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SELF-VALIDATED METHODS FOR THE SIMULTANEOUS INCLUSION OF POLYNOMIAL ZEROS

D.M. Milošević[1 §], Lj.D. Petković[2], M.S. Petković[3]

[1,3]Faculty of Electronic Engineering
University of Niš
Niš, 18000, SERBIA
[1]e-mail: dmilosev@elfak.ni.ac.yu
[2]Faculty of Mechanical Engineering
University of Niš
Niš, 18000, SERBIA

Abstract: The computed roots of algebraic equations are only approximations to the exact roots since there are errors originating from discretization, truncation and from rounding. For this reason, it is important to apply a root-finding procedure which simultaneously improves the approximations to the roots and also gives error bounds of the improved approximations. In this paper we study three types of self-validated methods that automatically provide upper error bounds of the computed approximations: (I) interval methods which deal with disks as arguments, (II) hybrid methods that combine a simultaneous method in ordinary complex arithmetic and an interval method in circular complex interval arithmetic, and (III) *a posteriori* bound error methods. Numerical examples illustrate each of the presented approaches.

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[§]Correspondence author

1. Introduction

Solving practical computational problems in applied mathematics, a natural question should be *"what is the error in the result?"* The computed solution of an algebraic equation is only an approximation to the exact solution due to errors originating from discretization, truncation and from rounding. Solving polynomial equations, the considerable amount of the applied procedure is to improve the approximate result and also to give error bounds for the improved approximations to the polynomial zeros.

In this paper we will study three types of self-validated methods for the simultaneous determination of polynomial zeros that overcome the aforementioned problems:

(I) Interval methods;

(II) Hybrid (combined) methods;

(III) A posteriori bound error methods.

Each of these classes of methods will be discussed in the next sections.

2. Interval Methods

Various authors developed techniques for the inclusion of polynomial zeros. These devices mostly use Gerschgorin's theorem, Rouché's theorem, fixed point principle. A quite different approach to error estimates for a given set of approximate zeros uses the so-called circular complex arithmetic, as pointed out by Gargantini and Henrici [5]. Simultaneous iterative methods, realized in circular arithmetic, produce resulting disks that contain the complex zeros of a polynomial. In this manner, not only very close approximations (given by the centers of disks) but also the upper error bounds for the zeros (given by the radii of disks) are obtained. For more details about simultaneous inclusion methods see the books [8] and [12], where the basic properties and operations of circular complex arithmetic are also reviewed.

Although there are several principles for constructing simultaneous inclusion methods, the most frequent and most efficient is the one based on fixed point relations, as done in the mentioned fundamental paper [5]. Let $\zeta_1, \dots, \zeta_n$ be the zeros of a given polynomial P and assume that we have found an array of n disks $\boldsymbol{Z} = (Z_1, \dots, Z_n)$ such that $\zeta_i \in Z_i$ $(i \in I_n := \{1, \dots, n\})$. Let $\boldsymbol{\zeta} = (\zeta_1, \dots, \zeta_n)$ and $\boldsymbol{z} = (z_1, \dots, z_n)$ be the vectors of the exact zeros of P and the centers of disks, $z_i = \operatorname{mid} Z_i$, and let us represent a fixed point relation in a general form

$$\zeta_i = G_i(\boldsymbol{z}, \boldsymbol{\zeta}). \tag{1}$$

For illustration, we give the following three examples of the fixed point relations:

$$\zeta_i = z_i - P(z_i) / \prod_{\substack{j=1 \\ j \neq i}}^{n} (z_i - \zeta_j) \quad (i \in I_n), \tag{$F1$}$$

$$\zeta_i = z_i - \Big(\frac{P'(z_i)}{P(z_i)} - \sum_{\substack{j=1 \\ j \neq i}}^{n} \frac{1}{z_i - \zeta_j} \Big)^{-1} \quad (i \in I_n), \tag{$F2$}$$

$$\zeta_i = z_i - W_i \Big(1 + \sum_{\substack{j=1 \\ j \neq i}}^{n} \frac{W_j}{\zeta_i - z_j} \Big)^{-1} \quad (i \in I_n), \tag{$F3$}$$

where $W_i = P(z_i) / \prod_{j \neq i} (z_i - z_j)$ is the so-called Weierstrass's correction.

Substituting the zeros on the right side of (1) by their inclusion disks and using the inclusion property, we obtain the inclusion

$$\zeta_i \in \hat{Z}_i := F_i(\boldsymbol{\zeta}, \boldsymbol{Z}) \tag{2}$$

Under suitable initial conditions (taking into account the size of initial disks and their distribution), the set $\hat{Z}_i$ is a new contracted disk containing the zero ζ_i. In general, we will use the symbol ˆ to denote quantities in the subsequent iteration.

Setting $(Z_1, \ldots, Z_n) =: (Z_1^{(0)}, \ldots, Z_n^{(0)})$, from (2) we can construct the following iterative methods for the simultaneous inclusion of all simple zeros of the polynomial P :

$$\boldsymbol{Z}^{(m+1)} = F_i(\boldsymbol{z}^{(m)}, \boldsymbol{Z}^{(m)}) \quad (m = 0, 1, \ldots). \tag{3}$$

Having in mind (2) and (3), we start from the fixed point relations $(F1)$, $(F2)$ and $(F3)$ and construct the following methods for the simultaneous inclusion of all simple zeros of the polynomial P :

Weierstrass-like method [8], [14], the convergence order 2:

$$\hat{Z}_i = z_i - \frac{P(z_i)}{\prod_{\substack{j=1 \\ j \neq i}}^{n} (z_i - Z_j)} \quad (i \in I_n), \tag{$I1$}$$

Ehrlich-like method [5], the convergence order 3:

$$\hat{Z}_i = z_i - \frac{1}{\dfrac{P'(z_i)}{P(z_i)} - \sum\limits_{\substack{j=1\\j\neq i}}^{n} \dfrac{1}{z_i - Z_j}} \quad (i \in I_n), \tag{I2}$$

Börsch-Supan-like method [7], the convergence order 3:

$$\hat{Z}_i = z_i - \frac{W_i}{1 + \sum\limits_{\substack{j=1\\j\neq i}}^{n} \dfrac{W_j}{Z_i - z_j}} \quad (i \in I_n). \tag{I3}$$

The main advantage of interval methods (3) is inclusion property; namely, in each iteration these interval methods produce the array of disks $Z_1^{(m)}, \ldots, Z_n^{(m)}$ such that $\zeta_i \in Z_i^{(m)},\ m = 0, 1, 2, \ldots$. In this way the automatic control of error is provided.

3. Hybrid Method

The main disadvantage of interval methods is their comparatively great computational amount of work. Following the idea of Caprani and Madsen [3], a few effective methods for the simultaneous inclusion of polynomial zeros were proposed by M. Petković [9]. These methods combine the efficiency of ordinary floating-point iterations with the accuracy control provided by interval arithmetic iterations.

First we list the following iterative methods in ordinary complex arithmetic which directly follow from the fixed point relations $(F1)-(F3)$ by substituting the exact zeros by their "point" approximations, that is, $\zeta_j := z_j\ (j \in I_n)$.

Durand-Kerner method [6], the convergence order 2:

$$\hat{z}_i = z_i - P(z_i) / \prod_{\substack{j=1\\j\neq i}}^{n} (z_i - z_j) \quad (i \in I_n), \tag{C1}$$

Ehrlich-Aberth's method [1], [4], the convergence order 3:

$$\hat{z}_i = z_i - \Big(\frac{P'(z_i)}{P(z_i)} - \sum_{\substack{j=1\\j\neq i}}^{n} \frac{1}{z_i - z_j} \Big)^{-1} \quad (i \in I_n), \tag{C2}$$

Börsch-Supan's method [2], the convergence order 3:

$$\hat{z}_i = z_i - W_i\Big(1 + \sum_{\substack{j=1\\ j\neq i}}^{n} \frac{W_j}{z_i - z_j}\Big)^{-1} \quad (i \in I_n), \tag{C3}$$

It is worth noting that these methods belong to the class of most efficient simultaneous methods for the determination of polynomial zeros.

The following procedure is used for the implementation of combined (hybrid) iterative methods:

1° Find initial disks (or rectangles) $Z_1^{(0)}, \ldots, Z_n^{(0)}$ containing the zeros $\zeta_1, \ldots, \zeta_n$ of a given polynomial;

2° Using a fast convergent iterative method in ordinary complex arithmetic (for examples, some of the listed methods $(C1)$, $(C2)$ or $(C3)$) compute the point approximations $z_i^{(m)}$ to any desired accuracy (after M iterative steps), starting from the centers $z_i^{(0)}$ of the initial disks $Z_i^{(0)}$ $(i = 1, \ldots, n)$;

3° Apply some interval method in circular arithmetic (say, $(I1)$, $(I2)$ or $(I3)$) only once in the final iterative step dealing with the initial disks $Z_1^{(0)}, \ldots, Z_n^{(0)}$ and improved approximations $z_1^{(M)}, \ldots, z_n^{(M)}$. The only purpose of interval iteration is to provide the inclusion of zeros, see [9].

For example let $z_1^{(M)}, \ldots, z_n^{(M)}$ be the array of n point approximations produced by one of the methods $(C1)$, $(C2)$ or $(C3)$. Applying Ehrlich-like interval method $(I2)$ in the final step, we find the improved circular approximations given by

$$Z_i^{(M,1)} = z_i^{(M)} - \cfrac{1}{\cfrac{P'(z_i^{(M)})}{P(z_i^{(M)})} - \displaystyle\sum_{\substack{j=1\\ j\neq i}}^{n} \big(z_i^{(M)} - Z_j^{(0)}\big)^{-1}}$$

for every $i \in I_n$. Let $r^{(0)} = \max\limits_{1\le i\le n} \operatorname{rad} Z_i^{(0)}$, $r^{(M,1)} = \max\limits_{1\le i\le n} \operatorname{rad} Z_i^{(M,1)}$ and let k be the order of convergence of iterative method realized in ordinary complex arithmetic. Then the following estimation is valid:

$$r^{(M,1)} = O\Big(\big(r^{(0)}\big)^{2k^M+1}\Big),$$

assuming that $r^{(0)} < 1$.

4. A Posteriori Error Bound Methods

Computationally verifiable initial conditions that guarantee the convergence of an iterative method for the simultaneous determination of polynomial zeros can be sutably expressed in the form (see, e.g., [10], [11], [13])

$$w^{(0)} \le c_n d^{(0)}, \tag{4}$$

where

$$w^{(m)} = \max_{1\le i\le n} |W(z_i^{(m)})|, \quad d^{(m)} = \min_{\substack{1\le i,j\le n\\ j\ne i}} |z_i^{(m)} - z_j^{(m)}|$$

and $m = 0, 1, 2, \ldots$ is the iteration index. The quantity c_n depends only on the polynomial degree n. When we omit the iteration index, then we write simply w and d.

The following assertion proved in [11] has the main role in our consideration.

Theorem 1. *Let the condition* (4) *with* $c_n < 1/(2n)$ *be valid, then disks* D_i *defined by*

$$D_i = \left\{ z_i; \frac{|W_i|}{1 - nc_n} \right\} = \left\{ z_i; \rho_i \right\} \quad (i \in I_n)$$

are mutually disjoint and each of them contains exactly one zero of P.

Let us assume that the centers z_i of disks D_i are calculated by an iterative method

$$z_i^{(m+1)} = \Phi_i(z^{(m)}) \quad (i \in I_n) \tag{5}$$

that converges under some suitable conditions, then we generate the sequences of disks $D_i^{(m)}$ $(m = 0, 1, \ldots)$ whose radii $\rho_i^{(m)} = |W_i^{(m)}|/(1 - nc_n)$ converge to 0. To provide a high computational efficiency it is necessary to apply only those methods which use quantities already calculated in the previous iterative step, in our case the corrections W_i since the radii ρ_i depend on Weierstrass' corrections W_i. For this reason, we restrict our choice to the class of derivative free methods which deal with Weierstrass' corrections, the so-called W*-class.* Let us note that the methods $(C1)$ and $(C3)$ belong to the W-class and, thus, they can be candidates for the iteration function Φ_i from (5).

Combining the results of Theorem 1 and an iterative simultaneous method of the form (5), we can state the following inclusion method:

A posteriori Error Bound Method: *is defined by the sequences of disks*

$\{D_i^{(m)}\}$ $(i \in I_n)$,

$$\begin{aligned} D_i^{(0)} &= \left\{ z_i^{(0)}; \frac{|W(z_i^{(0)})|}{1-nc_n} \right\}, \\ D_i^{(m)} &= \{z_i^{(m)}; \rho_i^{(m)}\}, \quad (i \in I_n;\ m = 1, 2, \ldots), \qquad (6) \\ z_i^{(m)} &= \Phi_i(z^{(m-1)}) \text{ by (5)}, \quad \rho_i^{(m)} = \frac{|W(z_i^{(m)})|}{1-nc_n}, \end{aligned}$$

assuming that the initial condition (4) (*with* $c_n \le 1/(2n)$) *holds.*

From (6) we observe that $\zeta_i \in D_i^{(m)}$ for each $i \in I_n$ and every $m = 0, 1, 2, \ldots$. The sequences of disks given by (6) can be regarded as a quasi-interval method, which differs structurally from usual interval methods that deal with disks as arguments, see Section 2.

5. Numerical Results

The convergence behavior of the presented self-validated methods was illustrated on a number of algebraic equations. We selected three examples to demonstrate their convergence properties. In our calculation we employed the programming package *Mathematica* 5.2 with multi-precision arithmetic since the tested methods converge very fast producing very small disks.

Example 1. We have applied the interval methods $(I1)$, $(I2)$ and $(I3)$ in circular arithmetic to find inclusion disks of the zeros of the polynomial

$$P(z) = z^9 + 3z^8 - 3z^7 - 9z^6 + 3z^5 + 9z^4 + 99z^3 + 297z^2 - 100z - 300.$$

The exact zeros are -3, ± 1, $\pm 2i$, $\pm 2 \pm i$. We have taken initial disks $\{z_i^{(0)}; r_i^{(0)}\}$ with the radii $r_i^{(0)} = 0.35$.

The largest radii of the resulting inclusion disks are given in Table 1, where $A(-q)$ means $A \times 10^{-q}$. The interval methods $(I2)$ and $(I3)$ are comparable; both converge cubically and give very tight inclusion disks. On the other side, Weierstrass-like interval method $(I1)$ is divergent. Besides, its convergence cost is pretty high so that this interval method is applied very seldom in practice.

Methods	max $r_i^{(1)}$	max $r_i^{(2)}$	max $r_i^{(3)}$
$(I1)$	*diverges*	—	—
$(I2)$	6.20(−2)	5.65(−5)	1.21(−17)
$(I3)$	6.63(−2)	2.69(−5)	3.82(−16)

Table 1 The largest disks of interval iterations

Example 2. For the comparison purpose, the combined methods were applied for the inclusion of zeros of the same polynomial given in Example 1. Ehrlich-Aberth's method ($C2$) was employed to improve the approximations to the zeros taking the centers $z_i^{(0)}$ of inclusion disks $Z_i^{(0)}$ from Example 1 as starting approximations. After two iterations we have obtained the approximations with the maximal error $\max_{1\le i\le 9} |z_i^{(2)} - \zeta_i| = 7.36\times 10^{-8}$.

In the final step we have applied only one interval iteration of the inclusion methods ($I1$), ($I2$) and ($I3$) taking the improved approximations $z_i^{(2)}$ and the initial disks $Z_i^{(0)} = \{z_i^{(0)}; 0.35\}$. The radii of the resulting inclusion disks are given in Table 2.

i	$(C2)-(I1)$	$(C2)-(I2)$	$(C2)-(I3)$
1	0.015	2.01(−15)	1.35(−15)
2	1.10(−3)	4.44(−15)	1.88(−15)
3	1.59(−3)	1.39(−17)	9.44(−17)
4	5.94(−2)	3.09(−15)	1.97(−15)
5	7.07(−3)	4.71(−17)	2.89(−16)
6	1.88(−4)	5.41(−19)	1.58(−17)
7	1.79(−3)	5.22(−17)	1.41(−16)
8	3.51(−4)	1.29(−15)	5.86(−16)
9	3.70(−4)	8.17(−19)	1.96(−17)

Table 2 The radii of disks produced by combined methods

Comparing the size of disks given in Table 2 (the second and the third column) and the size of disks obtained by the corresponding interval methods (Table 1), we conclude they there are comparable. However, the combined methods are realized by two point iterations and one interval iteration, while interval methods require three iterations in circular interval arithmetic. This fact obviously points to the greater computational efficiency of the combined methods in relation to the interval methods. We note that Weierstrass-like interval method ($I1$) gives again poor results.

Example 3. We considered the polynomial

$$\begin{aligned} P(z) &= z^{12} - (2+5i)z^{11} - (1-10i)z^{10} + (12-25i)z^9 \\ &\quad -30z^8 - z^4 + (2+5i)z^3 + (1-10i)z^2 - (12-25i)z + 30. \end{aligned}$$

Starting from the sufficiently close initial approximations $z_1^{(0)},\dots,z_{12}^{(0)}$ which give $\max \rho_i^{(0)} = 0.182$, we applied a posteriori error bound method (6) and obtained the inclusion disks $D_i^{(m)} = \{z_i^{(m)}; \rho_i^{(m)}\}$ ($i\in I_{12}$). The approximations $z_i^{(m)}$ $(m \geq 1)$ were calculated by the iterative formulas $(C1)$ and $(C3)$. The largest radii of the disks are presented in Table 3.

Methods	max $\rho_i^{(1)}$	max $\rho_i^{(2)}$	max $\rho_i^{(3)}$
$(C1)-(6)$	5.20(−2)	3.28(−3)	5.70(−6)
$(C3)-(6)$	8.54(−3)	1.14(−7)	2.68(−23)

Table 3 The largest radii of disks obtained by a posteriori error bound methods

A posteriori error bound methods are comparable or even better than interval methods and hybrid methods, but their computational cost is smallest so that they are the most efficient among the considered methods.

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