Optimal eighth-order simple root-finders free from derivative

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Abstract: The calculation of derivatives of a function mostly takes up a great deal of time and even in some cases, such as the existing problems in engineering and optimization, is impossible to be evaluated directly. Accordingly, an accurate derivative-free class of three-step methods is suggested for solving $f(x) = 0$. The proposed three-step technique comprises four evaluations of the function per iteration. The analytical proof of the main contribution is given. And finally, the accuracy of the developed techniques is tested numerically by solving numerical examples.

Keywords: Kung-Traub Hypothesis, fourth-order, eighth-order; iterative methods, efficiency index.

1. Prerequisites

Approximating the solution of $f(x) = 0$ is a classical problem. A practical tool to study the solution of such nonlinear equations is the use of iterative processes which are derivative-free [2] or derivative-involved [1] in essence. Beginning from an initial guess x_0 successive estimations (until some predetermined convergence criterion is satisfied) x_n are computed for any $n = 1, 2, \cdots$ with the help of a certain iteration function $\varphi: X \to X$ as follows: $x_{n+1} = \varphi(x_n)$.

Solving such equations by these iterative processes has so many applications. In engineering and optimization problems, we use the iterative processes to find the critical points of the given function. Newton's method is perhaps the best known method for finding the root of a nonlinear equation or for minimizing a general nonlinear function. To illustrate more, Newton's method can be used to find stationary points (such as local maxima and minima) of $f(x)$, as such points are the roots of the derivative function $f'(x) = 0$.

This method, also known as the Newton-Raphson method, can be traced back to Isaac Newton (1669) and Joseph Raphson (1690). Both Newton and Raphson appear to have derived essentially the same method independently. Newton based his derivation on a linearization of a higher-order polynomial and he showed how the method could be used to solve a particular cubic equation. Raphson's scheme on the other hand, more closely resembles what we now know as Newton's method. In its basic form, Newton's method is easy to implement and requires only the ability to compute a function and its first derivative (and second derivatives in optimization problems).

In practice, however, Newton's method needs to be modified to make it more robust and computationally efficient. With these modifications; Newton's method (or one of its many variations) is arguably the method of choice for a wide variety of problems. Mentioning that the geometric interpretation of the Newton's method in optimization problems is that at each iteration one approximates $f(x)$ by a quadratic function around x_n, and then takes a step towards the maximum/minimum of that quadratic function. Note that if $f(x)$ be a quadratic function, then the exact extremum is attained in one step.

As an another application-oriented example of iterations in solving nonlinear equations we can mention, if a is a number for which $f(a)$ vanishes mod p, it is often possible to lift a to a p-adic zero of $f(x)$. The standard technique for doing this is the p-adic analog of Newton's scheme, occasionally called Hensel's lemma. In numerical computation, one often replaces Newton's method by other schemes, chosen to avoid computation of derivatives to converge in very few iterations, or have other desirable properties, however see [3] for further information on the application of iterative root-solvers in Number Theory. For more application-oriented topics of root solvers in engineering problems, refer to the first chapter of [7].

In 1974, Kung and Traub [4] conjectured on the optimality of multi-point iterative schemes as comes next. An iterative method without memory for solving single variable nonlinear equation $f(x) = 0$, with $n + 1$ evaluations per iteration reaches to the maximum order of convergence 2^n and the optimal efficiency index $2^{n/(n+1)}$. Consequently, the efficiency of a p-th order method could be given by $p^{1/(n+1)}$ where $n+1$ is the whole number of evaluations per iteration.

Optimization problems defined by functions for which derivatives are unavailable or available at a prohibitive cost are emerging more and more frequently in computational science and engineering. Due to these, nowadays algorithms in which no derivative evaluation is needed are more in concentration by many researchers.

Accordingly, due to the vast need of derivative-free methods which are so useful when the calculations of derivatives of the given functions are impossible or difficult, in this study; we focus on optimal derivative-free methods without memory.

The paper unfolds the contents as follows. According to the conjecture of Kung-Traub (1974) a new class of derivative-free methods containing four evaluations per iteration to reach the convergence order eight is given in Section 2 as the central contribution. This section is followed by Section 3 wherein numerical reports and discussion on the comparisons with other famous derivative-free methods are presented. The conclusions have finally been drawn in Section 4.

2. Derivation of the new class

Let us consider the two-step cycle of Petkovic et al. [6] in which we have the Steffensen's method [8] in the first step and a modification of Newton's method in the second step as follows ($\beta \in \mathbb{R}-\{0\}$)

$$\begin{cases} y_n = x_n - \dfrac{\beta f(x_n)^2}{f(x_n+\beta f(x_n)) - f(x_n)}, \\ x_{n+1} = y_n \\ -\dfrac{\beta f(x_n) f(y_n)}{f(x_n+\beta f(x_n)) - f(x_n)} \left\{ \dfrac{1+\dfrac{f(y_n)}{f(x_n)}}{1-\dfrac{f(y_n)}{f(x_n+\beta f(x_n))}} \right\}, \end{cases} \tag{1}$$

with three evaluations of the function $f(x_n)$, $f(x_n+\beta f(x_n)), f(y_n)$ per iteration. For simplicity, we assume that $f(x_n+\beta f(x_n)) = f(w_n)$, that is $x_n+\beta f(x_n) = w_n$. Now by performing a new Newton's iteration after the second step as comes next we try to build a higher order class:

$$x_{n+1} = z_n - \frac{f(z_n)}{f'(z_n)}. \tag{2}$$

At this time, the main challenge is to approximate $f'(z_n)$ as efficiently as possible. Clearly, $f'(z_n)$ should be annihilated such as the order of convergence eight does not decrease. Thus, first we approximate it by an approximation through using the past three known data, i.e. $f(x_n)$, $f(y_n)$, $f(z_n)$. That is by taking into account of the following approximation function for $f(t)$ in the domain D as follows

$$f(t) \approx p(t) = a_0 + a_1(t-x_n) + a_2(t-x_n)^2, \tag{3}$$

which its first derivative has the form $p'(t) = a_1 + 2a_2(t-x_n)$. Obviously, the unknown three parameters a_0, a_1 and a_2 will be obtained by substituting of the known values in (3) as follows

$$\begin{cases} a_0 = f(x_n), \\ a_2 = \dfrac{f[y_n,x_n] - f[z_n,x_n]}{y_n - z_n} = f[y_n,x_n,z_n], \\ a_1 = f[z_n,x_n] - (z_n - x_n)a_2. \end{cases} \tag{4}$$

Hence, we have a more simplified three-step method without using any derivative in what follows by using weight function approach in the last step to keep the order at the highest level

$$\begin{cases} y_n = x_n - \dfrac{f(x_n)}{f[x_n,w_n]}, \\ z_n = y_n - \dfrac{f(y_n)}{f[x_n,w_n]} \left\{ \dfrac{1+\dfrac{f(y_n)}{f(x_n)}}{1-\dfrac{f(y_n)}{f(w_n)}} \right\}, \\ x_{n+1} = z_n - \dfrac{f(z_n)}{f[z_n,x_n] + f[y_n,x_n,z_n](z_n - x_n)} \\ \quad \times \{G(\varphi) + L(\pi) + P(\rho) + H(\tau) + K(\mu)\}, \end{cases} \tag{5}$$

wherein $w_n = x_n + \beta f(x_n)$, $G(\varphi)$, $L(\pi)$, $P(\rho)$, $H(\tau)$ and $K(\mu)$ are five real valued weight functions with $\varphi = \frac{f(y)}{f(w)}$, $\pi = \frac{f(y)}{f(x)}$, $\rho = \frac{f(z)}{f(x)}$, $\tau = \frac{f(z)}{f(w)}$ and $\mu = \frac{f(z)}{f(y)}$ (without the index n). Theorem 1 indicates that under what conditions the order of (5) is eight and hence, it is an optimal derivative-free class of without memory methods.

Theorem 1. *Assume f be a sufficiently continuous real function in the domain D. Then the sequence generated by (5) converges to the simple root $\alpha \in D$ with eighth-order convergence and it satisfies the follow-up error equation*

$$e_{n+1}=-\frac{1}{24c_1^7}(c_2(1+c_1\beta)^2(-c_1c_3+c_2^2(3+c_1\beta))(-24c_1^2c_2c_4(1+c_1\beta)^2+12c_1^2c_3^2(1+c_1\beta)^2K''(0)-24c_1c_3(c_2+c_1c_2\beta)^2\left(-2+(3+c_1\beta)K''(0)\right)+c_2^4(72+108K''(0)+G^{(4)}(0)+L^{(4)}(0)+c_1\beta(-24(-2+c_1\beta(2+c_1\beta))+12(4+c_1\beta)(6+c_1\beta(4+c_1\beta))K''(0)+(2+c_1\beta)\big(2+c_1\beta(2+c_1\beta)\big)L^{(4)}(0))))e_n^8+O(e_n^9), \quad (6)$$

when

$$\begin{cases} G(0)=1, G'(0)=G''(0)=0, G'''(0)=-18-24\beta f[x_n,w_n]-6(\beta f[x_n,w_n])^2, \left|G^{(4)}(0)\right|<\infty, \\ L(0)=L'(0)=L''(0)=L'''(0)=0, \left|L^{(4)}(0)\right|<\infty, \\ P(0)=P'(0)=0, \\ H(0)=0, H'(0)=1, \\ K(0)=K'(0)=0, \left|K''(0)\right|<\infty. \end{cases} \quad (7)$$

Proof. To prove that the order of (5) will arrive at eight by considering (7), we first consider $c_j=\frac{f^{(j)}(\alpha)}{j!}$, $j\ge 1$, and $e_n=x_n-\alpha$; now we should expand any terms of (2) around the simple root α in the *n*th iterate. Thus, we write

$$f(x_n)=c_1e_n+c_2e_n^2+c_3e_n^3+c_4e_n^4+c_5e_n^5+\cdots+O(e_n^9), \quad (8)$$

Accordingly, we attain

$$x_n-\frac{f(x_n)}{f[x_n,w_n]}=\alpha+\left(\beta+\frac{1}{c_1}\right)c_2e_n^2+\frac{\left(c_1c_3(1+c_1\beta)(2+c_1\beta)-c_2^2\big(2+c_1\beta(2+c_1\beta)\big)\right)}{c_1^2}e_n^3+\cdots+O(e_n^9). \quad (9)$$

Now, we should expand $f(y_n)$ around the simple root by using (9). We have

$$y_n-\frac{f(y_n)}{f[x_n,w_n]}\left\{\frac{1+f(y_n)/f(x_n)}{1-f(y_n)/f(w_n)}\right\}=\alpha-\frac{c_2(1+c_1\beta)^2\left(-c_1c_3+c_2^2(3+c_1\beta)\right)}{c_1^3}e_n^4-\frac{1}{c_1^4}(1+c_1\beta)(c_1^2c_3^2(1+c_1\beta)(2+c_1\beta)+c_1^2c_2c_4(1+c_1\beta)(2+c_1\beta)+c_2^4(3+c_1\beta)(6+c_1\beta(7+3c_1\beta))-c_1c_2^2c_3(20+c_1\beta(34+c_1\beta(19+3c_1\beta))))e_n^5+\cdots+O(e_n^9). \quad (10)$$

Using (9), (10), we attain

$$f(z_n)=\frac{c_2(1+c_1\beta)^2\left(-c_1c_3+c_2^2(3+c_1\beta)\right)}{c_1^2}e_n^4-\frac{1}{c_1^3}(1+c_1\beta)(c_1^2c_3^2(1+c_1\beta)(2+c_1\beta)+c_1^2c_2c_4(1+c_1\beta)(2+c_1\beta)+c_2^4(3+c_1\beta)(6+c_1\beta(7+3c_1\beta))-c_1c_2^2c_3(20+c_1\beta(34+c_1\beta(19+3c_1\beta))))e_n^5+\cdots+O(e_n^9). \quad (11)$$

Additionally, we attain

$$f[z_n,x_n]+f[y_n,x_n,z_n](z_n-x_n)=c_1-\frac{c_2c_3(1+c_1\beta)}{c_1}e_n^3+\cdots+O(e_n^9). \quad (12)$$

Considering (10)-(12) results in the following error in the third step

$$\frac{f(z_n)}{f[z_n,x_n]+f[y_n,x_n,z_n](z_n-x_n)}\times\{G(\varphi)+L(\pi)+P(\rho)+H(\tau)+K(\mu)\}=\frac{c_2(1+c_1\beta)^2\left(-c_1c_3+c_2^2(3+c_1\beta)\right)}{c_1^3}e_n^4+\cdots+O(e_n^9). \quad (13)$$

And finally by using (13) and again (7), we attain

$$e_{n+1}=x_{n+1}-\alpha=-\frac{1}{24c_1^7}(c_2(1+c_1\beta)^2(-c_1c_3+c_2^2(3+c_1\beta))(-24c_1^2c_2c_4(1+c_1\beta)^2+12c_1^2c_3^2(1+c_1\beta)^2K''(0)-24c_1c_3(c_2+c_1c_2\beta)^2\left(-2+(3+c_1\beta)K''(0)\right)+c_2^4(72+108K''(0)+G^{(4)}(0)+L^{(4)}(0)+c_1\beta(-24(-2+c_1\beta(2+c_1\beta))+12(4+c_1\beta)(6+c_1\beta(4+c_1\beta))K''(0)+(2+c_1\beta)\big(2+c_1\beta(2+c_1\beta)\big)L^{(4)}(0))))e_n^8+O(e_n^9). \quad (14)$$

This shows that any method from our class (5)-(7) will end up in eighth order of convergence using only four pieces of information per iteration. In consequence, our class of derivative-free methods satisfies the Kung-Traub conjecture for building optimal multi-point methods without memory. This ends the proof. ■

Some *typical* formats of the weight functions $G(\varphi), L(\pi), P(\rho), H(\tau)$ and $K(\mu)$ which satisfy the conditions of (7) are displayed in Table 1.

Table 1: Some forms of the weight functions $G(\varphi), L(\pi), P(\rho), H(\tau)$ and $K(\mu)$, $\theta \in \mathbb{R}$

Weight Function	Form 1	Form 2
$G(\varphi)$	$1-(3+4\beta f[x_n,w_n]+\beta(f[x_n,w_n])^2)\varphi^3$	$1-(3+4\beta f[x_n,w_n]+\beta(f[x_n,w_n])^2)\varphi^3+\theta\varphi^4$
$L(\pi)$	π^4	$\pi^4+\theta\pi^5$
$P(\rho)$	$\rho^2+\theta\rho^3$	$\frac{\rho^2}{1-\rho}$
$H(\tau)$	$\tau+\tau^2$	$\frac{\tau}{1-\tau}$
$K(\mu)$	$\mu^2+\theta\mu^3$	$\frac{\mu^2}{1-\mu}$

As a simple but efficient case of our suggested class (5)-(7), we can provide the following three-step optimal eighth-order method in which no derivative evaluation per step is needed to proceed

$$\begin{cases} y_n = x_n - \dfrac{f(x_n)}{f[x_n,w_n]}, \\ z_n = y_n - \dfrac{f(y_n)}{f[x_n,w_n]}\left\{\dfrac{1+\frac{f(y_n)}{f(x_n)}}{1-\frac{f(y_n)}{f(w_n)}}\right\}, \\ x_{n+1} = z_n - \dfrac{f(z_n)}{f[z_n,x_n]+f[y_n,x_n,z_n](z_n-x_n)}\{W_1\}, \end{cases} \tag{15}$$

with the following weight function

$$W_1 = 1-(3+4f[x_n,w_n]+(f[x_n,w_n])^2)\left(\frac{f(y_n)}{f(w_n)}\right)^3 + \left(\frac{f(y_n)}{f(x_n)}\right)^4 + \left(\frac{f(z_n)}{f(x_n)}\right)^2 + \frac{f(z_n)}{f(w_n)} + \left(\frac{f(z_n)}{f(y_n)}\right)^2, \tag{16}$$

where its error equation is as comes next

$$e_{n+1} = -\left(\frac{1}{c_1^7}\right)((1+c_1)^3 c_2((3+c_1)c_2^2 - c_1c_3)((13+c_1(17+c_1(9+2c_1)))c_2^4 - 2c_1(1+c_1)(2+c_1)c_2^2c_3 + c_1^2(1+c_1)c_3^2 - c_1^2(1+c_1)c_2c_4))e_n^8 + O(e_n^9). \tag{17}$$

Another very efficient three-step without memory iteration in which no derivative evaluation is needed per full cycle can be written in the following structure

$$\begin{cases} y_n = x_n - \dfrac{f(x_n)}{f[x_n,w_n]}, \\ z_n = y_n - \dfrac{f(y_n)}{f[x_n,w_n]}\left\{\dfrac{1+\frac{f(y_n)}{f(x_n)}}{1-\frac{f(y_n)}{f(w_n)}}\right\}, \\ x_{n+1} = z_n - \dfrac{f(z_n)}{f[z_n,x_n]+f[y_n,x_n,z_n](z_n-x_n)}\{W_2\}, \end{cases} \tag{18}$$

with the following weight function

$$W_2 = 1-(3+4f[x_n,w_n]+(f[x_n,w_n])^2)\left(\frac{f(y_n)}{f(w_n)}\right)^3 + \left(\frac{f(y_n)}{f(x_n)}\right)^5 + \left(\frac{f(z_n)}{f(x_n)}\right)^2 + \frac{f(z_n)}{f(w_n)} + \left(\frac{f(z_n)}{f(y_n)}\right)^3, \tag{19}$$

where its simple error equation is as follows

$$e_{n+1} = \left(\frac{1}{c_1^7}\right) \times ((1+c_1)^3 c_2^2\left((3+c_1)c_2^2 - c_1c_3\right) \times \left((-3+c_1+c_1^2)c_2^3 - 2c_1(1+c_1)c_2c_3 + c_1^2(1+c_1)c_4\right))e_n^8 + O(e_n^9). \tag{20}$$

In terms of computational point of view, each method from our proposed three-step class (5)-(7) of derivative-free methods include four evaluations to reach the convergence order 8, which implies $8^{1/4} \approx 1.682$ as its optimal efficiency index.

3. Numerical implementations

The objective of this section is to compare the most important existing optimal derivative-free methods with the novel methods under a fair circumstance. Liu et al. [5] gave an optimal quartically derivative-free technique consisting three evaluations of the function per iteration. Kung and Traub in their pioneer paper [4] provided a family of three-step derivative-free family of methods ($\beta \in \mathbb{R} - \{0\}$) by using the Inverse Interpolation.

To test the effectiveness of the new methods (15) and (18) from our classes of derivative-free methods, we have provided the test nonlinear functions in Table 2. The simple roots of each are listed in front of the nonlinear test function up to 15 decimal places when their simple roots are not integer.

For comparisons in this section, we have chosen the method of Steffensen (**SM2**) [8], the method of Liu et al. (**LM4**), the optimal Kung-Traub family with $\beta = 1$ (**KT8**).

Table 2: The examples considered in this study

Test Functions	Zeros
$f_1(x) = (\sin x)^2 + x$	$\alpha_1 = 0$
$f_2(x) = (1 + x^3)\cos\left(\frac{\pi x}{2}\right) + \sqrt{1 - x^2} - \frac{2(9\sqrt{2} + 7\sqrt{3})}{27}$	$\alpha_2 = 1/3$
$f_3(x) = (\sin x)^2 - x^2 + 1$	$\alpha_3 \approx 1.404491648215341$
$f_4(x) = e^{-x} + \sin(x) - 1$	$\alpha_4 \approx 2.076831274533113$
$f_5(x) = xe^{-x} - 0.1$	$\alpha_5 \approx 0.111832559158963$
$f_6(x) = \sqrt{x^4 + 8}\sin\left(\frac{\pi}{x^2 + 2}\right) + \frac{x^3}{x^4 + 1} - \sqrt{6} + \frac{8}{17}$	$\alpha_6 = -2$
$f_7(x) = \sqrt{x^2 + 2x + 5} - 2\sin(x) - x^2 + 3$	$\alpha_7 \approx 2.331967655883964$
$f_8(x) = \sin^{-1}(x^2 - 1) - \frac{x}{2} + 1$	$\alpha_8 \approx 0.594810968398369$
$f_9(x) = \left(\sin(x) - \frac{\sqrt{2}}{2}\right)(x + 1)$	$\alpha_9 \approx 0.785398163397448$
$f_{10}(x) = \tan(\sin(x^2 + \cos(x - 1)))$	$\alpha_{10} \approx 1.505551425951896$

The results are provided in Table 3. In fact, the absolute value of the given test functions after some full iterations are listed there. All calculations were done with MATLAB 7.6 using 800 digits floating point (Digits: =800) with VPA Command. In examples considered in this article, the stopping criterion is the $|f(x_n)| \leq \varepsilon$, where $\varepsilon = 10^{-800}$. Numerical results are in concordance with the theory developed in this paper. In most of the cases, the results obtained with our new methods are similar to the other optimal methods.

It is preferable to have a process that requires lesser number of iteration to reach its final solution, like (15) and (18). In general, computational accuracy strongly depends on the structures of the iterative methods, the sought zeros and the test functions as well as good initial approximations. One should be aware that no iterative method always shows best accuracy for all the test functions.

4. Conclusion and discussion

Many mathematical applications involve the solution of a nonlinear equation $f(x) = 0$.

There are many methods developed on the improvement of quadratically convergent Steffensen's method so as to get a superior convergence order than Steffensen using multi-step (multi-point methods). Multi-step iterative methods have multiple step process to follow the computation route of each step which is generally cumbersome to deal with.

In the language used thus far, a well-done three-step class which is free from any derivative-evaluation per iteration was constructed. The analytical proof of the related theorem was given thoroughly to show the eighth-order convergence. The contributed methods from this class includes four evaluations of the function per iteration and subsequently agrees with the Kung-Traub Hypothesis for constructing optimal multi-point iterative methods without memory for solving single variable nonlinear equations and reaches the efficiency index 1.682. Finally, a comparison with some famous methods in the literature was provided for a couple of hard test functions to demonstrate the accuracy of the novel methods from our contributed classes in practice.

Further investigation can be done in order to develop optimal 16th-order methods which are derivative-free and consistent with the Kung-Traub Hypothesis. However, interested readers may refer to [9-27] for understanding more on this topic.

Table 3: Results of convergence under fair circumstances for different derivative-free methods

f & $Guess$		SM2	LM4	KT8	**(15)**	**(18)**
$f_1, 0.5$	IT	8	4	3	3	3
	TNE	16	12	12	12	12
	$\|f\|$	0.1e-89	0.1e-84	0.7e-167	0.5e-162	0.4e-210
$f_2, 0.6$	IT	8	4	3	3	3
	TNE	16	12	12	12	12
	$\|f\|$	0.7e-325	0.1e-197	0.1e-395	0.1e-363	0.7e-359
$f_3, 1.7$	IT	8	4	3	3	3
	TNE	16	12	12	12	12
	$\|f\|$	0.3e-99	0.2e-172	0.5e-137	0.1e-198	0.2e-220
$f_4, 4.5$	IT	8	4	3	3	3
	TNE	16	12	12	12	12
	$\|f\|$	0.3e-272	0.5e-160	0.3e-301	0.8e-254	0.3e-349
$f_5, -0.2$	IT	8	4	3	3	3
	TNE	16	12	12	12	12
	$\|f\|$	0.1e-77	0.2e-101	0.3e-182	0.3e-138	0.4e-202
$f_6, -2.3$	IT	8	4	3	3	3
	TNE	16	12	12	12	12
	$\|f\|$	0.4e-337	0.5e-247	0.4e-460	0.1e-452	0.1e-476
$f_7, 1.6$	IT	8	4	3	3	3
	TNE	16	12	12	12	12
	$\|f\|$	0.1e-238	0.2e-178	0.1e-371	0.3e-324	0.4e-390
$f_8, 0.3$	IT	8	4	3	3	3
	TNE	16	12	12	12	12
	$\|f\|$	0.2e-243	0.7e-226	0.3e-466	0.1e-476	0.2e-507
$f_9, 1$	IT	8	4	3	3	3
	TNE	16	12	12	12	12
	$\|f\|$	0.2e-285	0.1e-192	0.1e-379	0.6e-307	0.1e-396
$f_{10}, 1.55$	IT	8	4	3	3	3
	TNE	16	12	12	12	12
	$\|f\|$	0.3e-470	0.1e-369	0.2e-771	0.3e-683	0.1e-773

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