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On an efficient simultaneous method for finding polynomial zeros

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ABSTRACT

A new iterative method for the simultaneous determination of simple zeros of algebraic polynomials is stated. This method is more efficient compared to the all existing simultaneous methods based on fixed point relations. A very high computational efficiency is obtained using suitable corrections resulting from the Kung–Traub three-step method of low computational complexity. The presented convergence analysis shows that the convergence rate of the basic third order method is increased from 3 to 10 using this special type of corrections and applying $2n$ additional polynomial evaluations per iteration. Some computational aspects and numerical examples are given to demonstrate a very fast convergence and high computational efficiency of the proposed zero-finding method.

1. Introduction

The aim of this paper is to construct an iterative method for the simultaneous determination of simple polynomial roots with a very high computational efficiency. The proposed method is ranked as the most efficient among existing methods in the class of simultaneous methods for approximating polynomial roots based on fixed point relations. The presented iterative formula relies on the fixed point relation of Gargantini–Henrici type [1]. A high computational efficiency is attained by employing suitable corrections which enable very fast convergence (equal to ten) with minimal computational costs. In fact, these corrections arise from the Kung–Traub three-point method [2].

2. Accelerated methods

Let $f(z) = \prod_{j=1}^{n}(z - \zeta_j)$ be a monic polynomial of degree n with simple real or complex zeros $\zeta_1, \dots, \zeta_n$ and let

$$u(z) = \frac{f(z)}{f'(z)} = \left[\frac{d}{dz}\log f(z)\right]^{-1} = \left(\sum_{j=1}^{n}\frac{1}{z-\zeta_j}\right)^{-1} \tag{1}$$

be Newton's correction appearing in the quadratically convergent Newton method. To construct an iterative method for the simultaneous inclusion of polynomial zeros, Gargantini and Henrici [1] started from (1) and derived the following fixed point relation

$$\zeta_i = z - \left(\frac{1}{u(z)} - \sum_{j\in \boldsymbol{I}_n\setminus\{i\}}\frac{1}{z-\zeta_j}\right)^{-1} \quad (i \in \boldsymbol{I}_n := \{1,\dots,n\}). \tag{2}$$

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Let $z_1, \dots, z_n$ be distinct approximations to the zeros $\zeta_1, \dots, \zeta_n$. Setting $z = z_i$ and substituting the zeros ζ_j by some approximations z_j^* in (2), the iterative method

$$\hat{z}_i = z_i - \left(\frac{1}{u(z_i)} - \sum_{j \in \mathbf{I}_n \setminus \{i\}} \frac{1}{z_i - z_j^*} \right)^{-1} \qquad (i \in \mathbf{I}_n) \tag{3}$$

for the simultaneous determination of all simple zeros of the polynomial f is obtained. The choice $z_j^* = z_j$ in (3) gives the well-known cubically convergent Ehrlich–Aberth method [3,4]

$$\hat{z}_i = z_i - \left(\frac{1}{u(z_i)} - \sum_{j \in \mathbf{I}_n \setminus \{i\}} \frac{1}{z_i - z_j} \right)^{-1} \qquad (i \in \mathbf{I}_n). \tag{4}$$

Comparing (2) and (3) it is evident that the better approximations z_j^* give the more accurate approximations $\hat{z}_i$; indeed, if $z_j^* \to \zeta_j$, then $\hat{z}_i \to \zeta_i$. This idea was employed by Nourein in [5] for the construction of the following fourth-order method by using the Newton approximations $z_j^* = z_j - u(z_j)$ in (3):

$$\hat{z}_i = z_i - \left(\frac{1}{u(z_i)} - \sum_{j \in \mathbf{I}_n \setminus \{i\}} \frac{1}{z_i - z_j + u(z_j)} \right)^{-1} \qquad (i \in \mathbf{I}_n). \tag{5}$$

In this paper we will prove that further increase of computational efficiency can be achieved by combining a suitable three-point method. More details about multipoint methods may be found in [6,7]. In fact, we construct a tenth-order simultaneous method of the form (3) using $2n$ additional polynomial evaluations. These additional evaluations provide a huge increase of the order of convergence from 3 (method (4)) to the incredible 10.

Let f be a function with an isolated zero ζ and let x_m be its approximation obtained at the mth iterative step. To achieve a very fast convergence of the method (3), we will apply a special case of the Kung–Traub family of multipoint methods of arbitrary order of convergence [2], given through the following three steps:

$$\begin{cases} y_m = x_m - \dfrac{f(x_m)}{f'(x_m)} = x_m - u(x_m), \qquad v_m = y_m - \dfrac{f(x_m) f(y_m) u(x_m)}{\big(f(x_m) - f(y_m)\big)^2}, \\ x_{m+1} = \mathcal{K}(x_m) := v_m - \dfrac{(y_m - v_m) f(v_m) u(x_m)}{\big(f(x_m) - f(v_m)\big)^2} \left[f(y_m) + \dfrac{f(x_m)^2}{f(y_m) - f(v_m)} \right]. \end{cases} \tag{6}$$

For simplicity, the three-point Kung–Traub iteration (6) is denoted as $x_{m+1} = \mathcal{K}(x_m)$.

Now we can construct a new simultaneous method taking the Kung–Traub approximations $z_j^* = \mathcal{K}(z_j)$ (given by (6)) in (3). If $z_1^{(0)}, \dots, z_n^{(0)}$ are initial approximations to the polynomial zeros $\zeta_1, \dots, \zeta_n$, then the new simultaneous method is defined by the iterative formula

$$z_i^{(m+1)} = z_i^{(m)} - \left(\frac{1}{u(z_i^{(m)})} - \sum_{j \in \mathbf{I}_n \setminus \{i\}} \frac{1}{z_i^{(m)} - \mathcal{K}(z_j^{(m)})} \right)^{-1}, \quad (i \in \mathbf{I}_n,\ m = 0, 1, \dots). \tag{7}$$

Remark 1. To decrease the total computational cost, before executing an iteration step it is first necessary to calculate all entries $\mathcal{K}(z_j^{(m)})$.

3. Convergence analysis

The following theorem deals with the order of convergence of the simultaneous method (7).

Theorem 1. *Assume that initial approximations $z_1^{(0)}, \dots, z_n^{(0)}$ are sufficiently close to the distinct zeros $\zeta_1, \dots, \zeta_n$ of the polynomial f. Then the order of convergence of the simultaneous method (7) is 10.*

Proof. For simplicity, we omit the iteration index m and denote all quantities at the $(m+1)$th iteration with the symbol $\widehat{\ }$. Let us introduce the errors $\varepsilon_j = z_j - \zeta_j$, $\hat{\varepsilon}_j = \hat{z}_j - \zeta_j$, and let

$$z_j^* = \mathcal{K}(z_j), \qquad \lambda_{ij} = z_i - \mathcal{K}(z_j), \qquad \theta_i = \sum_{j \in \mathbf{I}_n \setminus \{i\}} \frac{\mathcal{K}(z_j) - \zeta_j}{(z_i - \zeta_j)\lambda_{ij}}.$$

Then, starting from (7) and using (1) we obtain

$$\hat{z}_i = z_i - \left(\frac{1}{\varepsilon_i} + \sum_{j \in \mathbf{I}_n \setminus \{i\}} \frac{1}{z_i - \zeta_j} - \sum_{j \in \mathbf{I}_n \setminus \{i\}} \frac{1}{\lambda_{ij}} \right)^{-1} = z_i - \frac{\varepsilon_i}{1 - \varepsilon_i \theta_i},$$

and hence

$$\hat{\varepsilon}_i = \hat{z}_i - \zeta_i = \varepsilon_i - \frac{\varepsilon_i}{1 - \varepsilon_i\theta_i} = \frac{-\varepsilon_i^2\theta_i}{1 - \varepsilon_i\theta_i}. \tag{8}$$

According to the conditions of Theorem 1, we can assume that $\varepsilon_i = \mathcal{O}_M(\varepsilon_j)$ for any pair i, j; let $\varepsilon \in \{\varepsilon_1, \ldots, \varepsilon_n\}$ be the error of the maximal modulus. Here $\mathcal{O}_M$ is the symbol which points to the fact that two complex numbers w_1 and w_2 have moduli of the same order (that is, $|w_1| = \mathcal{O}(|w_2|)$, $\mathcal{O}$ is the Landau symbol), written as $w_1 = \mathcal{O}_M(w_2)$.

The order of convergence of the three-point method (6) is eight, that is, the following relation is valid

$$K(z_j) - \zeta_j = \mathcal{O}(\varepsilon_j^8). \tag{9}$$

See [2] for the proof. According to (9), we have $\theta_i = \mathcal{O}_M(\varepsilon^8)$ and from (8) we find

$$\hat{\varepsilon} = \mathcal{O}_M(\varepsilon^{10}),$$

which means that the order of convergence of the method (7) is 10. □

Remark 2. Exceptional acceleration of the order of convergence from 3 (the Ehrlich–Aberth method (4)) to 10 (the new method (7)) is attained using $2n$ additional evaluations of the polynomial f per iteration. As a consequence, the computational efficiency of the method (7) is increased, as shown in Section 4.

Let $\boldsymbol{\zeta} = (\zeta_1, \ldots, \zeta_n)$ and $\boldsymbol{z}^{(0)} = (z_1^{(0)}, \ldots, z_n^{(0)})$ be the vectors of simple polynomial zeros and distinct initial approximations to these zeros, respectively. One of the most interesting and challenging problems in studying iterative root-finding methods is to get a *ball of convergence* $B(\boldsymbol{\zeta}, \boldsymbol{R})$ with center $\boldsymbol{\zeta}$ and radius $\boldsymbol{R}$ such that the implemented method converges starting from any initial point $\boldsymbol{z}^{(0)}$ belonging to $B(\boldsymbol{\zeta}, \boldsymbol{R})$. A ball of convergence has been found for some relatively simple one-point methods for solving scalar equations of the form $f(x) = 0$ as well as systems of equations of Newton's and secant type, see [8] and references cited therein. In the case of n-point methods for scalar equations a ball of convergence has not been considered in the literature for $n \geq 3$ due to their very complicated structure. For this reason, the determination of a ball of convergence for the proposed method (7), involving the three-point method (6), also appears as a very difficult task.

Let $\{c; r\} := \{z : |z - c| \leq r\}$ denote a disk in the complex plane with center c and radius r. We consider a ball of convergence for an iterative method (IM) for the simultaneous determination of all n simple zeros $\zeta_1, \ldots, \zeta_n$ of a polynomial f of degree n. In general, the major problem in finding a ball of convergence of the form $B(\boldsymbol{\zeta}, \boldsymbol{R}) = (\{\zeta_1, R_1\}, \ldots, \{\zeta_n; R_n\})$ for the simultaneous methods for polynomial zeros is to state computationally verifiable conditions which guarantee the convergence starting with $\boldsymbol{z}^{(0)} \in B(\boldsymbol{\zeta}, \boldsymbol{R})$. Designing such a procedure is a very difficult task even for simple iterative methods. This fact has forced numerical analysts, beginning from the 1970s, to search for inclusion disks of the form $\{z_i; R_i\}$, centered at suitable approximations to the zeros, instead of $\{\zeta_i; R_i\}$. Here we present the following useful result:

Theorem 2. *For $n \geq 3$ let $W_i = f(z_i) / \prod_{j \in \boldsymbol{I}_n \setminus \{i\}} (z_i - z_j)$ and $\eta_i = z_i - W_i$. If the inequality*

$$\max_{1 \leq i \leq n} |W_i| < \frac{1}{2n} \min_{\substack{1 \leq i,j \leq n \\ j \neq i}} |z_i - z_j| \tag{10}$$

holds, then the disks

$$D_1 := \{\eta_1; |W_1|\}, \ldots, D_n := \{\eta_n; |W_n|\}$$

are mutually disjoint and each of them contains one and only one zero of f.

The proof of this assertion follows according to the study given in [9, pp. 28–31].

It remains to state convergence conditions for the guaranteed convergence which deal with the disks $D_1, \ldots, D_n$. For this purpose we use Smale's *point estimation theory* based on estimates in one point. This approach, introduced in [10,11], deals with the computationally verifiable domain of convergence. Following Smale's idea, point estimation theory for iterative methods for the simultaneous determination of simple polynomial zeros was developed in the book [9]. We briefly present this estimation procedure at an initial point.

Let $z_1^{(0)}, \ldots, z_n^{(0)}$ be components of the vector of initial approximations $\boldsymbol{z}^{(0)}$ and let

$$W_i^{(0)} = f(z_i^{(0)}) \Big/ \prod_{j \in \boldsymbol{I}_n \setminus \{i\}} \left(z_i^{(0)} - z_j^{(0)}\right) \ (i \in \boldsymbol{I}_n).$$

Following the result for the Ehrlich–Aberth method (5) with Newton's corrections, given in [9, pp. 102–111], the new method with Kung–Traub corrections (6) will converge under the following initial condition:

$$\max_{1 \leq i \leq n} |W_i^{(0)}| < c_n \cdot \min_{\substack{1 \leq i,j \leq n \\ j \neq i}} \left|z_i^{(0)} - z_j^{(0)}\right|, \tag{11}$$

where $c_n = 1/(\alpha n) < 1/(2n)$ $(\alpha > 2)$ is a constant that depends only on the polynomial degree n. Condition (11) is actually condition (10) with the constant c_n instead of $1/(2n)$. Since $c_n < 1/(2n)$, then the convergence condition (11) also provides the construction of non-overlapping disks $D_1, \ldots, D_n$ defined in Theorem 2. Let us emphasize that the initial condition (11) is computationally verifiable since it depends only on available data (initial approximations and coefficients of a given polynomial), which is of practical importance.

According to the values of c_n for the Ehrlich–Aberth method (4) (see [9, pp. 99–105]) and the Ehrlich–Aberth method with Newton's corrections (5) (see [9, pp. 105–111]), we may expect that α (appearing in the bound of c_n) belongs to the interval [2.5, 4]. However, the convergence analysis of the new method (7) is considerably more complicated than that of the methods (4) and (5) so that the determination of a sharp bound of c_n (that is, as small as possible parameter α) requires a laborious and very lengthy study. For this reason, this subject will be considered in a future work.

4. Computational aspects

In this section we compare the convergence behavior and computational efficiency of the Ehrlich–Aberth method (4), the Nourein method (5), the new simultaneous method (7), and two combined methods of order 10. The knowledge of the computational efficiency is of particular interest in designing a package of root-solvers. This comparison procedure is entirely justified since the analysis of efficiency given in [12, Chapter 6] for several computing machines showed that the Nourein method (5) has the highest computational efficiency in the class of simultaneous methods based on fixed point relations.

As presented in [13, Chapter 1], [12, Chapter 6] and [6, Chapter 1], the efficiency of an iterative method (IM) can be successfully estimated using the *efficiency index* given by

$$E(IM) = \frac{\log r}{d}, \tag{12}$$

where r is the R-order of convergence of the iterative method (IM), and d is the computational cost. The rank list of methods obtained by this formula mainly matches well a real CPU (central processor unit) time.

In order to evaluate the computation cost d it is preferable to use arithmetic operations per iteration taken with certain *weights* depending on the execution times of operations. Denote these weights with w_{as}, w_m and w_d for addition/subtraction, multiplication, and division, respectively. Let AS_n, M_n and D_n be the number of additions+subtractions, multiplications and divisions per iteration for all n zeros of a given polynomial of degree n. Then the computational cost d can be (approximately) expressed as

$$d = d(n) = w_{as}AS(n) + w_mM_n + w_dD_n \tag{13}$$

and from (12) and (13) we obtain

$$E(IM, n) = \frac{\log r}{w_{as}AS(n) + w_mM_n + w_dD_n}. \tag{14}$$

Introduce the abbreviations

$$A_{2,i} = \frac{f''(z_i)}{2f'(z_i)}, \qquad u_i = \frac{f(z_i)}{f'(z_i)}, \qquad S_{k,i} = \sum_{j\in \boldsymbol{I}_n\setminus\{i\}} \frac{1}{(z_i - z_j + u_j)^k}\ (k = 1, 2), \qquad h_i = \left(\frac{f'(z_i)}{f(z_i)} - \frac{f''(z_i)}{2f'(z_i)}\right)^{-1}.$$

In our numerical experiments we tested the simultaneous methods (4), (5), (7) and two combined methods of order 10. Namely, to the authors knowledge, there are no other simultaneous methods of order 10 apart from the new method (7). For this reason, in an artificial way we have constructed two methods of order 10 by combining Newton's method of order two and two simultaneous methods of order five given below.

Wang–Wu method [14]:

$$\hat{z}_i = z_i - \left[\frac{1}{h_i} - \frac{u_i}{2}\left(S_{1,i}^2 + S_{2,i}\right)\right]^{-1} \quad (i \in \boldsymbol{I}_n). \tag{15}$$

Farmer–Loizou-like method [15]:

$$\hat{z}_i = z_i - \frac{u_i(1 - u_iA_{2,i})}{1 - 2u_iA_{2,i} + (u_i^2/2)(A_{2,i}^2 - S_{2,i})} \quad (i \in \boldsymbol{I}_n). \tag{16}$$

We construct two combined methods, referred to as N–W–W and N–F–L, and execute one iteration through two steps:

1° Starting with approximations $z_1, \ldots, z_n$, apply Newton' method to obtain approximations $y_1, \ldots, y_n$.
2° Continue the iterative process employing either method (15) or (16) dealing with $y_1, \ldots, y_n$.

The order of convergence of the combined methods N–W–W and N–F–L is $2 \cdot 5 = 10$.

Table 1
The number of basic operations.

Methods	$A_n + S_n$	M_n	D_n
The Ehrlich–Aberth method (4)	$14n^2 + \mathcal{O}(n)$	$10n^2 + \mathcal{O}(n)$	$2n^2 + \mathcal{O}(n)$
The Nourein method (5)	$14n^2 + \mathcal{O}(n)$	$10n^2 + \mathcal{O}(n)$	$2n^2 + \mathcal{O}(n)$
The new method (7)	$22n^2 + \mathcal{O}(n)$	$18n^2 + \mathcal{O}(n)$	$2n^2 + \mathcal{O}(n)$
Combined N–W–W method	$29n^2 + \mathcal{O}(n)$	$26n^2 + \mathcal{O}(n)$	$2n^2 + \mathcal{O}(n)$
Combined N–F–L method	$27n^2 + \mathcal{O}(n)$	$26n^2 + \mathcal{O}(n)$	$2n^2 + \mathcal{O}(n)$

Table 2
The (percent) dominance of computational efficiency of the new method (7).

	$(X) = (4)$	$(X) = (5)$	$(X) =$ (N–W–W)	$(X) =$ (N–F–L)
$\rho((7), (X))$	41.6%	12.2%	32%	31%

We consider complex polynomials with real or complex zeros. The numbers of basic complex operations, reduced to operations of real arithmetic, are given in Table 1 as functions of the polynomial degree n taking the dominant terms of order $\mathcal{O}(n^2)$.

To compare the simultaneous methods (4), (5), (7), (N–W–W) and (N–F–L), we have used the weights (appearing in (14)) determined according to the estimation of complexity of basic operations in multiple-precision arithmetic. Without loss of generality, we assume that floating-point number representation is used, with a binary fraction of b bits. In other words, we deal with "*precision b*" numbers, giving results with a relative error of approximately 2^{-b}. Following results given in [16], the execution time $t_b(A)$ and $t_b(S)$ of addition and subtraction is $\mathcal{O}(b)$. Using Schönhage–Strassen multiplication (see [16]), we have $t_b(M) = \mathcal{O}\big(b \log b \ \log\log b\big)$ and $t_b(D) = 3.5 t_b(M)$. We chose the weights w_{as}, w_m and w_d proportional to $t_b(A)$, $t_b(M)$ and $t_b(D)$, respectively, for a 128-bit architecture.

Applying (14) and data given in Table 1, we calculated the percent ratios

$$\rho((7), (X)) = \left(\frac{E((7))}{E((X))} - 1\right) \cdot 100 \quad (\text{in } \%),$$

where (X) is one of the methods (4), (5), (N–W–W), (N–F–L). The entries of ρ are given in Table 2. Note that very similar values are obtained using the weights proportional to the processor execution times of basic operations for octuple precision (machine epsilon 10^{-67}) for a Pentium M 2.8 GHz running Fedora core 3 and an Opteron 64-bit processor (data taken from [17]).

It is evident from Table 2 that the new method (7) is more efficient than the tested methods (4), (5), (N–W–W) and (N–F–L). The dominant efficiency (about 30%) of method (7) in regard to (N–W–W) and (N–F–L) is expected since the latter methods require additional n polynomial evaluations. Having in mind the mentioned fact on the dominant efficiency of the Nourein method, it follows that the proposed simultaneous method (7) is the *most efficient method* for the simultaneous determination of polynomial zeros in the class of methods based on fixed point relations.

To demonstrate the convergence behavior of the methods (4), (5), (7), (N–W–W) and (N–F–L), we have tested a number of polynomial equations implementing the computational software package *Mathematica*. For illustration, among a number of tested algebraic polynomials we have selected one numerical example. As a measure of accuracy of the obtained approximations, we have calculated Euclid's norm

$$e^{(m)} := \|\boldsymbol{z}^{(m)} - \boldsymbol{\zeta}\|_2 = \left(\sum_{i=1}^{n} \left|z_i^{(m)} - \zeta_i\right|^2\right)^{1/2} \qquad (m = 0, 1, \ldots). \tag{17}$$

Example 1. We have applied the iterative methods (4), (5), (7), (N–W–W) and (N–F–L) for the simultaneous approximation of the zeros of the polynomial of the 21st degree

$$\begin{aligned} f_{21}(z) = {} & (z-4)(z^2-1)(z^4-16)(z^2+9)(z^2+16)(z^2+2z+5)(z^2+2z+2) \\ & \times (z^2-2z+2)(z^2-4z+5)(z^2-2z+10). \end{aligned}$$

The following initial approximations were used, yielding $e^{(0)} \approx 1.025$:

$$\begin{aligned} & z_1^{(0)} = 4.2 + 0.1i, \quad z_2^{(0)} = -1.2 + 0.1i, \quad z_3^{(0)} = 2.2 + 0.1i, \quad z_4^{(0)} = -2.2 - 0.1i, \\ & z_5^{(0)} = 0.2 + 2.1i, \quad z_6^{(0)} = 0.2 - 2.1i, \\ & z_7^{(0)} = 0.2 + 3.1i, \quad z_8^{(0)} = 0.2 - 3.1i, \quad z_9^{(0)} = -1.2 + 2.1i, \quad z_{10}^{(0)} = -1.2 - 2.1i, \\ & z_{11}^{(0)} = -1.2 + 1.1i, \quad z_{12}^{(0)} = -1.2 - 1.1i, \end{aligned}$$

Table 3
Norm of approximation errors.

Methods	$e^{(1)}$	$e^{(2)}$	$e^{(3)}$
The Ehrlich–Aberth method (4)	8.76(−2)	1.03(−4)	2.16(−13)
The Nourein method (5)	4.61(−2)	5.74(−7)	1.26(−26)
The new method (7)	1.33(−2)	1.75(−17)	7.09(−166)
Combined N–W–W method	3.24(−3)	1.05(−23)	1.17(−228)
Combined N–F–L method	1.21(−2)	6.18(−16)	2.57(−148)

$$z_{13}^{(0)} = 1.2 + 1.1i, \quad z_{14}^{(0)} = 1.2 - 1.1i, \quad z_{15}^{(0)} = 2.2 + 1.1i, \quad z_{16}^{(0)} = 2.2 - 1.1i,$$
$$z_{17}^{(0)} = 1.2 + 3.1i, \quad z_{18}^{(0)} = 1.2 - 3.1i,$$
$$z_{19}^{(0)} = 0.2 + 4.1i, \quad z_{20}^{(0)} = 0.2 - 4.1i, \quad z_{21}^{(0)} = 1.1 + 0.2i.$$

The errors $e^{(m)}$ calculated by (17) are given in Table 3, where the notation $A(-h)$ means $A \times 10^{-h}$.

From Table 3 and a number of tested polynomial equations we can conclude that the proposed method (7) produces approximations of considerable accuracy; two iterative steps are usually sufficient in solving most practical problems when initial approximations are reasonably good and polynomials are well conditioned. The third iteration is given only to demonstrate very fast convergence and, most frequently, it is not needed for real-life problems.

In this concrete example the new method (7) gives more accurate approximations than the N–F–L method but is less accurate compared to the N–W–W method. However, a lot of tested numerical examples showed that the mentioned methods of order 10 produce approximations of approximately the same quality and that none of these methods is the best for all the examples. On the other hand, from Table 2 it is evident that the proposed method (7) is considerably more efficient (about 30%) than the combined methods N–W–W and N–F–L, which is its main advantage among the methods of the same order of convergence.

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