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A NOTE ON THREE-STEP ITERATIVE METHODS FOR NONLINEAR EQUATIONS

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Dedicated to Professor Petru Blaga at his 60^{th} *anniversary*

Abstract. In this short note we give certain comments and improvements of some three-step iterative methods recently considered by N.A. Mir and T. Zaman (Appl. Math. Comput. (2007) doi: 10.1016/j.amc.2007.03.071).

1. Introduction

Very recently, N.A. Mir and T. Zaman [1] have considered three-step quadrature based iterative methods for finding a single zero $x = \alpha$ of a nonlinear equation

$$f(x) = 0. \tag{1.1}$$

All variants of their methods include the formula

$$x_{n+1} = x_n - \frac{f(x_n)f'(x_n)}{f'(x_n)^2 - \lambda f(x_n)f''(x_n)}, \tag{1.2}$$

obtained from the rectangular quadrature formula. It is clear that (1.2) reduces to Newton and Halley method for $\lambda = 0$ and $\lambda = 1/2$, respectively.

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As a variant with maximal order of convergence they have proposed the following three-step method

$$\left.\begin{aligned} y_n &= x_n - \frac{f(x_n)}{f'(x_n)}, \\ z_n &= y_n - \frac{f(y_n)f'(y_n)}{f'(y_n)^2 - \lambda f(y_n)f''(y_n)}, \\ x_{n+1} &= z_n - \frac{(y_n - z_n)f(z_n)}{f(y_n) - 2f(z_n)}, \end{aligned}\right\} \tag{1.3}$$

proving that for a sufficiently smooth function f and a starting point x_0 sufficiently close to the single zero $x = \alpha$, this method has eighth order convergence for $\lambda = 1/2$, i.e.,

$$e_{n+1} = (-c_3c_2^5 + c_2^7)e_n^8 + O(e_n^9),$$

where $e_n = x_n - \alpha$ and

$$c_k = \frac{1}{k!}\frac{f^{(k)}(\alpha)}{f'(\alpha)}, \quad k = 2, 3, \ldots \ . \tag{1.4}$$

As we can see this three-step method need six function evaluations per iteration: $f(x_n)$, $f(y_n)$, $f(z_n)$, $f'(x_n)$, $f'(y_n)$, and $f''(y_n)$. Without new function evaluations, in this note we show that the formula

$$x_{n+1} = S(y_n, z_n) = z_n - \frac{f(z_n)}{f'(y_n) + (z_n - y_n)f''(y_n)} \tag{1.5}$$

is a much better choice than the third formula in (1.3). In that case the corresponding three-step method has tenth order convergence. Moreover, the formula (1.5) is numerically stable in comparing with the previous one.

The paper is organized as follows. In Section 2 we give certain auxiliary formulae, which can be used also in other investigations in convergence analysis. The main results and a numerical example are given in Section 3.

2. **Some auxiliary formulae**

We suppose that the equation (1.1) has a single zero $x = \alpha$ in certain neighborhood $U_\varepsilon(\alpha) := (\alpha - \varepsilon, \alpha + \varepsilon)$, $\varepsilon > 0$, and that the function f is sufficiently differentiable in $U_\varepsilon(\alpha)$. Evidently, $f'(\alpha) \neq 0$.

Let $x_n \in U_\varepsilon(\alpha)$ and

$$e_n := x_n - \alpha, \quad \widetilde{e}_n := y_n - \alpha, \quad \hat{e}_n := z_n - \alpha.$$

Using (1.4) it is easy to get the following formula

$$\begin{aligned}\frac{f(x_n)}{f'(x_n)} &= e_n - c_2 e_n^2 + 2(c_2^2 - c_3)e_n^3 - (4c_2^3 - 7c_3c_2 + 3c_4)e_n^4 \\ &+ (8c_2^4 - 20c_3c_2^2 + 10c_4c_2 + 6c_3^2 - 4c_5)e_n^5 \\ &- [16c_2^5 - 52c_3c_2^3 + 28c_4c_2^2 + (33c_3^2 - 13c_5)c_2 - 17c_3c_4 + 5c_6]e_n^6 \\ &+ O(e_n^7). \end{aligned} \tag{2.1}$$

This formula is an inverse of the well-known Schröder formula (cf. [2, pp. 352–354]).

Therefore, in the case of the Newton method

$$\Phi_N(x_n) = x_n - \frac{f(x_n)}{f'(x_n)} \tag{2.2}$$

we have

$$\begin{aligned}\widetilde{e}_n &= \Phi_N(x_n) - \alpha \\ &= c_2 e_n^2 - 2(c_2^2 - c_3)e_n^3 + (4c_2^3 - 7c_3c_2 + 3c_4)e_n^4 \\ &- (8c_2^4 - 20c_3c_2^2 + 10c_4c_2 + 6c_3^2 - 4c_5)e_n^5 \\ &+ [16c_2^5 - 52c_3c_2^3 + 28c_4c_2^2 + (33c_3^2 - 13c_5)c_2 - 17c_3c_4 + 5c_6]e_n^6 \\ &+ O(e_n^7). \end{aligned} \tag{2.3}$$

Also, we need the corresponding expression for

$$\widetilde{C}_2(y_n) := \frac{f''(y_n)}{2f'(y_n)} = \frac{1}{2}\,\frac{f''(\alpha) + \dfrac{f'''(\alpha)}{1!}\,\widetilde{e}_n + \dfrac{f^{iv}(\alpha)}{2!}\,\widetilde{e}_n^2 + \cdots}{f'(\alpha) + \dfrac{f''(\alpha)}{1!}\,\widetilde{e}_n + \dfrac{f'''(\alpha)}{2!}\,\widetilde{e}_n^2 + \cdots},$$

i.e.,

$$\widetilde{C}_2(y_n) = \frac{1}{2}\cdot\frac{1\cdot 2\,c_2 + 2\cdot 3\,c_3\,\widetilde{e}_n + 3\cdot 4\,c_4\,\widetilde{e}_n^2 + \cdots}{1 + 2c_2\,\widetilde{e}_n + 3c_3\,\widetilde{e}_n^2 + \cdots},$$

where c_k are defined by (1.4). It gives

$$\widetilde{C}_2(y_n) = A_0 + A_1\widetilde{e}_n + A_2\widetilde{e}_n^2 + A_3\widetilde{e}_n^3 + \cdots , \tag{2.4}$$

where

$$\begin{aligned}
A_0 &= c_2, \quad A_1 = 3c_3 - 2c_2^2, \quad A_2 = 4c_2^3 - 9c_3c_2 + 6c_4,\\
A_3 &= -8c_2^4 + 24c_3c_2^2 - 16c_4c_2 - 9c_3^2 + 10c_5,\\
A_4 &= 16c_2^5 - 60c_3c_2^3 + 40c_4c_2^2 + 5(9c_3^2 - 5c_5)c_2 + 15(c_6 - 2c_3c_4),\\
A_5 &= -32c_2^6 + 144c_3c_2^4 - 96c_4c_2^3 + (60c_5 - 162c_3^2)c_2^2 + 36(4c_3c_4 - c_6)c_2\\
&\quad +3(9c_3^3 - 15c_5c_3 - 8c_4^2 + 7c_7),\\
A_6 &= 64c_2^7 - 336c_3c_2^5 + 224c_4c_2^4 + 28(18c_3^2 - 5c_5)c_2^3 - 84(6c_3c_4 - c_6)c_2^2\\
&\quad -7(27c_3^3 - 30c_5c_3 - 16c_4^2 + 7c_7)c_2 + 7(18c_4c_3^2 - 9c_6c_3 - 10c_4c_5 + 4c_8),
\end{aligned}$$

etc.

Now, for the Halley method

$$\Phi_H(y_n) = y_n - \frac{f(y_n)/f'(y_n)}{1 - \widetilde{C}_2(y_n)(f(y_n)/f'(y_n))} \tag{2.5}$$

we have

$$\hat{e}_n = \Phi_H(y_n) - \alpha = \widetilde{e}_n - g_n\Big(1 + \widetilde{C}_2(y_n)g_n + [\widetilde{C}_2(y_n)g_n]^2 + \cdots\Big), \quad g_n = \frac{f(y_n)}{f'(y_n)}.$$

Using (2.1), in this case, we get

$$\begin{aligned}
\hat{e}_n &= (c_2^2 - c_3)\widetilde{e}_n^3 - 3(c_2^3 - 2c_3c_2 + c_4)\widetilde{e}_n^4 + 6(c_2^4 - 3c_3c_2^2 + 2c_4c_2 + c_3^2 - c_5)\widetilde{e}_n^5\\
&\quad -[9c_2^5 - 37c_3c_2^3 + 29c_4c_2^2 + 4(7c_3^2 - 5c_5)c_2 - 19c_3c_4 + 10c_6]\widetilde{e}_n^6 + O(\widetilde{e}_n^7).
\end{aligned} \tag{2.6}$$

In our analysis we also need an expansion of $f(z_n)/f'(y_n)$ in terms of $\widetilde{e}_n$ ($= y_n - \alpha$), where $z_n - \alpha = \hat{e}_n$ is given by (2.6). Thus, we have

$$v_n = \frac{f(z_n)}{f'(y_n)} = \frac{\hat{e}_n + c_2\,\hat{e}_n^2 + c_3\,\hat{e}_n^3 + \cdots}{1 + 2c_2\,\widetilde{e}_n + 3c_3\,\widetilde{e}_n^2 + \cdots},$$

i.e.,

$$\begin{aligned} v_n &= (c_2^2 - c_3)\widetilde{e}_n^3 - (5c_2^3 - 8c_3c_2 + 3c_4)\widetilde{e}_n^4 \\ &\quad + (16c_2^4 - 37c_3c_2^2 + 18c_4c_2 + 9c_3^2 - 6c_5)\widetilde{e}_n^5 \\ &\quad - (40c_2^5 - 124c_3c_2^3 + 69c_4c_2^2 - (32c_5 - 69c_3^2)c_2 - 32c_3c_4 + 10c_6)\widetilde{e}_n^6 \\ &\quad + O(\widetilde{e}_n^7). \end{aligned} \tag{2.7}$$

In the case when $y_n = \Phi_N(x_n)$ and

$$z_n = y_n - \frac{(x_n - y_n)f(y_n)}{f(x_n) - 2f(y_n)}, \tag{2.8}$$

we are interested in

$$u_n = \frac{f(x_n)}{f(y_n)}, \quad t_n = \frac{f(x_n)}{f'(z_n)}, \quad s_n = \frac{f'(x_n)}{f'(z_n)}, \tag{2.9}$$

i.e.,

$$u_n = \frac{e_n + c_2\, e_n^2 + c_3\, e_n^3 + \cdots}{\widetilde{e}_n + c_2\, \widetilde{e}_n^2 + c_3\, \widetilde{e}_n^3 + \cdots}, \tag{2.10}$$

$$t_n = \frac{e_n + c_2\, e_n^2 + c_3\, e_n^3 + \cdots}{1 + 2c_2\, \bar{e}_n + 3c_3\, \bar{e}_n^2 + \cdots}, \quad \text{and} \quad s_n = \frac{1 + 2c_2\, e_n + 3c_3\, e_n^2 + \cdots}{1 + 2c_2\, \bar{e}_n + 3c_3\, \bar{e}_n^2 + \cdots},$$

where $e_n = x_n - \alpha$, $\widetilde{e}_n = y_n - \alpha$, and $\bar{e}_n = z_n - \alpha$.

Here, $\bar{e}_n = \widetilde{e}_n - (e_n - \widetilde{e}_n)/(u_n - 2)$. According to (2.3) and (2.10) we get

$$\begin{aligned} \bar{e}_n &= c_2(c_2^2 - c_3)e_n^4 - 2(2c_2^4 - 4c_3c_2^2 + c_4c_2 + c_3^2)e_n^5 \\ &\quad + [10c_2^5 - 30c_3c_2^3 + 12c_4c_2^2 + 3c_2(6c_3^2 - c_5) - 7c_3c_4]e_n^6 \\ &\quad + O(e_n^7). \end{aligned} \tag{2.11}$$

For t_n and s_n we obtain

$$\begin{aligned} t_n &= e_n + c_2e_n^2 + c_3e_n^3 + c_4e_n^4 - (2c_2^4 - 2c_3c_2^2 - c_5)e_n^5 \\ &\quad + (6c_2^5 - 14c_3c_2^3 + 4c_4c_2^2 + 4c_3^2c_2 + c_6)e_n^6 + O(e_n^7) \end{aligned} \tag{2.12}$$

and

$$\begin{aligned} s_n \; = \; & 1 + 2c_2 e_n + 3c_3 e_n^2 + 4c_4 e_n^3 - (2c_2^4 - 2c_3 c_2^2 - 5c_5) e_n^4 \\ & + (4c_2^5 - 12c_3 c_2^3 + 4c_4 c_2^2 + 4c_3^2 c_2 + 6c_6) e_n^5 \\ & - [4c_2^6 - 22c_3 c_2^4 + 16c_4 c_2^3 - (6c_5 - 22c_3^2) c_2^2 - 14c_3 c_4 c_2 - 7c_7] e_n^6 \\ & + O(e_n^7), \end{aligned} \tag{2.13}$$

respectively.

3. **Main results**

We consider now the third-step iterative formula given by (2.2), (2.5), and (1.5), i.e.,

$$y_n = \Phi_N(x_n), \quad z_n = \Phi_H(y_n), \quad e_{n+1} = S(y_n, z_n), \quad n = 0, 1, \ldots\,, \tag{3.1}$$

for finding a simple zero $x = \alpha$ of the equation (1.1).

Theorem 3.1. *For a sufficiently differentiable function f in $U_\varepsilon(\alpha)$ and x_0 sufficiently close to α, the third-step method* (3.1) *has tenth order of convergence, i.e.,*

$$e_{n+1} = 3c_2^5 c_3 (c_3 - c_2^2) e_n^{10} + 30 c_2^4 (c_2^2 - c_3)^2 c_3 e_n^{11} + O(e_n^{12}) \tag{3.2}$$

where $e_n = x_n - \alpha$ and c_k are given in (1.4).

Proof. According to (3.1) (and (1.5)) we have

$$e_{n+1} = x_{n+1} - \alpha = S(y_n, z_n) - \alpha = \hat{e}_n - \frac{f(z_n)/f'(y_n)}{1 + 2(\hat{e}_n - \widetilde{e}_n)\widetilde{C}_2(y_n)}\,,$$

where $\widetilde{e}_n = y_n - \alpha$, $\hat{e}_n = z_n - \alpha$, and $\widetilde{C}_2(y_n) = f''(y_n)/(2f'(y_n))$. Replacing $\widetilde{C}_2(y_n)$ and $v_n = f(z_n)/f'(y_n)$ by the corresponding expressions (2.4) and (2.7), we obtain

$$e_{n+1} = 3c_3(c_3 - c_2^2)\widetilde{e}_n^5 + (c_2^5 + 7c_3 c_2^3 - 8c_4 c_2^2 - 17c_3^2 c_2 + 17c_3 c_4)\widetilde{e}_n^6 + O(\widetilde{e}_n^7).$$

Finally, using (2.3) we get (3.2). □

In [1] the authors also considered the following three-step method

$$\left.\begin{aligned} y_n &= x_n - \frac{f(x_n)}{f'(x_n)}, \\ z_n &= y_n - \frac{(x_n - y_n)f(y_n)}{f(x_n) - 2f(y_n)}, \\ x_{n+1} &= z_n - \frac{f(z_n)f'(z_n)}{f'(z_n)^2 - \lambda\, f(z_n)\left\{\dfrac{2(f(z_n) - f(x_n))}{(z_n - x_n)^2} - \dfrac{2f'(x_n)}{z_n - x_n}\right\}}, \end{aligned}\right\} \tag{3.3}$$

with five function evaluations per iteration: $f(x_n)$, $f(y_n)$, $f(z_n)$, $f'(x_n)$, and $f'(z_n)$. Their Theorem 3 states that this method has seventh order of convergence for any value of λ. However, the order of convergence is bigger than seven. Namely, we have the following result:

Theorem 3.2. *For a sufficiently differentiable function f in $U_\varepsilon(\alpha)$ and x_0 sufficiently close to α, the third-step method* (3.3) *has eighth order of convergence for any $\lambda \neq 1/2$, except for $\lambda = 1/2$ when the convergence is of the order nine. Then,*

$$\begin{aligned} e_{n+1} &= -2c_3c_2^2(c_2^2 - c_3)^2 e_n^9 \\ &\quad + c_2(c_2^2 - c_3)(16c_3c_2^4 - 3c_4c_2^3 - 32c_3^2c_2^2 + 11c_2c_3c_4 + 8c_3^3)e_n^{10} \\ &\quad + O(e_n^{11}), \end{aligned} \tag{3.4}$$

where $e_n = x_n - \alpha$ and c_k are given in (1.4).

Proof. Using the expansion (2.1) for the Newton correction $f(x_n)/f'(x_n) =: h(e_n)$, we have $f(z_n)/f'(z_n) = h(\bar{e}_n)$, where $\bar{e}_n$ is given by (2.11). According to (2.9), for the third formula in (3.3) we get

$$e_{n+1} = \bar{e}_n - \frac{h(\bar{e}_n)}{1 - 2\lambda\left\{\dfrac{h(\bar{e}_n) - t_n}{(\bar{e}_n - e_n)^2} - \dfrac{s_n}{\bar{e}_n - e_n}\right\}}, \tag{3.5}$$

where the expansions for t_n and s_n are given by (2.12) and (2.13), respectively. This gives

$$\begin{aligned} e_{n+1} &= (1 - 2\lambda)c_2^3(c_2^2 - c_3)^2 e_n^8 + 4c_2^2(c_2^2 - c_3)\big[2(2\lambda - 1)c_2^4 + (4 - 9\lambda)c_3c_2^2 \\ &\qquad + (2\lambda - 1)c_4c_2 + (3\lambda - 1)c_3^2\big]e_n^9 + \cdots \end{aligned}$$

For $\lambda = 1/2$ it reduces to (3.4). $\square$

Thus, the computational efficiency of the method (3.3), for $\lambda = 1/2$, is EFF= $9^{1/5} \approx 1.55185$. With the same function evaluations we can get a slightly simpler method of order nine with the same efficiency.

Theorem 3.3. *For a sufficiently differentiable function f in $U_\varepsilon(\alpha)$ and x_0 sufficiently close to α, the third-step method*

$$\left.\begin{aligned} y_n &= x_n - \frac{f(x_n)}{f'(x_n)}, \\ z_n &= y_n - \frac{(x_n - y_n)f(y_n)}{f(x_n) - 2f(y_n)}, \\ x_{n+1} &= z_n - \frac{f(z_n)f'(z_n)}{f'(z_n)^2 - \dfrac{1}{2}\, f(z_n)\dfrac{f'(z_n) - f'(x_n)}{z_n - x_n}}, \end{aligned}\right\} \tag{3.6}$$

has ninth order of convergence, i.e.,

$$\begin{aligned} e_{n+1} &= -\frac{3}{2}c_3c_2^2(c_2^2 - c_3)^2 e_n^9 \\ &\quad + 2c_2(c_2^2 - c_3)(6c_2^4c_3 - 12c_2^2c_3^2 + 3c_3^3 - c_2^3c_4 + 4c_2c_3c_4)e_n^{10} \\ &\quad + O(e_n^{11}), \end{aligned} \tag{3.7}$$

where $e_n = x_n - \alpha$ and c_k are given in (1.4).

Proof. Similarly as in the proof of the previous theorem, we have now

$$e_{n+1} = \bar{e}_n - \frac{h(\bar{e}_n)}{1 - \dfrac{1}{2}\, h(\bar{e}_n)\dfrac{1 - s_n}{\bar{e}_n - e_n}}$$

instead of (3.5). This gives (3.7). $\square$

The number of function evaluations in (3.6) can be reduced to four if we take an approximation of $f'(z_n)$ in the form

$$f'(z_n) \approx \tilde{f}'(z_n) = p_n f(x_n) + q_n f(y_n) + r_n f(z_n) + w_n f'(x_n),$$

obtained by the Hermite interpolation (cf. [3, pp. 51–58]), where

$$\begin{aligned} p_n &= \frac{(y_n - z_n)(z_n + 2y_n - 3x_n)}{(x_n - y_n)^2(x_n - z_n)}, \quad q_n = \frac{(x_n - z_n)^2}{(x_n - y_n)^2(y_n - z_n)}, \\ r_n &= \frac{3z_n - 2y_n - x_n}{(x_n - z_n)(y_n - z_n)}, \qquad\qquad w_n = \frac{y_n - z_n}{x_n - y_n}. \end{aligned}$$

For a such modified three-step method, in notation (3.6^M), the following result holds:

Theorem 3.4. *For a sufficiently differentiable function f in $U_\varepsilon(\alpha)$ and x_0 sufficiently close to α, the third-step method (3.6^M) has eight order of convergence, i.e.,*

$$\begin{aligned} e_{n+1} &= (c_2^2 - c_3)c_2^2 c_4 e_n^8 - \frac{1}{2}\Big[3c_2^5(c_2c_3 + 4c_4) - 2c_2^4(3c_3^2 + 2c_5) \\ &\quad + c_2^2(3c_3^3 + 4c_3c_5 + 4c_4^2) + 8c_2c_3c_4(c_3 - 3c_2^2)\Big]e_n^9 + O(e_n^{10}), \end{aligned}$$

where $e_n = x_n - \alpha$ and c_k are given in (1.4).

The corresponding computational efficiency is now much better, EFF$=$ $8^{1/4} \approx 1.68179$.

Example 3.1. Consider the equation

$$f(x) = xe^{x^2} - \sin^2 x + 3\cos x + 5 = 0,$$

with a simple zero

$$\alpha = -1.2076478271309189270094167583560840977602358189495388152059 2\ldots$$

In order to show the behavior of three-step methods (1.3), (3.1), (3.3), (3.6) and (3.6^M) we need a multi-precision arithmetics. Starting with $x_0 = -1$, we use Mathematica with 10000 significant digits. The errors $e_n = x_n - \alpha$ are given in Table 3.1. Numbers in parentheses indicate decimal exponents. Besides the convergence order (r) we give also the corresponding computational efficiency (EFF).

TABLE 3.1. The errors $e_n = x_n - \alpha$, $n = 0, 1, 2, 3, 4$, in three-step methods

method	(1.3)	(3.1)	(3.3)	(3.6)	(3.6^M)
order	$r = 8$	$r = 10$	$r = 9$	$r = 9$	$r = 8$
EFF	1.41421	1.46780	1.55185	1.55185	1.68179
$n = 0$	$2.08(-1)$	$2.08(-1)$	$2.08(-1)$	$2.08(-1)$	$2.08(-1)$
$n = 1$	$-1.05(-5)$	$3.70(-6)$	$-1.19(-7)$	$-9.24(-8)$	$-2.25(-6)$
$n = 2$	$-2.87(-40)$	$5.66(-54)$	$2.74(-63)$	$2.15(-64)$	$-8.57(-46)$
$n = 3$	$-8.87(-317)$	$3.93(-532)$	$-5.05(-564)$	$-4.26(-574)$	$-3.77(-361)$
$n = 4$	$-7.48(-2529)$	$1.02(-5313)$	$1.26(-5070)$	$2.204(-5161)$	$-5.32(-2884)$

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