

On Constructing a Cubically Convergent Numerical Method for Multiple Roots

Young Hee Geum

Abstract—We propose the numerical method defined by

$$x_{n+1} = x_n - \lambda \frac{f(x_n - \mu h(x_n))}{f'(x_n)}, \quad n \in \mathbb{N},$$

and determine the control parameter λ and μ to converge cubically. In addition, we derive the asymptotic error constant. Applying this proposed scheme to various test functions, numerical results show a good agreement with the theory analyzed in this paper and are proven using Mathematica with its high-precision computability.

Keywords—Asymptotic error constant, iterative method, multiple root, root-finding.

1.. INTRODUCTION

THE iteration methods to find the roots of nonlinear equations have various applications in many science problems[1,2,3,4]. Among them, the Newton's method is one of the most well-known iteration schemes and is modified by many researchers[5,6,7].

Assume that a function $f : \mathbb{C} \rightarrow \mathbb{C}$ has a multiple root α with integer multiplicity $m \geq 1$ and is analytic in a small neighborhood of α . We find an approximated α by a scheme

$$x_{n+1} = g(x_n), \quad n = 0, 1, 2, \dots, \quad (1)$$

where $g : \mathbb{C} \rightarrow \mathbb{C}$ is an iteration function and $x_0 \in \mathbb{C}$ is given. Then we find an approximated α using an iterative method. The roots of the equation are obtained using the following scheme:

$$g(x) = x - \lambda \frac{f(x - \mu h(x))}{f'(x)} \quad (2)$$

where

$$h(x) = \begin{cases} f(x)/f'(x), & \text{if } x \neq \alpha \\ \lim_{x \rightarrow \alpha} f(x)/f'(x), & \text{if } x = \alpha. \end{cases} \quad (3)$$

For a given $p \in \mathbb{N}$, we suppose that

$$\begin{cases} \left| \frac{d^p}{dx^p} g(x) \right|_{x=\alpha} = |g^{(p)}(\alpha)| < 1, & \text{if } p = 1. \\ g^{(i)}(\alpha) = 0 \text{ for } 1 \leq i \leq p-1 \text{ and } g^{(p)}(\alpha) \neq 0, & \text{if } p \geq 2. \end{cases} \quad (4)$$

Let $z(x) = x - \mu h(x)$ and $F(x) = \frac{f(x - \mu h(x))}{f'(x)}$. Since $g(x)$ is continuous at $x = \alpha$, $g(x)$ is represented by

$$g(x) = \begin{cases} x - \lambda F(x), & \text{if } x \neq \alpha \\ x - \lambda \lim_{x \rightarrow \alpha} F(x), & \text{if } x = \alpha. \end{cases} \quad (5)$$

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By Corollary 1 and Corollary 2, we have $[f(z)]_{x=\alpha}^{(k)} = 0, 0 \leq k \leq m-1$ and $f(\alpha) = f'(\alpha) = \dots = f^{(m-1)}(\alpha) = 0, f^{(m)} \neq 0$. Using L'Hospital's rule repeatedly, we have

$$\lim_{x \rightarrow \alpha} F(x) = \frac{[f(z)]_{x=\alpha}^{(m-1)}}{[f'(x)]^{(m-1)}} = 0 \quad (6)$$

Corollary 1: Suppose $f : \mathbb{C} \rightarrow \mathbb{C}$ has a multiple root α with a given integer multiplicity $m \geq 1$ and is analytic in a small neighborhood of α . Then the function $h(x)$ and its derivatives up to order 3 evaluated at α has the following properties with $\theta_j = \frac{f^{(m+j)}(\alpha)}{f^{(m)}(\alpha)}, j \in \mathbb{N}$:

(i) $h(\alpha) = 0$

(ii) $h'(\alpha) = \frac{1}{m}$

(iii) $h''(\alpha) = -\frac{2}{m^2(m+1)}\theta_1$

(iv) $h^{(3)}(\alpha) = \frac{6}{m^3(m+1)} \left\{ \theta_1^2 - \frac{2m}{m+2}\theta_2 \right\}$

From Eq.(2), we need to investigate some local properties of $g(x)$ in a small neighborhood of α . From the definition of $g(x)$ as described in Eq.(2), we rewrite

$$(g - x) \cdot f'(x) = -\lambda f(z). \quad (7)$$

where $f = f(x), f' = f'(x), z = x - \mu h(x)$ are used for concise and the symbol ' denotes the derivative with respect to x . Using Eq.(4), our aim is to establish some relationships between $\lambda, m, g'(\alpha), g''(\alpha)$ and $g'''(\alpha)$, for maximum order of convergence[8,9]. The next corollary is useful to calculate $g'(\alpha), g''(\alpha)$ and $g'''(\alpha)$.

Corollary 2: Let f stated in Corollary 1 have a multiple root α with a given multiplicity $m \geq 1$. Let $z(x) = x - \mu h(x)$ and $h(x)$ be defined by Eq.(3). Then the following hold:

$$\frac{d^k}{dx^k} f(z) \Big|_{x=\alpha} = [f(z)]^{(k)} \Big|_{x=\alpha} = \begin{cases} 0, & \text{if } 0 \leq k \leq m-1 \\ f^{(m)}(\alpha) \cdot z'(\alpha)^m, & \text{if } k = m \\ f^{(m+1)}(\alpha) \cdot z'(\alpha)^{m+1} + f^{(m)}(\alpha) \frac{m(m+1)}{2} \cdot z'(\alpha)^{m-1} z''(\alpha), & \text{if } k = m+1 \\ f^{(m+2)}(\alpha) \cdot z'(\alpha)^{m+2} + f^{(m+1)}(\alpha) \frac{(m+1)(m+2)}{2} \cdot z'(\alpha)^m z''(\alpha) \\ + f^{(m)}(\alpha) \cdot L_{m+2}(\alpha), & \text{if } k = m+2 \end{cases}$$

where $L_k = \binom{k}{3} t^{k-4} \{ t \cdot (-\mu h''') + \frac{3}{4}(k-3)\mu^2 h''(\alpha)^2 \}$.

Proof. Since $f'(\alpha) = f''(\alpha) = \dots = f^{(m-1)}(\alpha) = 0$ and $f^{(m)}(\alpha) \neq 0$, the assertion follows.

2.. CONVERGENCE ANALYSIS

In this section, we analyze the convergent properties of this proposed scheme in Eq(7) and develop the order of convergence and the asymptotic error constant in terms of parameter μ and γ .

We differentiate both sides of Eq(7) with respect to x to obtain

$$(g' - 1) \cdot f' + (g - x) \cdot f''(x) = -\lambda[f(z)]^{(1)} \quad (8)$$

Let $F_1(x) = \frac{-(g-x)f''(x) - \lambda[f(z)]^{(1)}}{f'}$. Since g' is continuous at α , we have

$$g'(x) - 1 = \begin{cases} F_1(x), & \text{if } x \neq \alpha \\ \lim_{x \rightarrow \alpha} F_1(x), & \text{if } x = \alpha, \end{cases} \quad (9)$$

Using Corollary 2 and $g(\alpha) = \alpha$, we have the following:

$$(g-x)f''(x) \Big|_{x=\alpha}^{(k)} = \sum_{j=0}^k \binom{k}{j} (g-x)^{(j)} f^{(k+2-j)} \Big|_{x=\alpha}$$

$$= \begin{cases} 0, & \text{if } 0 \leq k \leq m-2, m \geq 2 \\ (m-1)(g'-1)f^{(m)}(\alpha), & \text{if } k = m-1, \end{cases} \quad (10)$$

$$[f(z)]^{(1)} \Big|_{x=\alpha}^{(k)} = \begin{cases} 0, & \text{if } 0 \leq k \leq m-2, m \geq 2 \\ f^{(m)}(\alpha)(1 - \frac{\mu}{m})^m, & \text{if } k = m-1, \end{cases} \quad (11)$$

Substituting Eq.(10) and Eq.(11) into Eq.(9) leads

$$g'(\alpha) - 1 = \frac{-(m-1)(g'(\alpha) - 1)f^{(m)}(\alpha) - \lambda f^{(m)}(\alpha)(1 - \frac{\mu}{m})^m}{f^{(m)}(\alpha)}$$

$$g'(\alpha) - 1 = -(m-1)(g'(\alpha) - 1) - \lambda(1 - \frac{\mu}{m})^m$$

To obtain $g'(\alpha) = 0$, we get

$$m = \lambda \left(1 - \frac{\mu}{m}\right)^m = \lambda t^m \quad (12)$$

where $t^m = 1 - \frac{\mu}{m}$.

We differentiate both sides of Eq(8) with respect to x to obtain

$$g'' + 2(g' - 1) \cdot f'' + (g - x) \cdot f^{(3)} = -\lambda[f(z)]^{(2)} \quad (13)$$

Let $F_2(x) = \frac{-2(g'-1) \cdot f'' - (g-x) \cdot f^{(3)} - \lambda[f(z)]^{(2)}}{f'}$. We rewrite

$$g''(x) = \begin{cases} F_2(x), & \text{if } x \neq \alpha \\ \lim_{x \rightarrow \alpha} F_2(x), & \text{if } x = \alpha, \end{cases} \quad (14)$$

We need the following manipulation:

$$(g' - 1) \cdot f''(x) \Big|_{x=\alpha}^{(k)} = \sum_{j=0}^k \binom{k}{j} (g' - 1)^{(j)} f^{(k+2-j)} \Big|_{x=\alpha}$$

$$= \begin{cases} 0, & \text{if } 0 \leq k \leq m-3 \\ (g' - 1)f^{(m)}(\alpha), & \text{if } k = m-2 \\ (g' - 1)f^{(m+1)}(\alpha) + (m-1)g''f^{(m)}(\alpha), & \text{if } k = m-1, \end{cases} \quad (15)$$

$$(g-x) \cdot f^{(3)} \Big|_{x=\alpha}^{(k)} = \sum_{j=0}^k \binom{k}{j} j(g-x)^{(j)} f^{(k+3-j)} \Big|_{x=\alpha}$$

$$= \begin{cases} 0, & \text{if } 0 \leq k \leq m-3 \\ (m-2)(g'-1)f^{(m)}(\alpha), & \text{if } k = m-2 \\ (m-1)(g'-1)f^{(m+1)}(\alpha) + \frac{(m-1)(m-2)}{2} g''f^{(m)}(\alpha), & \text{if } k = m-1, \end{cases} \quad (16)$$

$$[[f(z)]^{(2)}]_{x=\alpha}^{(k)} = \begin{cases} 0, & \text{if } 0 \leq k \leq m-3 \\ f^{(m)}(\alpha)t^m, & \text{if } k = m-2 \\ f^{(m+1)}(\alpha)(t^{m-1} - t^m + t^{m+1}), & \text{if } k = m-1, \end{cases} \quad (17)$$

Applying Eq.(15), Eq.(16) and Eq.(17) into the numerator of $F_2(x)$ yields

$$-2(g' - 1)f'' - (g - x)f^{(3)} - \lambda[f(z)]^{(2)}$$

$$= \begin{cases} 0, & \text{if } 0 \leq k \leq m-3 \\ f^{(m)}(\alpha)(m - \lambda t^m), & \text{if } k = m-2 \\ f^{(m+1)}(\alpha)[(m+1) - \lambda(t^{m+1} - t^m + t^{m-1})] \\ -g''f^{(m)}(\alpha)\frac{(m+2)(m-1)}{2}, & \text{if } k = m-1, \end{cases} \quad (18)$$

From Eq.(18) and Eq.(14), we obtain

$$g'' = \frac{2\theta_1}{m(m+1)} \{(m+1) - \lambda(t^{m+1} - t^m + t^{m-1})\} \quad (19)$$

From Eq.(19), to have $g''(\alpha) = 0$ we get the following relation,

$$m+1 = \lambda(t^{m+1} - t^m + t^{m-1}) \quad (20)$$

We differentiate both sides of Eq(6) with respect to x to obtain

$$g^{(3)} \cdot f' + 3g'' \cdot f'' + 3(g' - 1) \cdot f^{(3)} + (g - x) \cdot f^{(4)} = -\lambda[f(z)]^{(3)}. \quad (21)$$

We rewrite

$$g^{(3)}(x) = \begin{cases} F_3(x), & \text{if } x \neq \alpha \\ \lim_{x \rightarrow \alpha} F_3(x), & \text{if } x = \alpha, \end{cases} \quad (22)$$

where

$$F_3(x) = \frac{-3g''f'' - 3(g' - 1)f^{(3)} - (g - x)f^{(4)} - \lambda[f(z)]^{(3)}}{f'}$$

We need the following calculation:

$$g'' \cdot f'' \Big|_{x=\alpha}^{(k)} = \sum_{j=0}^k \binom{k}{j} g^{(j+2)} f^{(k+2-j)} \Big|_{x=\alpha}$$

$$= \begin{cases} 0, & \text{if } 0 \leq k \leq m-2 \\ (m-1)g^{(3)}f^{(m)}(\alpha), & \text{if } k = m-1, \end{cases} \quad (23)$$

$$(g' - 1) \cdot f^{(3)} \Big|_{x=\alpha}^{(k)} = \sum_{j=0}^k \binom{k}{j} (g' - 1)^{(j)} f^{(k+3-j)} \Big|_{x=\alpha}$$

$$= \begin{cases} 0, & \text{if } 0 \leq k \leq m-4 \\ (g' - 1)f^{(m)}(\alpha), & \text{if } k = m-3 \\ -f^{(m+1)}(\alpha), & \text{if } k = m-2 \\ -f^{(m+2)}(\alpha) + \frac{(m-1)(m-2)}{2} g^{(3)}f^{(m)}(\alpha), & \text{if } k = m-1, \end{cases} \quad (24)$$

$$(g-x) \cdot f^{(4)} \Big|_{x=\alpha}^{(k)} = \sum_{j=0}^k \binom{k}{j} (g-x)^{(j)} f^{(k+4-j)} \Big|_{x=\alpha}$$

$$= \begin{cases} 0, & \text{if } 0 \leq k \leq m-4 \\ -(m-3)f^{(m)}, & \text{if } k = m-3 \\ -(m-2)f^{(m+1)}, & \text{if } k = m-2 \\ -(m-1)f^{(m+2)}(\alpha) + \frac{(m-1)(m-2)(m-3)}{6} g^{(3)}f^{(m)}(\alpha), & \text{if } k = m-1. \end{cases} \quad (25)$$

$$[[f(z)]^{(3)}]_{x=\alpha}^{(k)}$$

$$= \begin{cases} 0, & \text{if } 0 \leq k \leq m-4 \\ f^{(m)}(\alpha)(1 - \frac{\mu}{m})^m, & \text{if } k = m-3 \\ f^{(m+1)}(\alpha)t^{m+1} + f^{(m)}(\alpha)\frac{m(m+1)}{2}t^{m-1}z''(\alpha), & \text{if } k = m-2 \\ f^{(m+2)}(\alpha)t^{m+2} + f^{(m+1)}(\alpha)\frac{m+2}{m}(t^m - t^{m+1})\theta_1 \\ + f^{(m)}(\alpha)L_{m+2}(\alpha), & \text{if } k = m-1, \end{cases} \quad (26)$$

Replacing the numerator of $F_3(x)$ by Eq.(23), Eq.(24), Eq.(25) and Eq.(26) leads

$$-3g''f''|_{x=\alpha} - 3(g' - 1)f^{(3)}|_{x=\alpha} - (g - x)f^{(4)}|_{x=\alpha} - \lambda[f(z)]^{(3)}|_{x=\alpha}$$

$$= \begin{cases} 0, & \text{if } 0 \leq k \leq m - 4 \\ f^{(m)}(\alpha)(m - \lambda t^m), & \text{if } k = m - 3 \\ f^{(m+1)}(\alpha)\{m + 1 - \lambda(t^{m+1} - t^m + t^{m-1})\}, & \text{if } k = m - 2 \\ -\frac{(m-1)(m^2+4m+6)}{6}g^{(3)}f^{(3)} + f^{(m+2)}(\alpha)(m+2) \\ -\lambda\{f^{(m+2)}(\alpha)t^{m+2} - f^{(m+1)}(\alpha)\theta_1\frac{m+2}{m}(t^m - t^{m+1}) \\ -f^{(m)}(\alpha)L_{m+2}(\alpha)\}, & \text{if } k = m - 1, \end{cases} \quad (27)$$

From Eq.(22) and Eq.(27), we have

$$g^{(3)}(\alpha) = \frac{6}{m(m+1)(m+2)}$$

$$\left[\theta_2(m+2) - \lambda\{\theta_2 t^{m+2} + \theta_1^2(t^m - t^{m+1})\frac{m+2}{m} + L_{m+2}(\alpha) \right]. \quad (28)$$

Consequently, to make $g^{(3)}(\alpha) \neq 0$, we have the following relation:

$$(m+2)\theta_2 \neq \lambda\{\theta_2 t^{m+2} + \theta_1^2(1-t)t^m\frac{m+2}{m} + L_{m+2}(\alpha)\} \quad (29)$$

$$L_k = \binom{k}{3} t^{k-4} \{t \cdot (-\mu h''(\alpha)) + \frac{3}{4}(k-3)\mu^2 h''(\alpha)^2\} \\ \begin{cases} m = \lambda t^m \quad (2.5) \\ m+1 = \lambda(t^{m+1} - t^m + t^{m-1}) \quad (2.13) \\ (m+2)\theta_2 \neq \lambda\theta_2 t^{m+2} + \theta_1^2(1-t)t^m\frac{m+2}{m} + L_{m+2}(\alpha)(30) \end{cases}$$

Theorem 1: Let $f : \mathbb{C} \rightarrow \mathbb{C}$ have a zero α with integer multiplicity $m \geq 1$ and be analytic in a small neighborhood of α . Let θ_1, θ_2 be defined as in Corollary 1. Let t be a root of $\rho(t)$ defined in (20). Let x_0 be an initial guess chosen in a sufficiently small neighborhood of α . Then iteration method (2) with $\mu = m(1-t)$ has order 3 and its asymptotic error constant η as follows:

$$\eta = \frac{1}{6} |g^{(3)}(\alpha)| = \frac{1}{m(m+1)(m+2)} |\phi_1 \theta_1^2 + \phi_2 \theta_2|,$$

where $\phi_1 = -t^{m-2} \lambda q_1(t)$, $\phi_2 = m+2 - \lambda t^{m-2} q_2(t)$, $q_1(t) = -\frac{(m+2)(t-1)^2 \{2(m+1)t - m+1\}}{2m(m+1)}$ and $q_2(t) = t(t^3 - 2t + 2)$.

From Eq.(12) and Eq.(20), we get

$$mt^2 - (2m+1)t + m = 0$$

Typical cases for $1 \leq m \leq 4$ are studied here and listed in Table 1 to confirm Theorem 2.1.

TABLE I
 VALUES ρ, t AND η FOR $1 \leq m \leq 4$

m	$\rho(t)$	t	η
1	$t^2 - 3t + 1 = 0$	$\frac{3+\sqrt{5}}{2}$	$\frac{1}{6}[\theta_2(4-3t) + 2\theta_1^2(1-t)]$
2	$2t^2 - 5t + 2 = 0$	$\frac{5+\sqrt{9}}{4}$	$\frac{1}{24}[\theta_2 \frac{5t^2+2t+4}{t} + \theta_1^2 \frac{7t^2-2t+2}{3t^2}]$
3	$3t^2 - 7t + 3 = 0$	$\frac{7+\sqrt{13}}{6}$	$\frac{1}{60}[\theta_2 \frac{-7t^2+2t+6}{t} + 5\theta_1^2 \frac{4t^3+t^2-6t+1}{4t^2}]$
4	$4t^2 - 9t + 4 = 0$	$\frac{9+\sqrt{17}}{8}$	$\frac{1}{20}[\theta_2 \frac{10t-8}{t} + \theta_1^2 \frac{30t^3-49t^2+28t-9}{5t^2}]$

3.. ALGORITHM, NUMERICAL RESULTS AND DISCUSSIONS

The symbolic and computational ability of *Mathematica*[11] leads us to a zero-finding algorithm based on the analysis studied in Sections 1 and 2.

Algorithm 1 (Zero-Finding Algorithm)

Step 1. For $k \in \mathbb{N} \cup \{0\}$, construct iteration scheme (1) with the given function f at a multiple zero α as stated in Section 1.

Step 2. Set the minimum number of precision digits. With exact zero α or most accurate zero, supply the theoretical asymptotic error constant η . Set the error range ϵ , the maximum iteration number n_{max} and the initial value x_0 . Compute $f(x_0)$ and $|x_0 - \alpha|$.

Step 3. Compute x_{n+1} in (1.1) for $0 \leq n \leq n_{max}$ and display the computed values of $n, x_n,$

$$f(x_n), |x_n - \alpha|, |e_{n+1}/e_n^p| \text{ and } \eta.$$

In these experiments, we choose 300 as the minimum number of digits of precision by assigning $\$MinPrecision=250$ in *Mathematica* to achieve the specified nominal accuracy. We set the error bound ϵ to 0.5×10^{-235} for $|x_n - \alpha| < \epsilon$ and evaluate the n^{th} order derivative of the complicated nonlinear functions using the *Mathematica* command $D[f, \{x, n\}]$.

As an example for the convergence, we first illustrate the order of convergence and the asymptotic error constant with a function

$$f(x) = (x - 2) \cos(\pi/x)$$

having a real zero $\alpha = 2.0$ of multiplicity 2. We choose $x_0 = 1.89$ as an initial guess. Table II verifies cubic convergence apparently.

As a second example, we illustrate the order of convergence and the asymptotic error constant with a function

$$f(x) = (x^2 + 16) \log(x^2 + 17)^2$$

having a multiple real zero $\alpha = 4i$ of multiplicity 3. We choose $x_0 = 3.87i$ as an initial guess. Table III shows a good agreement with the theory developed in this paper. Table III clearly reflects the theoretical convergence presented in this paper. The computed asymptotic error constants are in good agreement with theoretical asymptotic error constants η up to 10 significant digits. The computed root is rounded to be accurate up to the 235 significant digits.

TABLE II
 CONVERGENCE FOR $f(x) = (x - 2) \cos(\pi/x)$ WITH $m = 2, \alpha = 2$

$$(t, \mu, l) = (1/2, 1, 8)$$

n	x_n	$ x_n - \alpha $	e_{n+1}/e_n^3	η
0	1.89	0.11		0.08820
1	1.99988197105842	0.000118029	0.08867689075	209479
2	1.999999999999985	1.45027×10^{-13}	0.08820274944	
3	2.000000000000000	2.69043×10^{-40}	0.08820209479	
4	2.000000000000000	1.71769×10^{-120}	0.08820209479	
5	2.000000000000000	0.0×10^{-299}		

TABLE III
 CONVERGENCE FOR $f(x) = (x^2 + 16) \log(x^2 + 17)^2$ WITH
 $m = 3, \alpha = 4i$

$$(t, \mu, l) = \left(\frac{7-\sqrt{13}}{6}, 1.30278, \frac{648}{(7-\sqrt{13})^3} \right)$$

n	x_n	$ x_n - \alpha $	e_{n+1}/e_n^3	η
0	3.87i	0.130000		5.571505565
1	3.99405900753211i	0.00594099	2.704138583	05565
2	3.99999888367444i	1.11633×10^{-6}	5.323703698	
3	4.00000000000000i	7.75071×10^{-18}	5.571456971	
4	4.00000000000000i	2.59416×10^{-51}	5.571505565	
5	4.00000000000000i	9.72665×10^{-152}	5.571505565	
6	4.00000000000000i	0.0×10^{-299}		

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Let d denote the number of new function or derivative evaluations per iteration. For our proposed method, d is found to be 3. We remark from [10] that both the computational efficiency EFF

$$EFF = \frac{p}{d} = \begin{cases} \frac{3}{3}, & \text{if } m = 1 \\ \frac{3}{3} \approx 0.6667, & \text{if } m \geq 2, \end{cases}$$

and the efficiency index $*EFF$

$$*EFF = p^{1/d} = \begin{cases} 3^{\frac{1}{3}} \approx 1.44225, & \text{if } m = 1 \\ 2^{\frac{1}{3}} \approx 1.25992, & \text{if } m \geq 2, \end{cases}$$

display a good measure of computation compared to the classical newton's method with

$$EFF = \frac{p}{d} = \begin{cases} 1, & \text{if } m = 1 \\ \frac{1}{2}, & \text{if } m \geq 2, \end{cases}$$

and

$$*EFF = p^{1/d} = \begin{cases} 2^{\frac{1}{2}} \approx 1.41421, & \text{if } m = 1 \\ 1^{\frac{1}{2}} = 1, & \text{if } m \geq 2. \end{cases}$$

Various numerical experiments prove the order of convergence and the asymptotic error constant of the extended leap-frogging Newton's method. This proposed development will play a important part in finding zeros of the nonlinear equation with highly accuracy. The current investigation will be extended to different methods at a multiple zero.

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