equation. These methods are now called generalized bisection methods and have been developed and applied by several authors (see e.g., [12, 19, 22, 23, 24, 25, 26, 31, 44, 48, 53, 61, 68, 62, 63, 70, 71, 73]). The generalized bisection methods are related to simplicial continuation methods (see e.g., [2]) and they are particularly useful when the function F_n is not smooth or cannot be accurately evaluated. Also, another class of bisection methods, based on interval analysis, has been widely used. These methods are robust and appropriate for finding starting points for Newton-like methods (see e.g., [26, 27, 28, 30, 32, 40]).

The accurate computation of topological degree of the mapping F_n at Θ_n relative to the bounded domain $\mathcal{D}_n$ using Stenger's or other related methods [24, 25, 55, 56], is heavily based on suitable assumptions, including the appropriate representation of the oriented boundary of $\mathcal{D}_n$. In particular, if the boundary of

$\mathcal{D}_n$ can be subdivided in a certain way ("sufficiently refined") then Stenger's method gives exact value of topological degree. Otherwise, heuristic termination criteria have to be used and therefore one cannot be sure that the value of topological degree is given correctly. On the other hand, if moduli of continuity are known (see [57]), one can use a deterministic termination criterion in order to obtain the degree with certainty.

To this end, Boult and Sikorski proposed in their interesting paper [7] an optimal complexity algorithm for computing with certainty the topological degree for any function from a class $\mathcal{F}$. This class consists of functions $F_2 : \mathcal{B} \rightarrow \mathbb{R}^2$ defined on the unit square $\mathcal{B}$, which satisfy the Lipschitz condition with constant $K > 0$ and whose infinity norm along the boundary of $\mathcal{B}$ is at least $\delta > 0$. Also, they established a worst-case lower bound, $m^* = 4\lfloor K/(4\delta)\rfloor$, on the number of function evaluations necessary to compute the topological degree for any function F_2 from the class $\mathcal{F}$. Their algorithm calculates the degree using Stenger's method [53]. They have examined the complexity, i.e. minimal cost of the problem of the calculation of topological degree for functions from class $\mathcal{F}$. Notice that the value of δ is always positive since the topological degree is not defined in the case where a solution of the equation $F_2(x) = \Theta_2$ lie on the boundary of $\mathcal{D}_2$. This is also true in the Boult and Sikorski approach, since in this case the value of δ is zero and an infinite number of points has to be considered.

If the value of the Lipschitz constant K with respect to $\mathcal{D}_2$ and the infinity norm δ of F_2 along the boundary of $\mathcal{D}_2$ are known and we choose equally spaced points on the boundary of $\mathcal{D}_2$ separated by a distance $1/\lfloor K/(4\delta)\rfloor$ in the infinity norm, then Boult and Sikorski have shown that we are able to evaluate the topological degree with certainty using Stenger's method [7]. This is so because, in this case, a sufficient refinement is obtained.

On the other hand, the values of K and δ may not be known a priori and in many cases their computation is a heavy task. To this end, we propose an alternative procedure for computing with certainty the topological degree in two dimensions by using Stenger's method. Our method does not require the values of K and δ. Instead, we separate properly the boundary of $\mathcal{D}_2$ to obtain a sequence of subintervals along the boundary which form a sufficient refinement. This can be done by constructing the subintervals in such a way that at least one component of the function F_2 does not vanish on each subinterval. To this end, we "properly" approximate the considered function using univariate polynomials. Then we isolate each one of the intersection points of these polynomials with the boundary of $\mathcal{D}_2$ in various subintervals so that the sequence of these subintervals forms a sufficiently refined boundary relative to the sign of F_2.

The paper is organized as follows. In the next section an algorithm for isolating the real roots of a univariate polynomial is described and its complexity is analyzed. In section 3 we briefly give a background on topological degree and its complexity. We also present a fast and accurate method for computing the value of topological degree with certainty. Furthermore, we apply the proposed method for the isolation of complex roots of analytic functions. The paper ends in Section 4 with some concluding remarks and a short discussion of further research.

2 Isolating the roots of a univariate polynomial

The aim of this section is to describe an algorithm for isolating the real roots of a univariate polynomial, and to analyze its complexity. We will apply it in the next section, to compute the topological degree of a polynomial map, for which we need to isolate on the boundary of the considered region all the roots of its components.

In general, many problems in different areas of science are reduced to the problem of finding all roots or extrema of a function in a given interval. The importance of the problem has attracted the attention of many research efforts and, as a result, many different approaches to the problem exist. We briefly mention here the deflation techniques used for the calculation of further solutions [8] or other more efficient and more recent interval analysis based methods (see e.g. [17, 18, 28, 30, 32, 40]) and the methods described in [22, 23, 44]. The corresponding existence tool of interval analysis based methods is the availability of the range of the function in a given interval, which can be implemented using interval arithmetic, though range overestimation, and hence efficiency problems must be resolved. This tool will, with mathematical rigor, give either a "no" or an "unknown" answer. The former case proceeds by subdividing the interval into two halves and employing additional criteria. The way the evaluation of functions is encoded influences the answer, which is usually pessimistic (i.e. "unknown"). In the vicinity of a root, interval Newton method (see e.g. [28, 40]) may however with slightly more computational effort, give an unambiguous "yes" answer.

A more geometric method which gives the exact number of roots $\mathcal{N}^r$ is based on topological degree theory using Kronecker's integral on a Picard's extension [20, 42]. For the computation of the topological degree see e.g. [7, 25, 53, 55, 56]. This method can be used for the isolation of all simple roots of a function $f(x)$ in an interval (a, b) and returns the number of roots using the formula (9) which is given in the next section.

In our approach we will use the representation of a polynomial in the Bernstein basis and Descartes' rule, in order to guide the subdivision scheme and to obtain a sequence of intervals, each containing one and only one real root of the univariate polynomial.

2.1 Isolation of the roots

We will use Proposition A.1 to isolate the real roots of a B-spline function $f(t)$ on an interval $[m, M]$. The control polygon is a first approximation of the curve. It can be used to give an estimation of the roots. In order to separate the roots, we can insert additional points in order to refine the polygon.

According to Proposition A.1, if the number of crossing points of the subpolygon corresponding to the internal $[u_i, u_{i+1}]$ with the x-axis is 0 or 1, then we know the exact number of roots within this interval. If this is not the case, we perform the splitting procedure.

This algorithm is related to the algorithm proposed in [15] and [36] but the corresponding authors do not give any precise result of the complexity of this algorithm. This will be done in Section 2.2. Notice that this algorithm is also related to the Uspensky's method [59, 46], by applying the change of variable $t \in [0, +\infty[\rightarrow \frac{t}{1+t} \in [0, 1[$. Here is a more precise description of the algorithm:

Algorithm 2.1 *Isolate the real roots.*

```
localization:=proc(b,[m,M])
L := {[m,M]}
Z := empty set of intervals
if size(L)>0 then
    L:=L minus {[m,M]};
    n:= Var(b)
    if b0=0 then Z= Z union {[m,m]}
    if bd=0 then Z= Z union {[M,M]}
    if n=1 then Z:= Z union {[m,M]};
    elif n>1 then
        L:=L union [m,(m+M)/2],[(m+M)/2,M];
        [b⁻,b⁺]:=subdivide(b);
        localization(b⁻,[m,(m+M)/2]);
        localization(b⁺,[(m+M)/2,M]);
    fi
fi
end
Output : Z
```

where L is the set of intervals that contain the real roots, Z is the set of intervals containing one and only one real root, Var(**b**) is the number of sign changes of the sequence $\mathbf{b} = (b_0, \ldots, b_d)$ and subdivide is the de Casteljau subdivision procedure (see Appendix).

2.2 The complexity

The main result of this section gives the complexity of the previous algorithm. Because the B-spline insertion procedure is local, we can restrict ourself to the case where $f(t)$ is a polynomial of degree d, represented in the Bernstein Basis.

Theorem 2.1 *Let $f(t)=\sum_{k=0}^{d} a_k B_k^d(t)$ be a polynomial of degree d represented in the Bernstein basis. Let x_k, $k=1,\ldots,d$ be the roots of f and $s=\min_{x_i\neq x_j}|x_i-x_j|$. Suppose that all real roots of the polynomial f are simple. Then the procedure* localization *terminates. Moreover the following hold:*

1. *An upper bound on the number of recursion steps of the procedure* localization *is*
$$l=\left\lceil \log_2\left(\frac{2}{s}\right)\right\rceil,$$
where the notation $\lceil\cdot\rceil$ refers to the smallest integer, which is not less than the real number quoted.

2. *An upper bound on the number of arithmetic operations of the procedure* localization *is*
$$v=\frac{1}{2}d(d+1)r\left(\left\lceil \log_2\left(\frac{2}{s}\right)\right\rceil-\log_2(r)+4\right),$$
where r is the number of sign changes of the sequence $(a_k)_{0,\ldots,d}$.

3. *The number of intervals in Z is the number of real roots of f in $[0,1]$.*

The study of complexity of the algorithm requires a reciprocal result of the Descartes rule. In fact we need to know when the number of real roots of f on $[0,1]$, denoted by $\#Z_f(0,1)$, equals zero implies $Var(\mathbf{b})=0$ and when $\#Z_f(0,1)=1$ implies $Var(\mathbf{b})=1$.

These are given by two theorems that we recall and reformulated in our contexte. Given a polynomial polynomial $f(x)=\sum_{i=0}^{d} b_i\, B_d^i(x)$ written in the Bernstein basis, the transformation
$$\delta(f)(x)=(1+x)^d f(\frac{1}{1+x})$$
yields the polynomial
$$\delta(f)(x)=\sum_i b_i\binom{d}{i}x^i.$$
The sign variation of the coefficients of this polynomial in the monomial basis is equal to $Var(\mathbf{b})$. We recall the two following theorems, proved for the number of sign variations of the coefficients of $\delta(f)$ in the monomial basis, which is equal to $Var(\mathbf{b})$:

Theorem 2.2 *[60] Suppose that $f(x)$ has no (complex) root such that $|z-\frac{1}{2}|<\frac{1}{2}$ and let $\mathbf{b}$ be the sequence of coefficients of f in the Bernstein basis. Then $Var(\mathbf{b})=0$.*

Theorem 2.3 *[9] Suppose that $f(x)=0$ has one real root in $[0,1]$ and no other (complex) root z such that $|z|<1$ and $|z-1|<1$ and let $\mathbf{b}$ be the sequence of coefficients of f in the Bernstein basis. Then $Var(\mathbf{b})=1$.*

This result has been sharpened in [37], by replacing the two conditions $|z|<1$ and $|z-1|<1$ by the conditions $|z-\frac{1}{2}(1\pm \mathbf{i}\sqrt{3})|<\frac{1}{\sqrt{3}}$. See also [4]. As a consequence, we deduce that if $f(x)=0$ has one real root in $[0,1]$ and no roots such that $|z-\frac{1}{2}|<\frac{3}{2}$, then $Var(\mathbf{b})=1$

Proof of Theorem 2.1 At the level n of the recursion step, the algorithm localization computes polynomials $f^r(t)=f(t/2^n+r_n/2^n+\cdots+r_1/2)$ where $r=(r_1,\ldots,r_n)$, $r_i\in\{0,1\}$. A root t of f^r is linked with a root x of f by
$$x=t/2^n+r_n/2^n+\cdots+r_1/2.$$
If f has a multiple real root, the algorithm localization does not terminate since the condition $Var(f^r)\leqslant 1$ cannot to be reached.

We first compute an upper bound for the number of recursion steps to get $Var(f^r)=1$ in the case where f has simple real roots.

Let $x_1\in[0,1]$ be a simple real root of f. From theorem 2.3, we obtain sufficient conditions for which $Var(f^r)=1$. These are $|t_k-\frac{1}{2}|\geqslant\frac{3}{2}$ for $k\neq 1$. We now estimate n for which we have this inequality, that is
$$|t_k-\frac{1}{2}|\geqslant|t_k-t_1|-|t_1-\frac{1}{2}|\geqslant 2^n|x_k-x_1|-\frac{1}{2}\geqslant 2^n s-\frac{1}{2}\geqslant\frac{3}{2},\quad k=2,\ldots,d.$$

It implies that

$$n \geqslant \log_2\left(\frac{2}{s}\right).$$

Next, we give an upper bound for the number of recursion steps to get $Var(f^r) = 0$. From theorem 2.2, we have $Var(f^r) = 0$ when $|t_k - \frac{1}{2}| \geqslant \frac{1}{2}$ for $k = 1, \ldots, d$. Since the coefficients of f are real so that the non-real roots are conjugate and $|t_i - t_j| = 2^n\,|x_i - x_j|$, for all $i, j = 1, \ldots, d$, this previous inequality holds when $2^n\, s \geqslant 1$ i.e., $n \geqslant \log_2\left(\frac{1}{s}\right)$.

Finally, the number of recursion steps to isolate the roots is bounded by $\left\lceil \log_2\left(\frac{2}{s}\right)\right\rceil$.

There are 2^k polynomials of type f^r at the level k of recursion. The De Casteljau algorithm needs additions and divisions by 2: it is easy to see that there are $d(d+1)$ arithmetic operations. Moreover, when we split the interval, the total number r of sign variations can only decrease (because of the variation diminishing property). Moreover, we remove the interval with sign variation equal to 0 and do not split anymore those with sign variation equal to 1. Consequently, the recursion tree of height at most $l = \left\lceil \log_2\left(\frac{2}{s}\right)\right\rceil$ has a maximal number of edges when its $\log_2(\frac{r}{2})$ first levels are filled and the subtrees are of maximal height. The number of edges is thus bounded by:

$$\sum_{k=0}^{\log_2(r/2)} 2^k + \left(l - \log_2\left(\frac{r}{2}\right) + 1\right)\,\frac{r}{2} \leqslant \frac{1}{2} r(l - \log_2(r) + 4).$$

As each step requires $d(d+1)$ operations, we obtain the desired complexity bound. □

Remark 2.1 *Using [37], we can replace* $\log_2(\frac{2}{s})$ *by* $\log_2(\frac{1+\sqrt{3}}{2\,s})$ *in the previous complexity bounds.*

3 The topological degree and its complexity

We briefly outline topological degree theory for determining the exact number of zeros of a system of nonlinear transcendental equations by computing the value of the topological degree using Kronecker's integral [3, 16, 24, 33, 39, 53] on Picard's extension [20, 21, 42, 43, 52].

Suppose that a function $F_n = (f_1, f_2, \ldots, f_n)\colon \overline{\mathcal{D}_n} \subset \mathbb{R}^n \to \mathbb{R}^n$ is defined and twice continuously differentiable in an open and bounded domain $\mathcal{D}_n$ of $\mathbb{R}^n$ with boundary $\vartheta\mathcal{D}_n$. Suppose further that the zeros of the equation $F_n(x) = p$, where $p \in \mathbb{R}^n$ is a given vector, are not located on $\vartheta\mathcal{D}_n$, and that they are simple, i.e., the determinant, $\det J_{F_n}$, of the Jacobian matrix of F_n at these zeros is non–zero.

Definition 3.1 *The* topological degree of F_n at p relative to $\mathcal{D}_n$ *is denoted by* $\deg[F_n, \mathcal{D}_n,\, p]$ *and is defined by the following sum:*

$$\deg[F_n, \mathcal{D}_n, p] = \sum_{x \in F_n^{-1}(p) \cap \mathcal{D}_n} \operatorname{sgn}\bigl(\det J_{F_n}(x)\bigr), \tag{1}$$

where $\operatorname{sgn}(\psi)$ *defines the well known three valued sign function:*

$$\operatorname{sgn}(\psi) = \begin{cases} -1, & \text{if} \quad \psi < 0\,, \\ 0, & \text{if} \quad \psi = 0\,, \\ 1, & \text{if} \quad \psi > 0\,. \end{cases} \tag{2}$$

The topological degree is invariant under changes of the vector p in the sense that, if $q \in \mathbb{R}^n$ is any vector, then it holds that [41, p.157]:

$$\deg[F_n, \mathcal{D}_n, p] \equiv \deg[F_n - q, \mathcal{D}_n, p - q],$$

where $F_n - q$ denotes the mapping $F_n(x) - q$, $x \in \mathcal{D}_n$. Thus, for simplicity reason, we consider the case where the topological degree is defined at the origin $\Theta_n = (0, \ldots, 0)$ in $\mathbb{R}^n$.

The topological degree $\deg[F_n, \mathcal{D}_n, \Theta_n]$ can be represented by the Kronecker integral which is closely tied with facts used later and is defined as follows:

$$\deg[F_n, \mathcal{D}_n, \Theta_n] = \frac{\Gamma(n/2)}{2\pi^{n/2}} \int\!\!\int_{\vartheta\mathcal{D}_n}\!\cdots\!\int \frac{\sum_{i=1}^{n} A_i dx_1 \ldots dx_{i-1} dx_{i+1} \ldots dx_n}{\left({f_1}^2 + {f_2}^2 + \ldots + {f_n}^2\right)^{n/2}}, \tag{3}$$

where A_i define the following determinants:

$$A_i = (-1)^{n(i-1)} \det \left[F_n \quad \frac{\partial F_n}{\partial x_1} \quad \cdots \quad \frac{\partial F_n}{\partial x_{i-1}} \quad \frac{\partial F_n}{\partial x_{i+1}} \quad \cdots \quad \frac{\partial F_n}{\partial x_n} \right], \tag{4}$$

where $\frac{\partial F_n}{\partial x_k} = \left(\frac{\partial f_1}{\partial x_k}, \frac{\partial f_2}{\partial x_k}, \ldots, \frac{\partial f_n}{\partial x_k} \right)$ is the kth column of the determinant $\det J_{F_n}$ of the Jacobian matrix J_{F_n}.

Definition 3.1 can be generalized when the function is only continuous [11, 41]. In this case, Kronecker's theorem [3, 11, 41] states that $F_n(x) = \Theta_n$ has at least one zero in $\mathcal{D}_n$ if $\deg[F_n, \mathcal{D}_n, \Theta_n] \neq 0$. Furthermore, if $\mathcal{D}_n = \mathcal{D}_n^1 \cup \mathcal{D}_n^2$ where $\mathcal{D}_n^1$ and $\mathcal{D}_n^2$ have disjoint interiors and $F_n(x) \neq \Theta_n$ for all $x \in \vartheta\mathcal{D}_n^1 \cup \vartheta\mathcal{D}_n^2$, then the topological degree is additive, i.e.:

$$\deg[F_n, \mathcal{D}_n, \Theta_n] = \deg[F_n, \mathcal{D}_n^1, \Theta_n] + \deg[F_n, \mathcal{D}_n^2, \Theta_n]. \tag{5}$$

Now, since $\deg[F_n, \mathcal{D}_n, \Theta_n]$ is equal to the number of zeros of $F_n(x) = \Theta_n$ that give positive determinant of the Jacobian matrix minus the number of zeros that give negative determinant of the Jacobian matrix, the total number $\mathcal{N}^r$ of zeros of $F_n(x) = \Theta_n$ can, of course, be obtained by the value of $\deg[F_n, \mathcal{D}_n, \Theta_n]$ if all these zeros have the same sign of the determinant of the Jacobian matrix. Note that, by assumption, all the zeros of $F_n(x) = \Theta_n$ are simple. To this end, Picard considered the following extension of the function F_n and the domain $\mathcal{D}_n$:

$$F_{n+1} = (f_1, \ldots, f_n, f_{n+1}) \colon \mathcal{D}_{n+1} \subset \mathbb{R}^{n+1} \to \mathbb{R}^{n+1}, \tag{6}$$

where $f_{n+1} = y \det J_{F_n}$, and $\mathcal{D}_{n+1}$ is the direct product of the domain $\mathcal{D}_n$ with an arbitrary interval of the real y–axis containing the point $y = 0$. Then the zeros of the following system of equations:

$$\begin{aligned} &f_i(x_1, x_2, \ldots, x_n) = 0, \quad i = 1, \ldots, n, \\ &y \det J_{F_n}(x_1, x_2, \ldots, x_n) = 0, \end{aligned} \tag{7}$$

are the same as the zeros of $F_n(x) = \Theta_n$ provided that $y = 0$. On the other hand, it is easily seen that the determinant of the Jacobian matrix of (7) is equal to $[\det J_{F_n}(x)]^2$ which is always nonnegative (positive at the simple zeros). Thus we may conclude the following.

Theorem 3.1 [42, 43]. *The total number $\mathcal{N}^r$ of zeros of $F_n(x) = \Theta_n$ is given by*

$$\mathcal{N}^r = \deg[F_{n+1}, \mathcal{D}_{n+1}, \Theta_{n+1}], \tag{8}$$

under the hypotheses that F_n is twice continuously differentiable and that all the zeros are simple and lie in the strict interior of $\mathcal{D}_{n+1}$.

Based on this, we are able to give closed formulas for the total number of roots. As for example in the univariate case, let (a, b) be an open interval in $\mathbb{R}$, and suppose that $f \colon [a, b] \subset \mathbb{R} \to \mathbb{R}$ is twice continuously differentiable. Assume further that $f(a)\, f(b) \neq 0$ and that all the roots of f that lie in (a, b) are simple. Then, by applying (1) for $n = 2$ we obtain that the total number $\mathcal{N}^r$ of roots of f that lie in (a, b) is given by [23]:

$$\mathcal{N}^r = -\frac{\gamma}{\pi} \int_a^b \frac{f(x) f''(x) - f'^2(x)}{f^2(x) + \gamma^2 f'^2(x)}\, dx + \frac{1}{\pi} \arctan \left(\frac{\gamma\, [f(a) f'(b) - f(b) f'(a)]}{f(a) f(b) + \gamma^2 f'(a) f'(b)} \right), \tag{9}$$

where γ is an arbitrary small real positive constant. It was explicitly shown by Picard [42, 43] that Relation (9) is independent of the value of γ.

The formula (9) can be used for the isolation of all simple roots of a function f in a specific interval $[a, b]$. Results with this approach can be found in [22, 23, 44]. Also, in [22, 23] a framework for the study of the expected complexity of the problem of finding with certainty all simple roots of a function has been presented and results have been shown for the case when the roots are uniformly or arbitrarily distributed (with a continuous distribution) in the considered interval. Furthermore, in [22] it is proved that the expected value (with respect to the considered distribution) of the times that we need to apply the formula (9) in order to isolate n roots ($n \geqslant 2$) is $\mathcal{O}(n \log n)$. Notice that an optimal algorithm for sorting has complexity time $\mathcal{O}(n \log n)$. On the other hand, using our approach we are able to sort n numbers with the same cost if we consider them as roots of a univariate polynomial. We intend to present results in this direction in a future communication.

The Kronecker-Picard integral can be also applied for the determination of the total number of multiple roots [13, 21, 23, 58].

For the case of complex zeros the following theorem states that the total number of complex zeros can be obtained by the value of the topological degree without Picard's extension:

Theorem 3.2 [72]. *Let $\mathcal{D}_2 \subset \mathbb{C}$ be an open bounded region and let $f : \mathcal{D}_2 \to \mathbb{C}$ be analytic. Suppose that f has no zeros on $\vartheta\mathcal{D}_2$ and assume that all zeros of f that lie in $\mathcal{D}_2$ are simple. Then the total number $\mathcal{N}^r$ of zeros of f is equal to* $\deg[F_2, \mathcal{D}_2, \Theta_2]$, *where:*

$$F_2(x_1, x_2) = (f_1(x_1, x_2), f_2(x_1, x_2)) = \Big(\Re(f(x_1 + \mathbf{i}\, x_2)), \Im(f(x_1 + \mathbf{i}\, x_2))\Big),$$

where $\Re(z)$ is the real and $\Im(z)$ is the imaginary part of $z \in \mathbb{C}$.

3.1 Optimal computation of 2–D topological degree

Several methods for the computation of the topological degree have been proposed in the past few years (see e.g., [7, 24, 25, 53, 55, 56]). To evaluate the topological degree, we use Stenger's method that in some classes of functions is an almost optimal complexity algorithm (see for example [7, 50, 53]). The accurate computation of topological degree using Stenger's or other related methods [24, 25, 55, 56], is based on suitable assumptions, including appropriate representation of the boundary of $\mathcal{D}_n$. In particular, if the boundary of $\mathcal{D}_n$ can be "sufficiently refined" then Stenger's method gives the value of topological degree.

Definition 3.2 [24, 25, 53, 54, 55, 56, 57]. *Let Π^n be an n–polyhedron. Suppose that $F_n = (f_1, f_2, \ldots, f_n)$: $\Pi^n \subset \mathbb{R}^n \to \mathbb{R}^n$ is continuous with $\Theta_n \notin F_n(\vartheta\Pi^n)$. If $n = 1$, $\vartheta\Pi^1$ is said to be sufficiently refined relative to* $\operatorname{sgn} F_1$, *if $0 \notin F_1(\vartheta\Pi^1)$. If $n > 1$, $\vartheta\Pi^n$ is said to be sufficiently refined relative to* $\operatorname{sgn} F_n$, *if $\vartheta\Pi^n$ has been subdivided so that it may be written as a union of a finite number of $(n-1)$–dimensional regions $Q_1^{n-1}, Q_2^{n-1}, \ldots, Q_m^{n-1}$, each consisting of a union of a finite number of $(n-1)$–simplices with pairwise disjoint $(n-1)$–dimensional interiors and having the following properties:*

a) the interiors of the Q_i^{n-1} are pairwise disjoint and each Q_i^{n-1} is connected;

b) for each region Q_i^{n-1}, there exists at least one component of F_n, (for example f_{r_i}), that does not vanish on it;

c) if $f_{r_i} \neq 0$ on Q_i^{n-1}, then ϑQ_i^{n-1} is sufficiently refined relative to $\operatorname{sgn} F_{r_i}$ *where:*

$$F_{n-1}^{r_i} = (f_1, f_2, \ldots, f_{r_i-1}, f_{r_i+1}, \ldots, f_n).$$

We now concentrate on dimension 2, although many of the following results can be extended to a higher dimension.

Definition 3.3 *A segment $[p_i, p_j]$ is defined to be a* closed counterclockwise oriented portion of $\vartheta\mathcal{D}_2$ with endpoints p_i and p_j and interior (p_i, p_j). *A* partition *P of $\vartheta\mathcal{D}_2$ is either the empty set or a set $\{p_i\}_{i=1}^{g}$ of counterclockwise ordered points from $\vartheta\mathcal{D}_2$ such that*

$$\vartheta\mathcal{D}_2 = \sum_{i=1}^{g} [p_i, p_{i+1}], \qquad p_{g+1} = p_1. \tag{10}$$

Lemma 3.1 *A nonempty partition P forms a sufficient refinement of the boundary $\vartheta\mathcal{D}_2$ relative to the sign of a function $F_2 = (f_1, f_2)$ if and only if $(p_i, p_{i+1}) \cap (p_j, p_{j+1}) = \emptyset$ for all $i \neq j$ and on each $[p_i, p_{i+1}]$, there exists a component of F_2, say f_j, that is of constant sign (i.e., $\neq 0$) on $[p_i, p_{i+1}]$, and the remaining component of F_2 is nonzero at p_i and p_{i+1}.*

Proof. The proof is obvious (cf. Definition 3.2). $\square$

Stenger proved (see [53]) that, given a sufficient refinement of the boundary $\vartheta\mathcal{D}_2$ of $\mathcal{D}_2$, the topological degree can be computed as:

$$\deg\,[F_2, \mathcal{D}_2, \Theta_2] = \frac{1}{4}\sum_{i=1}^{g} (-1)^{j_i-1} \deg\,[f_{j_i+1}, [p_i, p_{i+1}], 0] \times \operatorname{sign} f_{j_i}(p_i), \tag{11}$$

where j_i is the index of the component of $F_2 = (f_1, f_2)$ that has constant sign on $[p_i, p_{i+1}]$, $f_3 = f_1$, $\deg\,[f_j, [p_i, p_{i+1}], 0] = \{\operatorname{sign} f_j(p_{i+1}) - \operatorname{sign} f_j(p_i)\}/2$, and $\operatorname{sign} f_j(p_i) = (1, \text{ if } f_j(p_i) > 0, -1 \text{ if } f_j(p_i) < 0)$.

A worst-case lower bound for the number of function evaluations needed by this algorithm is expressed in terms of the Lipschitz constant of F_2 with respect to $\mathcal{D}_2$ and the infinity norm of F_2 along the boundary of $\mathcal{D}_2$.

More specifically, let $\mathcal{B} \equiv [0,1] \times [0,1]$ be the unit square in $\mathbb{R}^2$ and $\|\cdot\|_\infty$ be the infinity norm in $\mathbb{R}^2$. For given positive δ and K define

$$\begin{aligned} \mathcal{F} = \Big\{F_2 : \mathcal{B} \to \mathbb{R}^2,\ \ F_2 = (f_1, f_2) :\ \ & \|F_2(x) - F_2(y)\|_\infty \leqslant K\|x - y\|_\infty \quad \forall\, x, y \in \mathcal{B} \\ & \|F_2(x)\|_\infty \geqslant \delta \quad \forall\, x \in \vartheta\mathcal{B} \ \text{ and } \ K/(4\delta) \geqslant 1\Big\}. \end{aligned} \tag{12}$$

Boult and Sikorski presented in [7] an optimal complexity algorithm for computing the topological degree for any function from the class $\mathcal{F}$. Their algorithm calculates the degree using (11). They have examined the complexity, i.e. minimal cost of the problem of the calculation of topological degree for functions from class $\mathcal{F}$ and concluded that it is an almost optimal complexity algorithm. They assumed that each arithmetic operation ($+$, $-$, $*$, $\div$, abs( )), each logical operation (and, or, not) or comparison ($>$, $<$, $\geqslant$, $\leqslant$, $=$, $\neq$) costs unity, and that each function evaluation costs c. Also, they proved that any algorithm that solves the problem must use at least $m^* = 4\lfloor K/(4\delta)\rfloor$ function evaluations and a lower bound on the computational complexity is $m^* \times (c+2) - 1$.

The above can be extended to the case where the domain of interest is an arbitrary polyhedron in $\mathbb{R}^2$ [7]. This extension consists of choosing points on the boundary of the polyhedron separated by a distance $1/\lfloor K/(4\delta)\rfloor$ in the infinity norm [7].

3.2 A new approach

To evaluate the topological degree using the optimal complexity algorithm of [7] we need the value of the Lipschitz constant

$$K = \max_{\substack{x \neq y \\ x, y \in \mathcal{D}_2}} \frac{\|F_2(x) - F_2(y)\|_\infty}{\|x - y\|_\infty},$$

with respect to $\mathcal{D}_2$ and the infinity norm δ of F_2 along the boundary of $\mathcal{D}_2$.

We propose another scheme that involves only $\delta = \min_{x \in \vartheta\mathcal{D}_2} \|F_2(x)\|_\infty$. The scheme consists of two steps:

- First, we approximate the function F_2 on the boundary by B-splines, controlling the error of approximation in terms of second derivatives. This approximation step is not required if map F_2 is a polynomial.

- Secondly, we use the B-spline approximation and the isolation procedure of Section 2, in order to compute the topological degree of F_2.

In order to compute topological degree of F_2 from an approximation of its components on the boundary of the domain, we will exploit the homotopy invariance of the degree. More precisely, we use the following definition:

Definition 3.4 *Suppose that $\varphi_1, \varphi_2 : \overline{\mathcal{D}}_n \subset \mathbb{R}^n \to \mathbb{R}^n$ are two continuous mappings defined on the closure $\overline{\mathcal{D}}_n$ of an open and bounded domain $\mathcal{D}_n$. If $p \in \mathbb{R}^n$ is any point such that $p \notin \varphi_1(\vartheta\mathcal{D}_n)$ and $p \notin \varphi_2(\vartheta\mathcal{D}_n)$, and if there is a homotopy:*

$$H : \overline{\mathcal{D}}_n \times I \subset \mathbb{R}^{n+1} \to \mathbb{R}^n, \qquad I = [0, 1],$$

such that $H(x, 0) = \varphi_1(x)$, $H(x, 1) = \varphi_2(x)$ with $H(x, t) \neq p$ for all $(x, t) \in \vartheta\mathcal{D}_n \times I$, then φ_1 and φ_2 are said to be homotopic avoiding *p.*

The homotopy invariance of the degree is given by:

Theorem 3.3 [**Homotopy Invariance**] [5, 11, 35, 41]. *If φ_1 and φ_2 are homotopic avoiding p then* $\deg[H(\cdot, t), \mathcal{D}_n, p]$ *has the same value for all $t \in I$ and consequently* $\deg[\varphi_1, \mathcal{D}_n, p] = \deg[\varphi_2, \mathcal{D}_n, p]$.

As conclusion of Theorem 3.3, we find that the topological degree depends only on the values of the considered function on the boundary $\vartheta\mathcal{D}_n$ of the domain $\mathcal{D}_n$. In particular, if $\varphi_1, \varphi_2 : \overline{\mathcal{D}}_n \subset \mathbb{R}^n \to \mathbb{R}^n$ are two continuous mappings defined on the closure $\overline{\mathcal{D}}_n$ of an open and bounded domain $\mathcal{D}_n$ and if $p \in \mathbb{R}^n$ is any point for which the $\deg[\varphi_1, \mathcal{D}_n, p]$, $\deg[\varphi_2, \mathcal{D}_n, p]$ are defined, then Theorem 3.3 implies the following three theorems:

Theorem 3.4 [**Boundary–Value**] [5, 11, 35, 41]. *If $\varphi_1(x) = \varphi_2(x)$ for $x \in \vartheta\mathcal{D}_n$, then* $\deg[\varphi_1, \mathcal{D}_n, p] = \deg[\varphi_2, \mathcal{D}_n, p]$.

Theorem 3.5 [**Poincaré–Bohl**] [5, 11, 35, 41]. *If for each $x \in \vartheta\mathcal{D}_n$ the line segment $[\varphi_1(x), \varphi_2(x)]$ does not intersect the point p, then* $\deg[\varphi_1, \mathcal{D}_n, p] = \deg[\varphi_2, \mathcal{D}_n, p]$.

Theorem 3.6 [**Rouché**] [5, p.226],[11, 35, 41]. *If for some positive number $\eta < \pi$ it holds that $\|\varphi_1(x) - p\| > \eta$ for $x \in \vartheta\mathcal{D}_n$ and if $\|\varphi_1(x) - \varphi_2(x)\| < \eta$ for $x \in \mathcal{D}_n$ then* $\deg[\varphi_1, \mathcal{D}_n, p] = \deg[\varphi_2, \mathcal{D}_n, p]$.

Thus, if F_2 does not vanish on the boundary of the domain and if its components are approximated closely enough on this boundary, the topological degree of the map and its approximation will be the same. We are going to approximate components of F_2 by B-splines within $\epsilon < \delta = \min_{x\in\vartheta\mathcal{D}_2} \|F_2(x)\|_\infty$. By Theorem 3.6, the topological degree will not change. The approximation error is controlled as follows. Let us denote by S_d the Schoenberg operator defined by:

$$S(F_2) = \sum_{i=0}^{L-d+1} F_2(\zeta_i) B_i^d$$

where $\zeta_i = \frac{1}{d}(u_i + \cdots + u_{i+d-1})$, B_i^d is the Bézier basis from Section A.2 and $u_d \leqslant a, b \leqslant u_L$. The fundamental property of S is that it reproduces straight lines, i.e. $S(f) = f$ when f is a polynomial of degree one. The following well known result, is given in e.g. [38, p.8], [45, p.36].

Theorem 3.7 *Let f be a function twice differentiable on the interval $[a, b]$. Suppose further that $|\mathbf{u}| = \sup_{d \leqslant i \leqslant L} |u_{i+1} - u_i|$. Then, for all $d \geqslant 1$, we have:*

$$\|f - S(f)\|_\infty \leqslant C_d |\mathbf{u}|^d \|f^{(d)}\|_\infty.$$

First, let us consider a rectangular domain $\mathcal{D}_2$. We approximate F_2 on the boundary $\vartheta\mathcal{D}_2$ by a univariate B-spline, which yields control polygons on the boundary $\vartheta\mathcal{D}_2$. The complete B-spline $2D$ map is obtained by constructing any mesh that fits with the control polygons on the boundary $\vartheta\mathcal{D}_2$ and by computing the corresponding *tensor* B-spline, corresponding to the representation in the bivariate basis $(B_i^d(t) B_j^d(s))_{0 \leqslant i,j \leqslant d}$, (see [14]).

If we consider triangular domain, then we will use triangular meshes and B-splines. We assume hereafter that the map $F_2 = (f_1, f_2)$ is twice continuously differentiable on the boundary $\vartheta\mathcal{D}_2$ and we denote by $S(F_2) = (S(f_1), S(f_2))$ the B-spline approximation associated with Schoenberg operator on segments defining the boundary of the domain.

Proposition 3.1 *Assume that* $\|F_2\| > \eta$ *on* $\vartheta\mathcal{D}_2$ *and that the perimeter of* $\mathcal{D}_2$ *is* σ. *Then a B-spline approximation of* F_2 *such that*

$$\deg[S(F_2), \mathcal{D}_2, \Theta_2] = \deg[F_2, \mathcal{D}_2, \Theta_2],$$

can be constructed with L *nodes if*

$$L \geqslant \left\lceil \sigma\, d \sqrt{\frac{\|F_2^{(2)}\|}{2\eta}} \right\rceil .$$

Proof. We take for $\mathbf{u}$ a regular subdivision of points on the boundary $\mathcal{D}_2$ such that $|\mathbf{u}| < \frac{\sigma}{L}$ where L is the number of nodes and we apply Theorem 3.6. Thus the proposition is proved. $\square$

This result suggests that linear approximation ($d = 1$) will yield the optimal number of nodes. Higher order spline approximations can be however be exploited if the function f is of class C^k with $k \leqslant 2$ by using Schoenberg-like operators which reproduce polynomial functions of degree $(k-1)$. For more details, see [47].

The next step consists of computing effectively the topological degree of the B-spline map $S(F_2)$. We use the following results.

Proposition 3.2 *Suppose that* $F_2 = (f_1, f_2)\colon \mathcal{D}_2 \subset \mathbb{R}^2 \to \mathbb{R}^2$ *is continuous and that* $\Theta_2 \notin F_2(\vartheta\mathcal{D}_2)$. *Then a partition* P *of counterclockwise ordered points* $\{p_i\}_{i=1}^{g}$ *from the boundary* $\vartheta\mathcal{D}_2$ *that forms a sufficient refinement of* $\vartheta\mathcal{D}_2$ *relative to the sign of* F_2 *can be obtained by* $g = 2 \times \min\{\mathcal{N}_j^r, j = 1, 2\}$ *points where* $\mathcal{N}_j^r$ *determines the total number of sign changes of* f_j *along the boundary* $\vartheta\mathcal{D}_2$.

Proof. By Bolzano's existence criterion for each sign change of a component of F_2, say f_j, there exists a closed counterclockwise oriented portion of $\vartheta\mathcal{D}_2$ with endpoints p_i and p_{i+1} such that f_j vanishes exactly once within (p_i, p_{i+1}), $f_j \neq 0$ at p_i and p_{i+1} and the remaining component of F_2 is of constant sign on $[p_i, p_{i+1}]$. The latter holds since $\Theta_2 \notin F_2(\vartheta\mathcal{D}_2)$. Then the proof follows by Lemma 3.1. $\square$

Hereafter, we will assume that F_2 is a B-spline map of degree d (and thus continuous).

Definition 3.5 *We define an* optimal partition P_{opt} *as the partition* $\{p_i\}_{i=1}^{g}$ *of* g *counterclockwise ordered points from the boundary* $\vartheta\mathcal{D}_2$ *forming a sufficient refinement of* $\vartheta\mathcal{D}_2$ *relative to the sign of a function* F_2 *obtained with the minimum number* g.

Remark 3.1 The optimal partition is obtained by applying Proposition 3.2 to the longest possible portions of the boundary $\vartheta\mathcal{D}_2$ with endpoints p_i and p_{i+1} such that a component of F_2, say f_j, vanishes exactly once within (p_i, p_{i+1}), $f_j \neq 0$ at p_i and p_{i+1} and the remaining component of F_2 is of constant sign on $[p_i, p_{i+1}]$.

In order to effectively compute this optimal partition, we use the isolation procedure of Section 2. We decompose the boundary $\vartheta\mathcal{D}_2$ into segments, on which we isolate the roots of the product $f_1 f_2$. Using Theorem 2.1 we get the following results.

Theorem 3.8 *Assume that* $\vartheta\mathcal{D}_2$ *is a rectangular cell and that* F_2 *does not vanish on* $\vartheta\mathcal{D}_2$. *Then the number of operations needed to compute a sufficiently refined subdivision of* $\vartheta\mathcal{D}_2$ *is bounded by*

$$\omega = 4d(d+1)(r_1 + r_2)\left(\log_2\left(\frac{2}{s}\right) + 4\right),$$

where $s = \min_{i \neq j} |x_i - x_j|$ *for* $x_i, x_j \in \left\{\left[f_1^{-1}(0) \cup f_2^{-1}(0)\right] \cap \vartheta\mathcal{D}_2\right\}$, *(*$x_i, x_j$ *are the zeros of* f_1 *or* f_2 *along the boundary* $\vartheta\mathcal{D}_2$*), and* r_i *is the number of sign changes of* f_i *along the boundary* $\vartheta\mathcal{D}_2$.

Proof. We apply Theorem 2.1 to the product $f_1 f_2$, each subdivision requiring $d\,(d+1)$ arithmetic operations and the number of segments on the boundary of a rectangular cell being 4. Thus the theorem is proved. $\square$

Once we have isolated the roots of f_1 and f_2 on the boundary, that is when we obtain a sequence of intervals containing exactly one of the roots of f_1 or f_2, we derive immediately an optimal partition of the boundary, by simplifying the resulting subdivision.

We summarize the algorithm for computing topological degree of F_2:

Algorithm 3.1 *Computing the topological degree*

Assume that $\mathcal{D}_2$ *is a rectangle in* $\mathbb{R}^2$.

1. *if* F_2 *is not polynomial, approximate* F_2 *on the boundary, by the B-spline map* $S(F_2) = (f_1, f_2)$ *of degree* d,
2. *for each segment of the boundary* $\vartheta\mathcal{D}_2$, *isolate the roots of* $f_1 f_2$, *using Algorithm 2.1,*
3. *deduce a sufficiently refined subdivision of the boundary (see Lemma 3.1),*
4. *compute the topological degree of* F_2, *according to the formula (11).*

Combining previous results, we get:

Theorem 3.9 *The total number of operations required to compute topological degree of polynomial map* $F_2 = (f_1, f_2)$ *of degree* d *on* $\mathcal{D}_2$ *is bounded by*

$$\mathcal{O}\left(d^2\,(r_1 + r_2)\log_2\left(\frac{2}{s}\right)\right),$$

where $s = \min_{i\neq j}|x_i - x_j|$ *for* $x_i, x_j \in \left\{\left[f_1^{-1}(0) \cup f_2^{-1}(0)\right] \cap \vartheta\mathcal{D}_2\right\}$ *and* r_i *is the number of sign changes of* f_i *along the boundary* $\vartheta\mathcal{D}_2$.

3.3 The characteristic polyhedron criterion and the characteristic bisection method

The aim of this section is to describe a generalized bisection method for the computation of a solution of

$$F_n(x) = \Theta_n, \tag{13}$$

where $F_n = (f_1, \ldots, f_n)\colon \overline{\mathcal{D}}_n \subset \mathbb{R}^n \to \mathbb{R}^n$ is continuous. This method of bisection avoids all calculations concerning the topological degree.

Once we have obtained a domain for which the value of the topological degree relative to this domain is nonzero, we are able to obtain upper and lower bounds for solution values. To this end, by computing a sequence of bounded domains with nonzero values of topological degree and decreasing diameters, we are able to obtain a region with arbitrarily small diameter that contains at least one solution of Equation (13). However, although the nonzero value of topological degree plays an inportant role in the existence of a solution of Equation (13), the computation of this value is a time-consuming procedure. The bisection method, on the other hand, which is briefly described below, avoids all calculations concerning the topological degree by implementing the concept of the *characteristic* n*-polyhedron criterion* for the existence of a solution of Equation (13) within a given bounded domain. This criterion is based on the construction of a *characteristic* n*–polyhedron* [68, 62, 63]. To define a characteristic n–polyhedron (n–dimensional convex polyhedron) we construct the n*–complete* $2^n \times n$ *matrix* $\mathcal{M}_n$ whose rows are formed by all possible combinations of -1 and 1. To this end we compute the n*-binary* $2^n \times n$ *matrix* $\mathcal{M}_n^* = \left[e_{ij}^*\right]_{i,j=1}^{2^n,n}$ where e_{ij}^* is the jth digit of the n–digit binary representation of the number $(i-1)$ counting the left-most digit first. Then the elements of $\mathcal{M}_n = \left[e_{ij}\right]_{i,j=1}^{2^n,n}$ are given by $e_{ij} = 2e_{ij}^* - 1$. Suppose now that $\Pi^n = \langle V_1, V_2, \ldots, V_{2^n}\rangle$ is an oriented (i.e., an orientation has been assigned to its vertices) n–dimensional convex polyhedron with 2^n vertices, $V_i \in \mathbb{R}^n$, and let $F_n = (f_1, f_2, \ldots, f_n)\colon \Pi^n \subset \mathbb{R}^n \to \mathbb{R}^n$ be a continuous mapping.

Definition 3.6 *The* $2^n \times n$ *matrix* $\mathcal{S}(F_n; \Pi^n)$ *whose entries in the* k*-th row are the corresponding coordinates of the vector:*

$$\operatorname{sgn}(F_n(V_k)) = \Big(\operatorname{sgn}(f_1(V_k)), \operatorname{sgn}(f_2(V_k)), \ldots, \operatorname{sgn}(f_n(V_k))\Big), \tag{14}$$

will be called matrix of signs associated with F_n and Π^n, *where* $\operatorname{sgn}(\psi)$ *defines the three valued sign function (2).*

Definition 3.7 *An* n*–polyhedron* Π^n *is called* characteristic n–polyhedron relative to F_n, *iff the matrix* $\mathcal{S}(F_n; \Pi^n)$ *is identical with the matrix* $\mathcal{M}_n$, *after some permutation of its rows.*

Definition 3.8 *A polyhedron which is a convex hull of 2^{n-1} vertices of a characteristic n–polyhedron Π^n relative to F_n, will be called* r-side *of Π^n and will be noted by P_r, $r = 1, 2, \dots, n$ iff for all its vertices V_k, $k = 1, 2, \dots, 2^{n-1}$ the corresponding vectors $\operatorname{sgn}(F_n(V_k))$ have their r-th coordinate equal to each other. Moreover, if this common r-th element is -1 (or 1) then the P_r will be called* negative *(or* positive*)* r-side.

Lemma 3.2 [68]. *In each characteristic n–polyhedron relative to F_n there are n positive and n negative sides. Moreover, each side P_r of a characteristic n–polyhedron Π^n relative to $F_n = (f_1, f_2, \dots, f_n) \colon \Pi^n \subset \mathbb{R}^n \to \mathbb{R}^n$ is itself a characteristic $(n-1)$–polyhedron relative to $F^r_{n-1} = (f_1, f_2, \dots, f_{r-1}, f_{r+1}, \dots, f_n) \colon P_r \to \mathbb{R}^{n-1}$.*

Now, if the boundary $\vartheta \Pi^n$ of a characteristic polyhedron Π^n can be sufficiently refined then there is (at least) one zero within Π^n. More specifically, the following theorem holds:

Theorem 3.10 [68]. *Let $\mathcal{V} = \langle V_i \rangle_{i=1}^{2^n}$ and $\mathcal{P} = \{P_i\}_{i=1}^{2n}$ be the ordered set of vertices and the set of the sides, respectively, of a characteristic n–polyhedron Π^n relative to continuous $F_n \colon \Pi^n \subset \mathbb{R}^n \to \mathbb{R}^n$ for which $\Theta_n \notin F_n(\vartheta \Pi^n)$. Suppose that $S = \{S_{i,j}\}_{i=1,\,j=1}^{2n,\;j_i}$ is a finite set of $(n-1)$–dimensional oriented simplices which lie on $\vartheta \Pi^n$ with the following properties:*

1) $\vartheta \Pi^n = \sum_{i=1}^{2n} \sum_{j=1}^{j_i} S_{i,j}$,

2) the interiors of the members of S are disjoint,

3) these simplices make $\vartheta \Pi^n$ sufficiently refined relative to $\operatorname{sgn}(F_n)$*, and*

4) the vertices of each simplex $S_{i,j}$ are a subset of vertices of P_i.

Then, it holds that $\deg[F_n, \Pi^n, \Theta_n] = \pm 1$.

The above result implies the existence of at least one solution of Equation (13) within Π^n. For more details on how to construct a characteristic n–polyhedron and locate a desired solution see [62, 63, 65]. The characteristic polyhedron can be considered as a translation of the Poincaré–Miranda hypercube [34, 53, 64].

Next, we describe a generalized bisection method. This method combined with the above mentioned criterion, produces a sequence of characteristic polyhedra of decreasing size always containing the desired solution. We call it *Characteristic Bisection.* This version of bisection does not require the computation of the topological degree at each step, as others do [12, 25, 61]. It can be applied to problems with imprecise function values, since it depends only on their signs. The method simply amounts to constructing another refined characteristic polyhedron, by bisecting a known one, say Π^n. To do this, we compute the midpoint M of the longest edge $\langle V_i, V_j \rangle$, of Π^n (where the distances are measured in Euclidean norms). Then we obtain another characteristic polyhedron, Π^n_*, by comparing the sign, $\operatorname{sgn}(F_n(M))$, of $F_n(M)$ with that of $F_n(V_i)$ and $F_n(V_j)$ and substituting M for that vertex for which the signs are identical [62, 63, 65]. Then we select the longest edge of Π^n_* and continue the above process. If the assumptions of Theorem 3.10 are satisfied, one of the $\operatorname{sgn}(F_n(V_i))$, $\operatorname{sgn}(F_n(V_j))$ coincides with $\operatorname{sgn}(F_n(M))$, otherwise, we continue with another edge.

Theorem 3.11 [68]. *Suppose that Π^n is a characteristic n-polyhedron whose longest edge length is $\Delta(\Pi^n)$. Then, the minimum number ζ of bisections of the edges of Π^n required to obtain a characteristic polyhedron Π^n_* whose longest edge length satisfies $\Delta(\Pi^n_*) \leqslant \varepsilon$, for some accuracy $\varepsilon \in (0, 1)$, is given by*

$$\zeta = \left\lceil \log_2 \left(\Delta(\Pi^n)\, \varepsilon^{-1} \right) \right\rceil . \tag{15}$$

Notice that ζ is independent of the dimension n and that the bisection algorithm has the same number of iterations as the bisection in one-dimension which is optimal and possesses asymptotically the best rate of convergence [49].

3.4 Application to the isolation of complex roots of an analytic function

These tools can now be combined to compute complex roots of an analytic function in a bounded domain. Let $f : \mathbb{C} \to \mathbb{C}$ be an analytic map and let

$$\begin{aligned} F_2 : \mathbb{R}^2 \quad &\to \quad \mathbb{R}^2, \\ (x_1, x_2) \quad &\mapsto \quad \Big(\Re(f(x_1 + \mathbf{i}\, x_2)), \Im(f(x_1 + \mathbf{i}\, x_2)) \Big), \end{aligned}$$

where $\Re(z)$ is the real and $\Im(z)$ is the imaginary part of $z \in \mathbb{C}$. Suppose that $\mathcal{D}_2$ is a bounded domain of $\mathbb{R}^2$ and let us assume that F_2 does not vanish on its boundary. According to Theorem 3.1, the topological degree of F_2 on $\mathcal{D}_2$ is the number of complex roots in the domain $\mathcal{D}_2$. This criterion can be used to split a rectangular domain $\mathcal{D}_2$, as described in the following algorithm[1]:

Algorithm 3.2 *Isolating the complex roots within a precision s.*

While $\deg[F_2, \mathcal{D}_2, \Theta_2] > 1$ *and diameter*$(\mathcal{D}_2) > s$,

1. *split $\mathcal{D}_2$ along its longest dimension (edge) into $\mathcal{D}_2^1$ and $\mathcal{D}_2^2$,*
2. *compute* $\deg[F_2, \mathcal{D}_2^1, \Theta_2]$ *and* $\deg[F_2, \mathcal{D}_2^2, \Theta_2]$.

Notice that, if the topological degree is not well defined at Step (2), that is if F_2 vanishes on the new edge (or if the isolation process cannot separate the roots of F_2 by intervals of size greater than ϵ), we perturb the splitting by using an edge which do not split exactly into equal parts.

Proposition 3.3 *Assume that $\mathcal{D}_2$ is a rectangle of width a and height b. Then, the number of recursion steps in Algorithm 3.2 is bounded by*

$$\beta = 2\log_2\left(\frac{\sqrt{a^2+b^2}}{s}\right),$$

where $s = \min_{i\neq j}|z_i - z_j|$ and z_i is a root of f in $\mathcal{D}_2$.

Proof. Every two steps we divide the diameter by two and we stop when this diameter is less than s. Thus, if k is the number of steps, we have:

$$\frac{\sqrt{a^2+b^2}}{2^{\frac{k}{2}}} < s \qquad \Rightarrow \qquad k < 2\log_2\left(\frac{\sqrt{a^2+b^2}}{s}\right).$$

Thus the proposition is proved. □

Once the roots have been isolated, we can refine the isolation by using the characteristic polyhedron approach of the previous section.

This algorithm can be applied directly to a complex polynomial of degree d to compute all its roots in the complex plane, as follows. We replace its real part f_1 and imaginary part f_2 by the polynomials

$$\tilde{f}_i = (1-t_1)^d(1-t_2)^d f_i\left(\frac{t_1}{1-t_1}, \frac{t_2}{1-t_2}\right), \qquad i = 1, 2,$$

and isolate the roots of $\tilde{F}_2 = (\tilde{f}_1, \tilde{f}_2)$ on the domain $\mathcal{D}_2 = [0,1[\times[0,1[$, which will yield the roots of F_2 on $[0,+\infty[\times[0,+\infty[$. Using symmetry along the axes, we compute in a similar way the roots in the other quadrants.

4 Conclusions and further research

The approach that we proposed for the computation of the topological degree consists of:

1. approximation (if required) of a function by a B-spline map on the boundary of the domain,
2. isolating of the real zeros of its components on this boundary, and
3. computation of the topological degree by direct sign computations.

[1] it can be extended to general polygonal domains

We focused on the two dimensional case and analyzed in detail different steps of this approach. We provided new complexity results, that improve previously known bounds. We mentioned a direct application of this method to the isolation of complex roots of a univariate polynomial.

The interesting feature of this approach is that it is based on very simple operations such as sign evaluations, additions, divisions by 2, which may be of importance in the practical implementation of the algorithm. Also, the method can be adapted to a specific domain of interest, which is not the case of algebraic methods.

Many improvements can be added. First, most of the operations can be extended to higher dimensions, by applying recursively topological degree computation. Second, several steps can be adapted to a local behavior of the function, refining for instance the approximation where the function is small or adapting the domain to the geometry of the zeros. The validation of numerical stability of the method in the context of equations with approximate coefficients is under study. The topological degree theory should provide pertinent answers to problems for which the roots move from the complex domain to the real domain in a neighborhood of the input coefficients.

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A B-spline representation

We recall here the basic results that we use on Bezier polynomials and B-spline representations. For more details see e.g. [14].

A.1 Bézier curves.

Let $f : \mathbb{R} \to \mathbb{R}$ be a polynomial of degree d, with coefficients in $\mathbb{R}$. A possible representation for this polynomial is its $(d+1)$–array of coefficients in the monomial basis $1, t, \ldots, t^d$:

$$f(t) = \sum_{k=0}^{d} f_k \, t^k.$$

We will consider here another basis, given by the Bézier polynomials:

$$B_i^d(t) = \binom{d}{i} t^i \, (1-t)^{d-i}, \quad i = 0, \ldots, d.$$

We denote by $(a_i)_{i=0,\ldots,d}$ the coefficients of f in this basis:

$$f(t) = \sum_{i=0}^{d} a_i \, B_i^d(t).$$

The points $(p_i)_{i=0,\ldots,d}$ where $p_i = \left[\frac{i}{d}, a_i\right]$ form what is called the control polygon of the polynomial f (see [14]).

A value of a polynomial f can be easily computed from this representation, using the de Casteljau algorithm:

$$b_i^0 = a_i, \quad i = 0, \ldots, d,$$
$$b_i^r = (1-t)\, b_i^{r-1} + t\, b_{i+1}^{r-1}(t), \quad i = 0, \ldots, d-r.$$

The value of $f(t)$ is $b_0^d(t)$. This algorithm requires $\mathcal{O}(d^2)$ arithmetic operations and $\mathcal{O}(d)$ memory space. Moreover, the control polygons $\mathbf{P}^-(t) = (p_0^0, p_0^1, \ldots, p_0^d)$ and $\mathbf{P}^+(t) = (q_0^d, q_1^{d-1}, \ldots, q_d^0)$ (where $p_i^j = \left[\frac{j}{d}, b_i^j\right]$ and $q_i^j = \left[\frac{i}{d}, b_i^j\right]$) refer to the restriction of f on $[0,t]$ and $[t,1]$. We consider the special value $t = \frac{1}{2}$, for the subdivision step in our algorithm. The two control polygons $\mathbf{P}^-(t), \mathbf{P}^+(t)$ describe the functions $f^0(t) = f\left(\frac{t}{2}\right)$ and $f^1(t) = f\left(\frac{t+1}{2}\right)$ on the interval $[0,1]$.

A fundamental property of the Bernstein representation is that the curve defined by:

$$t \in [0,1] \to (t, f(t)) \in \mathbb{R}^2,$$

is contained in the convex hull of the points $(k/d, a_k)$, $k = 0, \ldots, d$. This follows easily from the classical equality $t = \sum_{k=0}^{d} \frac{k}{d} B_k^d(t)$.

We denote by $f^*(t)$ the following polynomial:

$$f^*(t) = (1+t)^d f\left(\frac{1}{1+t}\right) = \sum_{k=0}^{d} \binom{d}{k} a_k t^{d-k}.$$

Consequently, the localization of the real roots of $f(t)$ in the interval $[0,1]$ is equivalent to the localization of the real roots of $f^*(t)$ in the interval $[0, +\infty[$.

Another interesting property of this representation is the following:

Proposition A.1 *The number of sign changes of the sequence* $\mathbf{a} = (a_i)_{i=0,\ldots,d}$ *bounds the number of roots of* f *in the interval* $[0,1]$. *Moreover, this bound is equal to the number of roots modulo* 2.

Proof. The first point is a direct consequence of the Variation Diminishing property of Bézier curves [14, p.54].

For the second point, we remark that, by applying the change of variables $t \to \frac{t}{1+t}$, we can use the classical Descartes rule for f^*, giving a bound and the parity of the number of positive real roots of a univariate polynomial [45]. Thus the proposition is proved. □

The control polygon of a curve is a very rough but quite intuitive description of the curve. This description can be refined by insertion of points, given by the following formula:

$$p_i^{'} = \frac{i}{d+1}\, p_{i-1} + \left(1 - \frac{i}{d+1}\right) p_i, \qquad i = 0, \ldots, d+1,$$

which requires $\mathcal{O}(d)$ arithmetic operations. Iterating this refinement yields a sequence of polygons which converge to the curve [14].

A.2 B-splines

In our approach we also use B-splines. We briefly recall their construction (for more details see for instance [14]). Let $u_0 = a, \ldots, u_L = b$ be a set of non-decreasing numbers, also called a *subdivision* of $[a,b]$. A *B-spline curve of order d associated with the subdivision* $\mathbf{u} = (u_0, \ldots, u_L)$, is a curve which is piecewise polynomial of degree d on the interval $[a,b]$, and of class C^{r_i} at the node u_i. Notice that these nodes may not be distinct. The curve is polynomial (of degree d) on the interval $[u_i, u_{i+1}]$ and defined by the control polygon $([\xi_{i+j}, b_{i+j}])_{j=0,\ldots,d-1}$ where:

$$\xi_i = \frac{1}{d}(u_i + \cdots + u_{i+d-1}).$$

In order to represent a polynomial P of degree d with control values $b_0, \ldots, b_L$ on the interval $[0,1]$, we take the subdivision $u_0 = \cdots = u_{d-1} = 0$, $u_d = \cdots = u_{2d-1} = 1$. Thus we have $\xi_j = \frac{j}{d}$, and the control polygon defining the curve is the following:

$$[\xi_0, b_0], \ldots, [\xi_{L-d+1}, b_{L-d+1}].$$

The internal representation of such a B-spline is thus given by:

- the sequence of nodes $u_0, \ldots, u_L$,
- the control values $b_0, \ldots, b_L$.

The abscissas $(\xi_i)_{i=0,\ldots,L-d}$ can be computed directly from these values.

Refining the representation. Given a B-spline, in order to get a more precise representation of the same curve we can refine the subdivision. This task is performed by the insertion algorithm described in [14], and similar to de Casteljau algorithm. This refinement procedure has the following properties:

- Variation diminishing property: a line intersects the control polygon in more points than the number of real zeros of the polynomial P on the interval $[a,b]$.
- By inserting a sequence of equidistant points in $[a,b]$, the sequence of polygons converge to the curve.

Consequently, the number of sign changes in the sequence b_i bounds the number of real roots in the interval $[a,b]$. This bound is equal to the actual number of real roots, modulo 2.