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Higher-order iterative methods for approximating zeros of analytic functions

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Abstract

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Iterative methods with extremely rapid convergence in floating-point arithmetic and circular arithmetic for simultaneously approximating simple zeros of analytic functions (inside a simple smooth closed contour in the complex plane) are presented. The R-order of convergence of the basic total-step and single-step methods, as well as their improvements which use Newton's and Halley's corrections, is given. Some hybrid algorithms that combine the efficiency of ordinary floating-point iterative methods with the accuracy control provided by interval arithmetic are also considered.

Keywords: Iterative methods, zeros of analytic functions, inclusion methods, convergence order.

1. Introduction

In the recent paper [8] a class of iterative methods of a high order of convergence for the simultaneous determination of simple zeros of analytic functions was constructed. These methods are based on the logarithmic derivative of a considered analytic function and they can be regarded as a generalization of the algorithms presented in [9] for polynomials. In the present paper we establish a new class of iterative methods for approximating zeros of analytic functions with improved order of convergence.

Let $z \mapsto \Phi(z)$ be an analytic function inside and on the simple smooth closed contour Γ without zeros on Γ and with a known number n of simple zeros inside Γ. Then Φ will be of the form

$$\Phi(z) = X(z) \prod_{j=1}^{n} (z - \zeta_j), \tag{1}$$

inside Γ, where ζ_j are the zeros of Φ and X is an analytic function, but without zeros inside Γ (see [18]). The number of zeros n of Φ inside Γ is determined from the argument principle [7]

$$n=\frac{1}{2\pi \mathrm{i}}\int_{\Gamma}\frac{\Phi'(w)}{\Phi(w)}\,\mathrm{d}w. \tag{2}$$

Following [18] the analytic function X can be written as

$$X(z)=\exp(Y(z)), \tag{3}$$

inside Γ, where Y is also an analytic function inside Γ given by

$$Y(z)=\frac{1}{2\pi \mathrm{i}}\int_{\Gamma}\frac{\log\left[(w-c)^{-n}\Phi(w)\right]}{w-z}\,\mathrm{d}w \tag{4}$$

(see [3]). In (4) c is an arbitrary point inside Γ such that $\Phi(c)\neq 0$.

Using the logarithmic derivative of Φ from (1) it follows that

$$\frac{\Phi'(z)}{\Phi(z)}=Y'(z)+\sum_{j=1}^{n}(z-\zeta_j)^{-1},\quad z\neq\zeta_j,$$

wherefrom

$$\zeta_i=z-\left[\frac{\Phi'(z)}{\Phi(z)}-Y'(z)-\sum_{\substack{j=1\\ j\neq i}}^{n}(z-\zeta_j)^{-1}\right]^{-1},\quad i=1,\dots,n. \tag{5}$$

Starting from the fixed-point relation (5) in [8] a class of methods for simultaneously improving the zeros $\zeta_1,\dots,\zeta_n$ of Φ was developed. For example, if $z_1,\dots,z_n$ are approximations to the zeros $\zeta_1,\dots,\zeta_n$, then the formula

$$\hat{z}_i=z_i-\left[\frac{\Phi'(z_i)}{\Phi(z_i)}-Y'(z_i)-\sum_{\substack{j=1\\ j\neq i}}^{n}(z_i-\zeta_j)^{-1}\right]^{-1},\quad i=1,\dots,n, \tag{6}$$

(obtained from (5)), where $\hat{z}_i$ is the new approximation to ζ_i, defines the iterative method with cubic convergence.

Remark 1. The fixed-point relation of the form (5) for entire functions with infinitely many zeros and exponent of convergence <1 was previously derived in [5] and applied for the inclusion of zeros by circular complex regions.

2. The fixed-point relations

Applying a procedure presented in [11] we now derive a fixed-point relation similar to (5). Let us define

$$f_k(z)=\frac{\Phi^{(k)}(z)}{\Phi(z)},\quad k=1,2.$$

Using the logarithmic derivative, from (1) we find

$$f_1(z)=\frac{\Phi'(z)}{\Phi(z)}=Y'(z)+\sum_{j=1}^{n}(z-\zeta)^{-1} \tag{7}$$

and

$$f_1'(z)=\frac{\Phi''(z)\Phi(z)-\Phi'(z)^2}{\Phi(z)^2}=Y''(z)-\sum_{j=1}^{n}(z-\zeta_j)^{-2}. \tag{8}$$

It is evident that

$$f_2(z)=\frac{\Phi''(z)}{\Phi(z)}=f_1(z)^2+f_1'(z). \tag{9}$$

From (7)–(9) we obtain for $z\neq\zeta_j$,

$$\begin{aligned}\left[\sum_{\substack{j=1\\ j\neq i}}^{n}(z-\zeta_j)^{-1}\right]^2+\sum_{\substack{j=1\\ j\neq i}}^{n}(z-\zeta_j)^{-2}&=\left[f_1(z)-Y'(z)-(z-\zeta_i)^{-1}\right]^2\\ &\quad-\left[f_1'(z)+(z-\zeta_i)^{-2}-Y''(z)\right]\\ &=\left[f_1(z)-Y'(z)\right]^2-2\left[f_1(z)-Y'(z)\right](z-\zeta_i)^{-1}\\ &\quad+f_1(z)^2-f_2(z)+Y''(z).\end{aligned}$$

Hence

$$\zeta_i=z-\frac{2\left[f_1(z)-Y'(z)\right]}{f_1(z)^2-f_2(z)+\left[f_1(z)-Y'(z)\right]^2+Y''(z)-s_{1,i}^2-s_{2,i}},\quad i=1,\ldots,n, \tag{10}$$

where

$$s_{k,i}=\sum_{\substack{j=1\\ j\neq i}}^{n}(z-\zeta_j)^{-k},\quad k=1,2. \tag{11}$$

The fixed-point relation (10) is the basis for constructing a class of algorithms for finding zeros of analytic functions in (ordinary) complex arithmetic as well as in circular arithmetic. According to (4) the derivatives $Y'(z)$ and $Y''(z)$ are given by

$$Y'(z)=\frac{1}{2\pi\mathrm{i}}\int_\Gamma\frac{\log\left[(w-c)^{-n}\Phi(w)\right]}{(w-z)^2}\mathrm{d}w \tag{12}$$

and

$$Y''(z)=\frac{1}{\pi\mathrm{i}}\int_\Gamma\frac{\log\left[(w-c)^{-n}\Phi(w)\right]}{(w-z)^3}\mathrm{d}w. \tag{13}$$

Remark 2. If $\Phi(z)$ is a monic polynomial with simple zeros $\zeta_1, \ldots, \zeta_n$, that is,

$$X(z)=1, \qquad Y(z)=0, \qquad \Phi(z)=P_n(z)=\prod_{j=1}^{n}(z-\zeta_j),$$

then (10) reduces to the fixed-point relation derived in [19] (see also [11]).

3. Algorithms in complex arithmetic

Starting from the fixed-point relation (10), in a similar manner as for the class of iterative methods of Halley's type [11], we can construct total-step and single-step methods of higher order of convergence. For $z \in \mathbb{C}$ let us define

$$v(z)=f_1(z)-Y'(z), \qquad h(z)=f_1(z)^2-f_2(z)+Y''(z),$$

$$\Sigma_i(a, b)=\left[\sum_{j=1}^{i-1}(z_i-a_j)^{-1}+\sum_{j=i+1}^{n}(z_i-b_j)^{-1}\right]^2 + \sum_{j=1}^{i-1}(z_i-a_j)^{-2}+\sum_{j=i+1}^{n}(z_i-b_j)^{-2},$$

where $a=(a_1,\ldots, a_n)^{\mathrm{T}}$ and $b=(b_1,\ldots, b_n)^{\mathrm{T}}$ are some vectors. Further, we denote

$$N(z)=\frac{\Phi(z)}{\Phi'(z)} \qquad \text{(Newton's correction)},$$

$$H(z)=\left[\frac{\Phi'(z)}{\Phi(z)}-\frac{\Phi''(z)}{2\Phi'(z)}\right]^{-1} \qquad \text{(Halley's correction)},$$

and introduce the vectors

$$z=(z_1,\ldots, z_n)^{\mathrm{T}} \qquad \text{(the former approximations)},$$

$$\hat{z}=(\hat{z}_1,\ldots, \hat{z}_n)^{\mathrm{T}} \qquad \text{(the new approximations)},$$

$$z_N=(z_{N,1},\ldots, z_{N,n})^{\mathrm{T}}, \quad z_{N,i}=z_i-N(z_i) \qquad \text{(Newton's approximations)},$$

$$z_H=(z_{H,1},\ldots, z_{H,n})^{\mathrm{T}}, \quad z_{H,i}=z_i-H(z_i) \qquad \text{(Halley's approximations)}.$$

Assume that reasonably good approximations $z_1,\ldots, z_n$ to the zeros $\zeta_1,\ldots, \zeta_n$ were found. Letting $z=z_i$ and $\zeta_i:=\hat{z}_i$ in (10), and taking certain approximations of ζ_j in the sum Σ_i on the right-hand side of (10), we obtain the whole set of iterative methods for the simultaneous determination of the zeros $\zeta_1,\ldots, \zeta_n$ of an analytic function Φ.

(TS) For $\zeta_j:=z_j$, $j \neq i$, we obtain the Total-Step method (TS):

$$\hat{z}_i=z_i-\frac{2v(z_i)}{h(z_i)+v(z_i)^2-\Sigma_i(z, z)}, \quad i=1,\ldots, n. \tag{14}$$

(SS) Let $\zeta_j := \hat{z}_j$, $j < i$, and $\zeta_j := z_j$, $j > i$ (the Gauss—Seidel approach); then we get from (10) the Single-Step method (SS):

$$\hat{z}_i = z_i - \frac{2v(z_i)}{h(z_i) + v(z_i)^2 - \Sigma_i(\hat{z}, z)}, \quad i = 1, \ldots, n. \tag{15}$$

(TSN) Substituting $\zeta_j := z_{N,j} = z_j - N(z_j)$, $j \neq i$, in (10) one obtains the Total-Step method with Newton's correction (TSN):

$$\hat{z}_i = z_i - \frac{2v(z_i)}{h(z_i) + v(z_i)^2 - \Sigma_i(z_N, z_N)}, \quad i = 1, \ldots, n. \tag{16}$$

(SSN) The TSN method can be accelerated by applying the Gauss–Seidel approach: setting $\zeta_j := \hat{z}_j$, $j < i$, and $\zeta_j := z_{N,j} = z_j - N(z_j)$, $j > i$, in (10) we get the Single-Step method with Newton's correction (SSN):

$$\hat{z}_i = z_i - \frac{2v(z_i)}{h(z_i) + v(z_i)^2 - \Sigma_i(\hat{z}, z_N)}, \quad i = 1, \ldots, n. \tag{17}$$

(TSH) Taking $\zeta_j := z_{H,j} = z_j - H(z_j)$, $j \neq i$, in (10), similarly as for the TSN method we construct the Total-Step method with Halley's correction (TSH):

$$\hat{z}_i = z_i - \frac{2v(z_i)}{h(z_i) + v(z_i)^2 - \Sigma_i(z_H, z_H)}, \quad i = 1, \ldots, n. \tag{18}$$

(SSH) The Single-Step method with Halley's correction (SSH) is obtained by substituting $\zeta_j := \hat{z}_j$, $j < i$, and $\zeta_j := z_{H,j} = z_j - H(z_j)$, $j > i$, in (10):

$$\hat{z}_i = z_i - \frac{2v(z_i)}{h(z_i) + v(z_i)^2 - \Sigma_i(\hat{z}, z_H)}, \quad i = 1, \ldots, n. \tag{19}$$

We will now consider the convergence speed of the iterative methods (14)–(19). First, for the derived Total-Step methods we have the following assertions.

Theorem 3. *The order of convergence of the total-step methods TS* (14), *TSN* (16) *and TSH* (18) *is four, five and six, respectively.*

Proof. Let $z^{(\lambda)} = (z_1^{(\lambda)}, \ldots, z_n^{(\lambda)})^{\mathrm{T}}$, $\lambda \in \{1, 2, 3\}$, be the vector of approximations given by

$$\begin{aligned} z_i^{(1)} &= z_i && \text{(the current approximations)},\\ z_i^{(2)} &= z_i - N(z_i) && \text{(the Newton approximations)},\\ z_i^{(3)} &= z_i - H(z_i) && \text{(the Halley approximations)}. \end{aligned}$$

In the proof of this theorem the upper index indicates the type of approximation and it should be strongly distinguished from the iteration index. Using this notation the total-step methods (14), (16) and (18) can be represented by the unique formula as

$$\hat{z}_i = z_i - \frac{2v(z_i)}{h(z_i) + v(z_i)^2 - \Sigma_i(z^{(\lambda)}, z^{(\lambda)})}, \quad i = 1, \ldots, n, \ \lambda = 1, 2, 3. \tag{20}$$

Let us introduce the abbreviations

$$s_{k,i}^{(\lambda)}=\sum_{\substack{j=1\\ j\neq i}}^{n}\left(z_i-z_j^{(\lambda)}\right)^{-k},\quad k=1,2,\ \lambda=1,2,3,$$

$$q_{k,i}=\sum_{j=1}^{n}\left(z_i-\zeta_j\right)^{-k},\quad k=1,2,\qquad a_i=\sum_{\substack{j=1\\ j\neq i}}^{n}\left(z_i-\zeta_j\right)^{-1},$$

$$d_i^{(\lambda)}=\left(\sum_{\substack{j=1\\ j\neq i}}^{n}\frac{z_j^{(\lambda)}-\zeta_j}{(z_i-\zeta_j)\left(z_i-z_j^{(\lambda)}\right)}\right)\left(\sum_{\substack{j=1\\ j\neq i}}^{n}\frac{2z_i-z_j^{(\lambda)}-\zeta_j}{(z_i-\zeta_j)\left(z_i-z_j^{(\lambda)}\right)}\right)$$
$$+\sum_{\substack{j=1\\ j\neq i}}^{n}\frac{\left(z_j^{(\lambda)}-\zeta_j\right)\left(2z_i-z_j^{(\lambda)}-\zeta_j\right)}{(z_i-\zeta_j)^2\left(z_i-z_j^{(\lambda)}\right)^2}.$$

Let $\epsilon_i=z_i-\zeta_i$ and $\hat{\epsilon}_i=\hat{z}_i-\zeta_i$, and let $|\epsilon|=\max_i|\epsilon_i|$, $|\hat{\epsilon}|=\max_i|\hat{\epsilon}_i|$. Assuming that all approximations $z_1^{(\lambda)},\ldots,z_n^{(\lambda)}$ are sufficiently close to the zeros $\zeta_1,\ldots,\zeta_n$ and taking into account the quadratic convergence of Newton's method and the cubic convergence of Halley's method, we can write

$$\left|z_j^{(\lambda)}-\zeta_j\right|\leqslant\alpha_j^{(\lambda)}|\epsilon|^{\lambda},\quad j=1,\ldots,n,\ \lambda=1,2,3,$$

where $\alpha_j^{(\lambda)}$ are some positive numbers. According to (7)–(9) we obtain

$$2v(z_i)=2q_{1,i}=\frac{2}{\epsilon_i}(1+a_i\epsilon_i) \tag{21'}$$

and

$$h(z_i)+v(z_i)^2-\Sigma_i(z^{(\lambda)},z^{(\lambda)})$$
$$=h(z_i)+v(z_i)^2-\left[s_{1,i}^{(\lambda)}\right]^2-s_{2,i}^{(\lambda)}=q_{1,i}^2+q_{2,i}-\left[s_{1,i}^{(\lambda)}\right]^2-s_{2,i}^{(\lambda)}$$
$$=\left[(z_i-\zeta_i)^{-1}+\sum_{j\neq i}(z_i-\zeta_j)^{-1}\right]^2+(z_i-\zeta_i)^{-2}+\sum_{j\neq i}(z_i-\zeta_j)^{-2}$$
$$-\left[\sum_{j\neq i}\left(z_i-z_j^{(\lambda)}\right)^{-1}\right]^2-\sum_{j\neq i}\left(z_i-z_j^{(\lambda)}\right)^{-2}$$
$$=2(z_i-\zeta_i)^{-2}+2(z_i-\zeta_i)^{-1}\sum_{j\neq i}(z_i-\zeta_j)^{-1}+\left[\sum_{j\neq i}(z_i-\zeta_j)^{-1}\right]^2$$
$$-\left[\sum_{j\neq i}\left(z_i-z_j^{(\lambda)}\right)^{-1}\right]^2+\sum_{j\neq i}\left[\frac{1}{(z_i-\zeta_j)^2}-\frac{1}{\left(z_i-z_j^{(\lambda)}\right)^2}\right]$$
$$=2(z_i-\zeta_i)^{-2}+2(z_i-\zeta_i)^{-1}\sum_{j\neq i}(z_i-\zeta_j)^{-1}-\left(\sum_{j\neq i}\frac{z_j^{(\lambda)}-\zeta_j}{(z_i-\zeta_j)\left(z_i-z_j^{(\lambda)}\right)}\right)$$
$$\times\left(\sum_{j\neq i}\frac{2z_i-z_j^{(\lambda)}-\zeta_j}{(z_i-\zeta_j)\left(z_i-z_j^{(\lambda)}\right)}\right)-\sum_{j\neq i}\frac{\left(z_j^{(\lambda)}-\zeta_j\right)\left(2z_i-z_j^{(\lambda)}-\zeta_j\right)}{(z_i-\zeta_j)^2\left(z_i-z_j^{(\lambda)}\right)^2},$$

that is,

$$h(z_i)+v(z_i)^2-\Sigma_i(z^{(\lambda)},\, z^{(\lambda)})=\frac{2}{\epsilon_i^2}+\frac{2a_i}{\epsilon_i}-d_i^{(\lambda)}. \tag{21''}$$

Let us define

$$\beta_1=\min_{i,j}|z_i-\zeta_j|,\quad \beta_2^{(\lambda)}=\min_{i,j}\left|z_i-z_j^{(\lambda)}\right|,\quad \rho_1=\max_{i,j}|z_i-\zeta_j|,\quad \rho_2^{(\lambda)}=\max_{i,j}\left|z_i-z_j^{(\lambda)}\right|.$$

Then we have

$$\begin{aligned}\left|d_i^{(\lambda)}\right| &\leqslant \left(\sum_{j\neq i}\frac{\left|z_j^{(\lambda)}-\zeta_j\right|}{|z_i-\zeta_j|\left|z_i-z_j^{(\lambda)}\right|}\right)\left(\sum_{j\neq i}\frac{\left|2z_i-z_j^{(\lambda)}-\zeta_j\right|}{|z_i-\zeta_j|\left|z_i-z_j^{(\lambda)}\right|}\right)\\ &\quad+\sum_{j\neq i}\frac{\left|z_j^{(\lambda)}-\zeta_j\right|\left|2z_i-z_j^{(\lambda)}-\zeta_j\right|}{\left|z_i-\zeta_j\right|^2\left|z_i-z_j^{(\lambda)}\right|^2}\\ &<\frac{n\left(\rho_1+\rho_2^{(\lambda)}\right)}{\left(\beta_1\beta_2^{(\lambda)}\right)^2}\sum_{j\neq i}\alpha_j^{(\lambda)}|\epsilon|^\lambda=\gamma_i^{(\lambda)}|\epsilon|^\lambda\leqslant\gamma^{(\lambda)}|\epsilon|^\lambda,\end{aligned}$$

where

$$\gamma_i^{(\lambda)}=\frac{n\left(\rho_1+\rho_2^{(\lambda)}\right)}{\left(\beta_1\beta_2^{(\lambda)}\right)^2}\sum_{j\neq i}\alpha_j^{(\lambda)}\quad\text{and}\quad\gamma^{(\lambda)}=\max_i\gamma_i^{(\lambda)}.$$

Besides, for sufficiently small $|\epsilon_i|$, $i=1,\dots,n$, there exist positive constants $\tau_i^{(\lambda)}$ so that

$$\left|2+2a_i\epsilon_i-\epsilon_i^2d_i^{(\lambda)}\right|\geqslant\tau_i^{(\lambda)}\geqslant\tau^{(\tau)},\quad \tau^{(\lambda)}=\min_i\tau_i^{(\lambda)}.$$

Using (21′) and (21″) we get from (20)

$$\hat{\epsilon}_i=\epsilon_i-\frac{\dfrac{2}{\epsilon_i}(1+a_i\epsilon_i)}{\dfrac{2}{\epsilon_i^2}+\dfrac{2a_i}{\epsilon_i}-d_i^{(\lambda)}}=\frac{-\epsilon_i^3d_i^{(\lambda)}}{2+2a_i\epsilon_i-\epsilon_i^2d_i^{(\lambda)}}.$$

By the previous estimations we find

$$|\hat{\epsilon}_i|=\frac{\left|\epsilon_i^3d_i^{(\lambda)}\right|}{\left|2+2a_i\epsilon_i-\epsilon_i^2d_i^{(\lambda)}\right|}<\frac{\gamma^{(\lambda)}|\epsilon_i|^3|\epsilon|^\lambda}{\tau^{(\lambda)}},$$

wherefrom

$$|\hat{\epsilon}_i|\leqslant|\hat{\epsilon}|<\frac{\gamma^{(\lambda)}|\epsilon|^{\lambda+3}}{\tau^{(\lambda)}}.$$

Taking $\lambda=1$, 2 and 3, we prove that the order of convergence of the total-step methods (14), (16) and (18) is four, five and six, respectively. □

For the single-step methods we will use the notion of the R-order of convergence, introduced in [10]. The R-order of convergence of the iterative process $\mathbb{P}$ with the limit point $\zeta=(\zeta_1,\dots,\zeta_n)^{\mathrm{T}}$ (the vector of exact zeros) will be denoted by $O_{\mathrm{R}}(\mathbb{P},\zeta)$.

Theorem 4. *The R-order of convergence of the single-step methods SS* (15), *SSN* (17) *and SSH* (19) *is bounded below by*

$$O_{\mathrm{R}}(\mathrm{SS},\zeta)\geqslant 3+t_n,\qquad O_{\mathrm{R}}(\mathrm{SSN},\zeta)\geqslant 3+x_n,\qquad O_{\mathrm{R}}(\mathrm{SSH},\zeta)\geqslant 3+y_n,$$

where t_n, x_n and y_n are the unique positive roots of the equations

$$t^n-t-3=0,\qquad x^n-x\cdot 2^{n-1}-3\cdot 2^{n-1}=0,\qquad y^n-y\cdot 3^{n-1}-3^n=0,$$

respectively.

Proof. The convergence analysis of the single-step methods (15), (17) and (19) is performed by the same procedure which has already been applied in the papers [1,11,14–16]. For this reason we will only sketch the proof of Theorem 4.

Let $u_i^{(m)}$ be a multiple of $|z_i^{(m)}-\zeta_i|$, $i=1,\dots,n$, where $m=0,1,\dots$ is the iteration index. As in the mentioned papers, it can be shown that the single-step methods (15), (17) and (19) belong to a class of iterative simultaneous methods for which the following relation can be derived:

$$u_i^{(m+1)}\leqslant\frac{1}{n-1}\left(u_i^{(m)}\right)^p\left(\sum_{j<i}u_j^{(m+1)}+\sum_{j>i}\left(u_j^{(m)}\right)^q\right),$$
$$i=1,\dots,n,\quad m=0,1,\dots,\quad p,q\in\mathbb{N}. \tag{22}$$

We introduce the ordered pair $U(\mathbb{P})=(p,q)$ as an *exponent characteristic* of the relation (22) for the iterative process $\mathbb{P}$, where p and q are the corresponding exponents in (22). An extensive but elementary analysis (similar to that presented in [1,11,14] etc.) shows that the considered iterative methods SS (15), SSN (17) and SSH (19) have the following exponent characteristics:

$$U(\mathrm{SS})=(3,1),\qquad U(\mathrm{SSN})=(3,2),\qquad U(\mathrm{SSH})=(3,3).$$

For the single-step iterative process $\mathbb{P}$ with $U(\mathbb{P})=(p,q)$ it was proved in [16] that

$$O_{\mathrm{R}}(\mathbb{P},\zeta)\geqslant 3+\tau_n,$$

where τ_n is the unique positive root of the equation

$$\tau^n-\tau q^{n-1}-pq^{n-1}=0.$$

Taking into account this result with specific values for p and q, we immediately obtain the assertions of Theorem 4. □

The values of the lower bounds of the R-order of convergence for the considered single-step methods, in dependence of the number of zeros n, are displayed in Table 1.

Table 1

Method	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$	$n=8$	$n=9$	$n=10$
SS (15)	5.303	4.672	4.453	4.341	4.274	4.229	4.196	4.172	4.153
SSN (17)	6.646	5.862	5.585	5.443	5.357	5.299	5.257	5.225	5.200
SSH (19)	7.854	6.974	6.662	6.502	6.404	6.338	6.291	6.255	6.227

4. Algorithms in circular arithmetic

In this section we present some algorithms for the inclusion of zeros of an analytic function. For the construction of these algorithms the complex interval arithmetic will be used. More about inclusion methods can be found in [12] and the references cited therein. We only emphasize the main advantage of inclusion methods which consists of the determination of resulting disks or rectangles containing the sought zeros. In this manner the automatic determination of the upper error bounds, given by radii or semidiagonals of inclusion complex intervals, is provided.

Algorithms presented in this section are realized in circular interval arithmetic. In what follows a circular closed region (disk) $Z=\{z: |z-c| \leqslant r\}$ with center $c = \operatorname{mid} Z$ and radius $r = \operatorname{rad} Z$ will be denoted by the parametric notation $Z=\{c; r\}$. For the reader's convenience we briefly review some properties of circular arithmetic (see, e.g., [2,4]):

$$\{c_1; r_1\} \pm \{c_2; r_2\} = \{c_1 \pm c_2; r_1 + r_2\},$$

$$\{c_1; r_1\} \cdot \{c_2; r_2\} = \{c_1 c_2; |c_1| r_2 + |c_2| r_1 + r_1 r_2\},$$

$$Z^{-1} = \{c; r\}^{-1} = \frac{\{\bar{c}; r\}}{|c|^2 - r^2}, \quad |c| > r, \text{ i.e., } 0 \notin Z,$$

$$Z_1 : Z_2 = Z_1 \cdot Z_2^{-1}, \quad 0 \notin Z_2,$$

$$W^{-1} = \{z: |z-c| \geqslant r\}^{-1} = \frac{\{-\bar{c}; r\}}{r^2 - |c|^2}, \quad |c| < r, \text{ i.e., } 0 \notin W,$$

(the inverse of a closed exterior of a circle which does not contain the origin).

Assume that we found n disjoint disks $Z_i^{(0)} = \{z_i^{(0)}; r_i^{(0)}\}$ containing the simple zeros $\zeta_1, \ldots, \zeta_n$ of an analytic function Φ, $\zeta_i \in Z_i^{(0)}$, $i = 1, \ldots, n$. Let z be an arbitrary complex number such that $z \notin Z_i^{(0)}$, $i = 1, \ldots, n$, and let

$$S_{k,i}^{(m)} = \sum_{\substack{j=1 \\ j \neq i}}^{n} \left(\frac{1}{z - Z_j^{(m)}} \right)^k, \quad k = 1, 2.$$

Then obviously

$$s_{k,i} \in S_{k,i}^{(0)},$$

where $s_{k,i}$ is given by (11). By this fact from the fixed-point relation (10) it follows that

$$\zeta_i \in z - \frac{2v(z)}{h(z) + v(z)^2 - \left[S_{1,i}^{(0)}\right]^2 - S_{2,i}^{(0)}}, \quad i = 1, \ldots, n, \tag{23}$$

where v and h are the functions introduced in Section 3.

If the denominator of (23) does not contain the number 0, then the inverse in (23) is defined and the set on the right-hand side of (23) is also a disk. Evidently the relation (23) suggests the construction of an iterative interval method for the inclusion of the zeros $\zeta_1, \ldots, \zeta_n$.

Let $Z_i^{(m)} = \{z_i^{(m)}; r_i^{(m)}\}$, $m = 0, 1, \ldots$, and let Σ_i be the sum defined in Section 3 with $z = z_i^{(m)}$. Besides, let $r^{(m)} = \max_i r_i^{(m)}$. The successive inclusion approximations to ζ_i are given by

$$Z_i^{(m+1)} = z_i^{(m)} - \frac{2v\left(z_i^{(m)}\right)}{h\left(z_i^{(m)}\right) + v\left(z_i^{(m)}\right)^2 - \Sigma_i\left(\mathbf{Z}^{(m)}, \mathbf{Z}^{(m)}\right)}, \quad i = 1, \ldots, n, \ m = 0, 1, \ldots, \tag{24}$$

where $\mathbf{Z}^{(m)} = (Z_1^{(m)}, \ldots, Z_n^{(m)})^{\mathrm{T}}$.

The properties of the interval method (24) are given in the next theorem.

Theorem 5. *For the sequences* $\{Z_i^{(m)}\}$, $i = 1, \ldots, n$, *of disks, produced by the total-step iterative method* (24) *we have for each* $i = 1, \ldots, n$ *and* $m = 0, 1, \ldots,$

(i) $\zeta_i \in Z_i^{(m)}$;

(ii) $r^{(m+1)} = O((r^{(m)})^4)$.

Proof. Since the convergence analysis of the interval method (24) is essentially the same as the one presented in [4,11], we briefly outline the proof of Theorem 5.

First we prove (i). Assuming that $\zeta_i \in Z^{(m)}$, $i = 1, \ldots, n$, $m \geqslant 0$, and using the relation

$$s_{1,i}^2 + s_{2,i} \in \Sigma_i(\mathbf{Z}^{(m)}, \mathbf{Z}^{(m)}),$$

from (24) and (10) we obtain that $\zeta_i \in Z_i^{(m+1)}$. Since $\zeta_i \in Z_i^{(0)}$, assertion (i) follows according to mathematical induction.

For simplicity, in proving (ii) we will omit the iteration index and write $\hat{Z}_i$, $\hat{r}_i$, Z_i, r_i, $\hat{r}$, r instead of $Z_i^{(m+1)}$, $r_i^{(m+1)}$, $Z_i^{(m)}$, $r_i^{(m)}$, $r^{(m+1)}$, $r^{(m)}$. Besides, let us introduce

$$\Sigma_i(\mathbf{Z}, \mathbf{Z}) = \{w_i; \eta_i\}, \quad \mathbf{Z} = (Z_1, \ldots, Z_n)^{\mathrm{T}}.$$

Interval formula (24) now becomes

$$\hat{Z}_i = z_i - \frac{2v(z_i)}{h(z_i) + v(z_i)^2 - \{w_i; \eta_i\}} = z_i - \frac{2v(z_i)}{\left\{h(z_i) + v(z_i)^2 - w_i; \eta_i\right\}}.$$

Using the properties of circular arithmetic, from the last formula we find

$$\hat{r}_i = \operatorname{rad}\left(\hat{Z}_i\right) = \frac{2\,|v_i(z_i)|\,\eta_i}{\left|h(z_i) + v(z_i)^2 - w_i\right|^2 - \eta_i^2}. \tag{25}$$

By circular arithmetic it is easy to show that

$$\eta_i = \operatorname{rad}(\Sigma_i(\mathbf{Z}, \mathbf{Z})) = O(r).$$

Furthermore, starting from the factorization (1) we obtain

$$\frac{1}{|\Phi(z_i)|} = O\left(\frac{1}{|z_i - \zeta_i|}\right) = O\left(\frac{1}{r_i}\right),$$

so that

$$|h(z_i)+v(z_i)^2-w_i| = \frac{1}{|\Phi(z_i)|^2}\big|\Phi'(z_i)^2-\Phi''(z_i)\Phi(z_i)+[\Phi'(z_i)-Y'(z_i)\Phi(z_i)]^2 + [Y''(z_i)-w_i]\Phi(z_i)^2\big| = \mathrm{O}\left(\frac{1}{r_i^2}\right).$$

According to the previous estimations, we can write

$$\eta_i=\alpha_i r,\qquad |v(z_i)|=\frac{\beta_i}{r_i},\qquad |h(z_i)+v(z_i)^2-w_i|=\frac{\gamma_i}{r_i^2},$$

where α_i, β_i, $\gamma_i \in \mathbb{R}^+$ are some positive numbers. From (25) we get

$$\hat{r}_i=\frac{2\dfrac{\beta_i}{r_i}\cdot\alpha_i r}{\dfrac{\gamma_i^2}{r_i^4}-\alpha_i^2 r^2}=\frac{2\alpha_i\beta_i r_i^3 r}{\gamma_i^2-\alpha_i^2 r_i^4 r^2}\leqslant\frac{2\alpha_i\beta_i r^4}{\gamma_i^2-\alpha_i^2 r_i^4 r^2}.$$

Assuming that all r_i are small enough, the denominator can be bounded by some positive constant, that is,

$$\gamma_i^2-\alpha_i^2 r_i^4 r^2>\tau>0,\quad \text{for every } i=1,\ldots,n.$$

Taking $\rho=\max_i(\alpha_i\beta_i)$ we find

$$\hat{r}_i\leqslant\hat{r}<\frac{2\rho}{\tau}r^4,$$

which means that the order of convergence of the interval method (24) is four. □

The convergence of the iterative method can be accelerated by computing the new approximation $Z_i^{(m+1)}$ serially, using the already calculated approximations $Z_1^{(m+1)},\ldots,\ Z_{i-1}^{(m+1)}$ as soon as they are available. In this way we establish the single-step interval method

$$Z_i^{(m+1)}=z_i^{(m)}-\frac{2v(z_i^{(m)})}{h(z_i^{(m)})+v(z_i^{(m)})^2-\Sigma_i(Z^{(m+1)},\ Z^{(m)})},$$

$$i=1,\ldots,n,\ m=0,1,\ldots\ . \tag{26}$$

The R-order of convergence of this method is the same as for the single-step method SS (15).

Remark 6. Since $\mathrm{rad}((1/Z)^2)<\mathrm{rad}(1/Z^2)$, in order to obtain small disks in calculating the sum Σ_i, it is better to sum the squares of inverse disks rather than the inversion of disks' squares.

Sometimes, it is of interest to find only k $(<n)$ including approximations, for example when the improvement of only a certain group of zeros, clustered around a center c, is of importance. Assume that we found k disjoint disks $Z_i^{(0)}=\{z_i^{(0)},\ r_i^{(0)}\}$ $i=1,\ldots,\ k$, containing the zeros

$\zeta_1, \ldots, \zeta_k$ and that these disks were included inside the disk $\{c; R\}$. All remaining zeros $\zeta_{k+1}, \ldots, \zeta_n$ are supposed to lie in the region $W = \{z; |z - c| > R\}$ (the exterior of the disk $\{c; R\}$). Starting from (10) and using the inclusion isotonicity property we construct the following iterative method for simultaneous improving of k inclusion disks:

$$Z_i^{(m+1)} = z_i^{(m)} - \frac{2v(z_i^{(m)})}{h(z_i^{(m)}) + v(z_i^{(m)})^2 - [A_{1,i}^{(m)}]^2 - A_{2,i}^{(m)}}, \quad i = 1, \ldots, k, \ m = 0, 1, \ldots, \tag{27}$$

where

$$A_{\lambda,i}^{(m)} = \sum_{\substack{j=1 \\ j \neq i}}^{k} \left(\frac{1}{z_i^{(m)} - Z_j^{(m)}} \right)^{\lambda} + (n-k) \left(\frac{1}{z_i^{(m)} - W} \right)^{\lambda}, \quad \lambda = 1, 2.$$

We note that the inverse of the exterior of a circle $(z_i^{(m)} - W)^{-1}$ is a closed disk if it is provided that $z_i^{(m)} \notin W$ in each iteration. Furthermore, since

$$\operatorname{rad}\left(\frac{1}{z_i^{(m)} - W} \right) = O(1),$$

the order of convergence of the iterative method (27) is only *three*.

A particular case of interest appears when only one simple zero, say $\zeta = \zeta_1$, is isolated in a disk $Z^{(0)} = \{c; R\}$ and $\zeta_j \in \{z; |z - c| > R\} = \operatorname{ext}(Z^{(0)})$. Then the iterative formula (27) reduces to

$$Z^{(m+1)} = z^{(m)} - \frac{2v(z^{(m)})}{h(z^{(m)}) + v(z^{(m)})^2 - n(n-1)\left(\dfrac{1}{z^{(m)} - \operatorname{ext}(Z^{(0)})} \right)^2},$$

$$m = 0, 1, \ldots, \quad z^{(m)} = \operatorname{mid}(Z^{(m)}). \tag{28}$$

The order of convergence of the last iterative method is also three.

As it is well known, the main objection to interval methods is their comparatively great computational amount of work because interval computations require extra operations. Their computational efficiency can be increased if these methods are combined with iterative methods in ordinary floating-point arithmetic (see [13]). Such *combined methods* consist of two steps:

(1) Compute complex approximations $z_i^{(m)}$, $i = 1, \ldots, k$, $1 \leqslant k \leqslant n$, appearing in (24), (27) or (28) to any wanted accuracy by some algorithms in (ordinary) complex arithmetic starting with the centers $z_i^{(0)} = \operatorname{mid}(Z_i^{(0)})$.

(2) Apply the desired interval method ((24), (27) or (28)) only once dealing with the improved approximations $z_i^{(m)}$ and the initial complex intervals $Z_i^{(0)}$.

For example, the combined method which uses the interval formula (24) has the form

$$Z_i^{(m,1)} = z_i^{(m)} - \frac{2v(z_i^{(m)})}{h(z_i^{(m)}) + v(z_i^{(m)})^2 - \Sigma_i(\mathbf{Z}^{(0)}, \mathbf{Z}^{(0)})}, \quad i = 1, \ldots, n.$$

The upper "index" $(m, 1)$ indicates that the inclusion disk $Z_i^{(m,1)}$ is furnished by m iterations in floating-point arithmetic and one interval iteration. As emphasized in [13], the contraction of the inclusion complex intervals $Z_i^{(m,1)}$ is attained due to the influence of the term $\Phi(z_i^{(m)})$ which is very small (in magnitude) when $z_i^{(m)}$ is a sufficiently good approximation. The main role of the initial complex intervals $Z_i^{(0)}$ is to provide the inclusion of zeros.

Finally, we observe that the computational efficiency of the combined methods which apply some of the interval methods (24), (27) or (28) can be further improved if we use some of the simpler iterative methods in floating-point arithmetic (to obtain the "point" approximation $z_i^{(m)}$) which does not require the computation of $Y'(z)$ and $Y''(z)$ in each iteration. For example, Newton's method

$$z_i^{(\lambda+1)} = z_i^{(\lambda)} - \frac{\Phi\left(z_i^{(\lambda)}\right)}{\Phi'\left(z_i^{(\lambda)}\right)}, \quad \lambda = 0, 1, \ldots, m-1,$$

or Halley's method

$$z_i^{(\lambda+1)} = z_i^{(\lambda)} - \frac{\Phi\left(z_i^{(\lambda)}\right)}{\Phi'\left(z_i^{(\lambda)}\right)}\left[1 - \frac{\Phi''\left(z_i^{(\lambda)}\right)\Phi\left(z_i^{(\lambda)}\right)}{2\Phi'\left(z_i^{(\lambda)}\right)^2}\right]^{-1}, \quad \lambda = 0, 1, \ldots, m-1,$$

could be usefully applied.

Remark 7. The inclusion methods (24), (27) and (28) and the corresponding combined methods can also be realized in rectangular arithmetic and all derived results remain valid. Although the operations of rectangular arithmetic are more complicated (than circular arithmetic operations), this arithmetic realized by the rounded real interval arithmetic (so-called rounded rectangular arithmetic, see [17]) possesses a useful property that takes into account rounding errors.

5. Some computational aspects

The presented algorithms possess extremely rapid convergence. As it can be seen from Table 1 and Theorem 3 the R-order of convergence is between 4 and 7. Numerical examples have shown that a high accuracy of the approximative solutions may be obtained by only few (three or even two) iterations. In order to avoid the effect of rounding errors, in the implementation of the suggested methods multiple-precision arithmetic should be employed.

The behaviour of the presented methods for the simultaneous determination of zeros of analytic functions is almost the same as in the case of polynomial zeros. For this reason and the fact that computational aspects of the iterative methods of the same type were presented in [8] in detail, we will not discuss further the mentioned points. Instead, our attention will be restricted to the computation of the number of zeros n (by using (2)), $Y'(z)$ and $Y''(z)$ (by using (12) and (13), respectively). Besides, we will consider the influence of the approximative values of $Y'(z)$ and $Y''(z)$ and the rounding errors appearing in the evaluation of Φ, Φ' and Φ'' on the accuracy of approximations of the sought zeros of Φ. Some of these points have already been considered in [8] so that we will give in short some necessary remarks.

As it was noted in [8], the number of zeros n, given by (2), $Y'(z)$ and $Y''(z)$, given by (12) and (13), should be computed in practice by applying a suitable sufficiently accurate quadrature rule for contours. In [8] the authors proposed the trapezoidal quadrature rule of the form

$$\frac{1}{2\pi \mathrm{i}} \int_\Gamma G(w)\, \mathrm{d}w \cong \sum_{k=1}^{m} A_{km} G(w_{km}),$$

where A_{km} are the weights and w_{km} the corresponding nodes of the quadrature rule. It is convenient to apply this quadrature rule along the circumference $\Gamma = \{w: |w| = R\}$ with nodes

$$w_{km} = R \exp(\mathrm{i}\Theta_{km}), \quad \Theta_{km} = \frac{(2k-1)\pi}{m}, \qquad k = 1, \ldots, m.$$

In some cases considerably better results can be obtained by using complex polynomials $\{\omega_m\}$ orthogonal on the semicircle, introduced in [6]. Using the orthogonal polynomials ω_m the Gauss–Christoffel quadrature rule of Legendre's type

$$\int_0^\pi g(\mathrm{e}^{\mathrm{i}\Theta})\, \mathrm{d}\Theta \cong \sum_{k=1}^{m} \sigma_k^{(m)} g(\xi_k^{(m)}) \tag{29}$$

for integrals over the unit semicircle was constructed in [6]. The nodes $\xi_k^{(m)}$ are the zeros of $\omega_m(z)$ which are all simple and lie in the interior of the upper unit half disk. The weights $\sigma_k^{(m)}$ in (29) are obtained by solving the corresponding linear system of equations (see [6] for more details). The tabulated values of $\sigma_k^{(m)}$ and $\xi_k^{(m)}$ for various m can be found in [6]. Taking the circumference $\Gamma = \{w: |w| = R\}$ as the contour of integration, an integral can be computed numerically by (29) in the following manner:

$$\begin{aligned}
\frac{1}{2\pi \mathrm{i}} \int_\Gamma G(w)\, \mathrm{d}w &= \frac{R}{2\pi} \int_0^{2\pi} \mathrm{e}^{\mathrm{i}\Theta} g(R\, \mathrm{e}^{\mathrm{i}\Theta})\, \mathrm{d}\Theta = \frac{R}{2\pi} \int_0^{2\pi} g(R\, \mathrm{e}^{\mathrm{i}\Theta})\, \mathrm{d}\Theta \\
&= \frac{R}{2\pi} \left[\int_0^\pi g(R\, \mathrm{e}^{\mathrm{i}\Theta})\, \mathrm{d}\Theta + \int_0^\pi g(R\, \mathrm{e}^{\mathrm{i}(\Theta+\pi)})\, \mathrm{d}\Theta \right] \\
&\cong \frac{R}{2\pi} \sum_{k=1}^{m} \sigma_k^{(m)} \left[g(R\xi_k^{(m)}) + g(-R\xi_k^{(m)}) \right].
\end{aligned}$$

It was remarked in [8] that the influence of the approximation to $Y'(z)$ (obtained by an appropriate quadrature rule) on the numerical results for the zeros ζ_i of Φ is very small for increasing values of the number of iterations and, consequently, this influence is not of particular importance. The authors came to this conclusion considering (6) in the form

$$\hat{z}_i = z_i - \Delta_i - (\Delta_i)^2 [Y'(z_i) + \hat{s}_{1,i}] + O((\Delta_i)^3), \tag{30}$$

where $\Delta_i = \Phi(z_i)/\Phi'(z_i)$ is Newton's correction and $\hat{s}_{k,i} = s_{k,i}$, $k = 1, 2$. Namely, $Y'(z_i)$ is multiplied by the quantity $(\Delta_i)^2$ which is very small (in absolute value) if z_i is a sufficiently good approximation to the zero ζ_i.

Similarly, formula (14) can be rewritten in the form

$$\begin{aligned}
\hat{z}_i = z_i - \Delta_i - (\Delta_i)^2 \frac{\Phi''(z_i)}{2\Phi'(z_i)} \\
+ \tfrac{1}{2}(\Delta_i)^3 \left[Y'(z_i)^2 + Y''(z_i) - \hat{s}_{1,i}^2 - \hat{s}_{2,i} - \frac{\Phi''(z_i)}{\Phi'(z_i)} \left(\frac{\Phi''(z_i)}{2\Phi'(z_i)} + Y'(z_i) \right) \right] \\
+ o((\Delta_i)^3),
\end{aligned} \tag{31}$$

wherefrom we note that the quantities $Y'(z_i)^2$ and $Y''(z_i)$ are multiplied by $(\Delta_i)^3$. This means that the influence of $Y'(z_i)$ and $Y''(z_i)$ is even smaller than in the iterative formula (6).

From the previous consideration we may conclude that the influence of the quadrature errors in (6) and (14) is neutralized due to the very small factors $(\Delta_i)^2$ and $(\Delta_i)^3$, respectively. But, in spite of the quadrature errors (if they are reasonably small), the convergence of the mentioned methods is practically ensured by the main correction terms; in (30) Newton's method (with quadratic convergence)

$$\hat{z}_i = z_i - \Delta_i = z_i - \frac{\Phi(z_i)}{\Phi'(z_i)}$$

appears, while the main part

$$\hat{z}_i = z_i - \Delta_i - (\Delta_i)^2 \frac{\Phi''(z_i)}{2\Phi'(z_i)} = z_i - \frac{\Phi(z_i)}{\Phi'(z_i)} \left(1 - \frac{\Phi''(z_i)\Phi(z_i)}{2\Phi'(z_i)^2}\right)$$

in (31) is the well-known Chebyshev's method of the third order. Nevertheless, taking into account the remark given in [8], in order to avoid some critical cases (for example, when one or more zeros of Φ lie very close to the boundary Γ), it is advisable to calculate $Y'(z_i)$ and $Y''(z_i)$ with reasonably sufficient accuracy.

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