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An Optimally Convergent Three-step Class of Derivative-free Methods

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Abstract: In this paper, a new optimally convergent eighth-order class of three-step without memory methods is suggested. We here pursue derivative-free algorithms, i.e., algorithms requiring only the ability to evaluate the (objective) function. Since the types of problems that these algorithms can solve are extremely diverse in nature. The analysis of convergence shows that each derivative-free method of our class requires four pieces of information per full iteration to obtain the optimal efficiency index 1.682. Numerical experiments with comparison to some existing derivative-free methods are furnished to support the underlying theory.

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Key words: Multi-point methods . derivative-free . optimal order . error equation . Kung-Traub conjecture . efficiency index

INTRODUCTION

For approximating a root α of a nonlinear equation $f(x) = 0$, a variety of high-order two-or three-step multi-point iterative methods free from second derivatives have been developed by Heydari-Hosseini-Loghmani [3], Sharma-Guha-Sharma [12], Kung-Traub [7], Soleymani [13], Soleymani [16] and even higher orders schemes by Sargolzaei-Soleymani [11] and Geum-Kim [2]. The efficiency index of these methods is found to be high in contrast to the efficiency of one-point methods. On the other hand, these new methods can be extended to solve system of nonlinear equations, see e.g. Darvishi [1].

To shortly mention on the applications of the topic of nonlinear equations solving, we can mention the following: the various types of space structures differ in their behavior under load and so a different method of analysis must be used for each type. Space truss (a space frame truss is a three-dimensional framework of members pinned at their ends; a tetrahedron shape is the simplest space truss, consisting of six members which meet at four joints) systems are one of the most popular forms of space frames [10] which needs to be solved by iterative root solvers.

Many iterative methods have been offered for improving Newton-Raphson approach for solving nonlinear equations. However, many depend on the second or higher derivatives in the computing process, which restricts their practical application because of inherently intensive and extensive nature of the computation involved.

In recent years, also there has been some progress in devising iterative methods designed to improve application of the Newton-Raphson method, while at the same time, not requiring the computation of second derivatives (as mentioned above) [4, 9, 14]. However, there are some situations in which the calculation of the first derivatives is difficult or even impossible, thus root solvers in which there is no need of derivative calculation per iteration are needed.

Here, we focus on the simple roots of nonlinear scalar equations by iterative processes. The prominent one-point (or one-step) Newton's method of order two, which is a basic tool in numerical analysis has widely been discussed in literature [8, 18]. This scheme has 1.414 as its efficiency index. Newton's iteration and any variant of it include derivative-calculation per full cycle to proceed, which is not useful in engineering problems, mentioned above. To remedy this, first Steffensen coined the follow-up quadratically method [19]

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

Inspired by this method, so many derivative-free techniques with better orders of convergence have been provided through two-or three-step cycles. In between, the concept of optimality, which was mooted by Kung-Traub [7] plays a crucial role; a multi-point method for solving nonlinear scalar equations without memory has the optimal order $2^{(n-1)/n}$, where n is the

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total number of evaluations per full cycle. In what follows, we shortly give some of the high-order methods in which no derivative-evaluation per iteration is needed.

Khattri and Argyros in [6] formulated a sixth-order method as follows

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

Soleymani and Hosseinabadi in [15] suggested another sixth-order variant of Steffensen's technique as comes next

$$\begin{cases} y_n = x_n - \dfrac{f(x_n)}{f[x_n, w_n]}, w_n = x_n + f(x_n) \\ z_n = x_n - \dfrac{f(x_n)}{f[x_n, w_n]}\left[1 + \dfrac{f(y_n)}{f(x_n)}\left(1 + 2\dfrac{f(y_n)}{f(x_n)}\right)\right] \\ x_{n+1} = z_n - \dfrac{f(z_n)}{f[y_n, z_n]}\left[1 - \dfrac{1 + f[x_n, w_n]}{f[x_n, w_n]}\dfrac{f(z_n)}{f(w_n)}\right] \end{cases} \tag{3}$$

where $f[x_n,w_n]$ is the divided difference of $f(x_n)$, and

$$f(w_n) = f(x_n + f(x_n))$$

and could be given by

$$f[x_n, w_n] = \frac{f(w_n) - f(x_n)}{w_n - x_n}$$

Kung and Traub gave the following family of one-parameter methods by using inverse interpolation for annihilating the new-appeared first derivatives of the function in the Steffensen-Newton-Newton structure

$$\begin{cases} y_n = x_n + \beta f(x_n) \\ z_n = y_n - \beta\dfrac{f(x_n)f(y_n)}{f(y_n) - f(x_n)} \\ w_n = z_n - \dfrac{f(x_n)f(y_n)}{f(z_n) - f(x_n)}\left[\dfrac{1}{f[y_n, x_n]} - \dfrac{1}{f[z_n, y_n]}\right] \\ x_{n+1} = w_n - \dfrac{f(x_n)f(y_n)f(z_n)}{f(w_n) - f(x_n)}[W] \end{cases} \tag{4}$$

where

$$\begin{aligned} W = {} & \frac{1}{f(w_n) - f(y_n)}\left\{\frac{1}{f[w_n, z_n]} - \frac{1}{f[z_n, y_n]}\right\} \\ & - \frac{1}{f(z_n) - f(x_n)}\left\{\frac{1}{f[z_n, y_n]} - \frac{1}{f[y_n, x_n]}\right\} \end{aligned} \tag{5}$$

with $\beta \in R - \{0\}$.

In this work, we suggest a new class of three-step derivative-free methods consuming four pieces of information per full cycle to reach the optimal order of convergence eight. Clearly, the index of efficiency for our class is 1.682. Some numerical examples are also given to support the underlying theory developed in this paper. From the results displayed in Tables 3-6 and a number of numerical experiments, it will be concluded that the proposed multipoint class in this work is competitive with existing three-point methods of optimal order eight and possesses very fast convergence for good initial approximations, while it is completely free from derivative.

A NEW CLASS OF METHODS

In order to construct an optimal class of methods without computation of derivatives, we should consider a three steps cycle in which the first step is (1) and the second step provides the fourth-order convergence with only three evaluations and the Newton's method at the end. Here, we consider the second step of our cycle by a similar fourth-order derivative-free method of Khattri and Agarwal [5] and suggest the following iteration

$$y_n = x_n - \frac{f(x_n)}{f[x_n, w_n]}$$

$$z_n = y_n - \frac{f(y_n)}{f[x_n, w_n]}\left\{1 + \frac{f(y_n)}{f(x_n)} + \frac{f(y_n)}{f(w_n)}\right\}$$

$$x_{n+1} = z_n - \frac{f(z_n)}{f'(z_n)} \tag{6}$$

where $w_n = x_n + f(x_n)$. In the structure (6), $f'(z_n)$ should be annihilated as the order (eight) does not fall down. To do this, we first approximate it by the linear combination of the past two points x_n and y_n, i.e. $f'(z_n) \approx f[x_n,y_n]$. Then, we make use of weight function approach to reach the convergence order eight with only four pieces of information per full cycle. Thus, we suggest

$$\begin{cases} y_n = x_n - \dfrac{f(x_n)}{f[x_n, w_n]}, w_n = x_n + \beta f(x_n) \\ z_n = y_n - \dfrac{f(y_n)}{f[x_n, w_n]}\left\{1 + \dfrac{f(y_n)}{f(x_n)} + \dfrac{f(y_n)}{f(w_n)}\right\} \\ x_{n+1} = z_n - \dfrac{f(z_n)}{f[x_n, y_n]}\{G(t) + H(\tau) + K(\sigma) + L(\varphi) + P(\pi)\} \end{cases} \quad (7)$$

in which $t = \frac{f(z)}{f(x)}, \tau = \frac{f(z)}{f(y)}, \sigma = \frac{f(z)}{f(w)}, \varphi = \frac{f(y)}{f(x)}, \pi = \frac{f(y)}{f(w)}$ without the index n. Theorem 1 shows that how the structure (7) arrives at eighth order of convergence.

Theorem 1: Let $\alpha \in D$, be a simple zero of a sufficiently differentiable function $f: D \subseteq R \to R$ and let that $c_j = f^{(j)}(\alpha)/j!$, $j \geq 1$, $\beta \in R-\{0\}$. If x_0 is sufficiently close to α, then, (i): the order of convergence of the solution by the without memory derivative-free class defined in (7) is eight, when

$$\begin{cases} G(0) = G'(0) = 1, |G''(0)| \leq \infty \\ H(0) = 0, H'(0) = 1, |H''(0)| \leq \infty \\ K(0) = 0, K'(0) = 2, |K''(0)| \leq \infty \\ L(0) = L'(0) = L'''(0) = 0, L''(0) = -2, |L^{4}(0)| \leq \infty \\ P(0) = P''(0) = 0, P'(0) = 1 \\ P'''(0) = -(30 + 6\beta f[x_n, w_n](8 + \beta f[x_n, w_n](5 + \beta f[x_n, w_n]))), |P^{4}(0)| \leq \infty \end{cases} \quad (8)$$

and (ii): this solution reads the error equation

$$\begin{aligned} e_{n+1} = &-\frac{1}{24c_1^7}(c_2(1+c_1\beta)(-c_1c_3(1+c_1\beta)+c_2^2(5+c_1\beta(5+c_1\beta)))(-24c_1^2c_2c_4(1+c_1\beta)^2 \\ &+12c_1^2c_3^2(1+c_1\beta)^2(-2+H''(0))-24c_1c_2^2c_3(1+c_1\beta)(5(-3+H''(0))+c_1\beta(-13-c_1\beta \\ &+(5+c_1\beta)H''(0)))+c_2^4(-696+300H''(0)+L^{(4)}(0)+c_1\beta(12(5+c_1\beta)(-20-6c_1\beta+(10 \\ &+c_1\beta(5+c_1\beta)H''(0))+(2+c_1\beta)(2+c_1\beta(2+c\beta(2+c_1\beta))L^{(4)}(0))+P^{4}(0))))e_n^8+0(e_n^9). \end{aligned} \quad (9)$$

Proof: We simply provide the order of convergence by expanding Taylor's series around the simple root for the iteration function in the nth iterate. We seek this problem with the following Mathematica program (Matlab and Maple are also convenient). The following terms are used in the program given below.

$$\begin{aligned} &e = x - \alpha, u = y - \alpha, v = z - \alpha, b = x + \beta f(x) \\ &q_1 = \beta, fx = f(x), fy = f(y) \\ &fz = f(z), d = f[x, w] \end{aligned}$$

Mathematica Program

```
(*e=x-a;*)fx[e_]=c1*e+c2*e^2+c3*e^3+c4*e^4+c5*e^5+c6*e^6+c7*e^7+c8*e^8;
b=e+q1*fx[e];fw[b_]=c1*b+c2*b^2+c3*b^3+c4*b^4+c5*b^5+c6*b^6+c7*b^7+c8*b^8;d=(fw[b]-fx[e])/
(q1*fx[e]);(*u=y-a;*)u=e-Series[fx[e]/d,{e,0,8}];fy[u_]=c1*u
+c2*u^2+c3*u^3+c4*u^4+c5*u^5+c6*u^6+c7*u^7+c8*u^8;(*v=z-a;*)v=u(fy[u]
/d)*(1+fy[u]/fx[e]+fy[u]/fw[b]);fz[v_]=c1*v+c2*v^2+c3*v^3+c4*v^4+c5*v^5
+c6*v^6+c7*v^7+c8*v^8;G[0]=G'[0]=P'[0]=H'[0]=1;H[0]=K[0]=L[0]=L'[0]=P[0]=P''[0]=0;L''[0]=-
2;K'[0]=2;L'''[0]=0;
P'''[0]=-(30+6*q1*d*(8+q1*d*(5+q1*d)));e[n+1]=v-(fz[v]/((fy[u]-fx[e])/(u-e)))*(G[fz[v]/fx[e]]
+H[fz[v]/fy[u]]+K[fz[v]/fw[b]]+L[fy[u]/fx[e]]+P[fy[u]/fw[b]])//FullSimplify
```

Clearly, by considering (8), the order of the scheme (7) arrives at eight with only four evaluations per full cycle. Thus, the proof is complete.

In terms of computational efficiency, each method of our class (7)-(8) possesses 1.682 as its efficiency index which is the same to (4) and greater than 1.565 of (2) and (3) and 1.414 of Steffensen's method (1). Some typical forms of the real valued weight functions $G(t)$, $H(\tau)$, $K(\sigma)$, $L(\varphi)$ and $P(\pi)$ which satisfy (8) are listed in Table 1. The simplest method in terms of arithmetic calculation is given below

$$\begin{cases} y_n = x_n - \dfrac{f(x_n)}{f[x_n, w_n]} \\ z_n = y_n - \dfrac{f(y_n)}{f[x_n, w_n]}\left\{1 + \dfrac{f(y_n)}{f(x_n)} + \dfrac{f(y_n)}{f(w_n)}\right\} \\ x_{n+1} = z_n - \dfrac{f(z_n)}{f[x_n, y_n]}\{W_1\} \end{cases} \tag{10}$$

where $w_n = x_n + f(x_n)$ and

$$\begin{aligned} W_1 = {} & 1 + \frac{f(z_n)}{f(x_n)} + \frac{f(z_n)}{f(y_n)} + 2\frac{f(z_n)}{f(w_n)} - \left(\frac{f(y_n)}{f(x_n)}\right)^2 + \frac{f(y_n)}{f(w_n)} \\ & - \frac{1}{6}\Big(30 + 6f[x_n, w_n](8 + f[x_n, w_n](5 + f[x_n, w_n]))\Big) \times \left(\frac{f(y_n)}{f(w_n)}\right)^3 \end{aligned} \tag{11}$$

with the following error equation

$$\begin{aligned} e_{n+1} = {} & \frac{1}{c_1^7}(1 + c_1)\, c_2 \left((5 + c_1(5 + c_1))c_2^2 - c_1(1 + c_1)c_3\right) \\ & \times \left((29 + c_1(5 + c_1)(10 + 3c_1))c_2^4 - c_1(1 + c_1)(15 + c_1(13 + c_1))c_2^2 c_3 + c_1^2(1 + c_1)^2 c_3^2 + c_1^2(1 + c_1)^3 c_2 c_4\right)e_n^8 + 0(e_n^9) \end{aligned} \tag{12}$$

As an another example, we can have the following derivative-free eighth-order method from our proposed class of without memory iterations

$$\begin{cases} y_n = x_n - \dfrac{f(x_n)}{f[x_n, w_n]} \\ z_n = y_n - \dfrac{f(y_n)}{f[x_n, w_n]}\left\{1 + \dfrac{f(y_n)}{f(x_n)} + \dfrac{f(y_n)}{f(w_n)}\right\} \\ x_{n+1} = z_n - \dfrac{f(z_n)}{f[x_n, y_n]}\{W_2\} \end{cases} \tag{13}$$

where $w_n = x_n + f(x_n)$ and

$$\begin{aligned} W_2 = {} & 1 + \frac{f(z_n)}{f(x_n)} + \frac{f(z_n)}{f(y_n)} + \left(\frac{f(z_n)}{f(y_n)}\right)^2 + 2\frac{f(z_n)}{f(w_n)} - \left(\frac{f(y_n)}{f(x_n)}\right)^2 + \frac{f(y_n)}{f(w_n)} \\ & - \frac{1}{6}\Big(30 + 6f[x_n, w_n](8 + f[x_n, w_n](5 + f[x_n, w_n]))\Big) \times \left(\frac{f(y_n)}{f(w_n)}\right)^3 \end{aligned} \tag{14}$$

Table 1: Some typical forms of the real valued weight functions in (8)

Weight function	$G(t)$	$H(\tau)$	$K(\sigma)$	$L(\varphi)$	$P(\pi)$
Forms	$1 + t + \gamma_1\tau^2$	$\tau + \gamma_2\tau^2$	$2\sigma + \gamma_3\sigma^2$	$-\varphi^2$	$\pi - \frac{1}{6}\left(30 + 6\beta f[x_n, w_n](8 + \beta f[x_n, w_n](5 + \beta f[x_n, w_n]))\right)\pi^3$

$t = \frac{f(z_n)}{f(x_n)}, \tau = \frac{f(z_n)}{f(y_n)}, \sigma = \frac{f(z_n)}{f(w_n)}, \varphi = \frac{f(y_n)}{f(x_n)}, \pi = \frac{f(y_n)}{f(w_n)}, \gamma_1, \gamma_2, \gamma_3 \in R$

Such classes of methods (7)-(8) in which the highest possible order has been obtained by the smallest use of evaluations per iteration and moreover, no derivative evaluation is needed per step to proceed, are so useful in engineering and optimization problems. An example of the use of derivative-free algorithms in optimization (Air Pollution) can be the following: an application of derivative-free optimization involves function evaluation by numerical simulation.

The existence of several models for air pollution allows the possibility of computing the maximum air pollution concentration in a given region. The existent models, available both for fixed and mobile sources, allow also the planning of the sampling stations positions (maximizers). The refined models provide a more detailed treatment of physical and chemical processes, but have higher computational costs and the available software is usually written in a computer language where derivatives are not available or are very expensive to compute. Thus, the users refer to derivative-free algorithms, such as (10)-(11).

The informational efficiency is defined as the quotient of the convergence order of an iteration function and the informational usage of an iteration function (new pieces of information required per iteration) and denoted as IF. Thus IF = p/n where p is the convergence order and n is the whole number of evaluations. According to this, the informational efficiency for each member from our proposed class is 2 which is much better that 1 of Steffensen's, 1.5 of (2) and (3).

NUMERICAL TESTING

The results given in the previous section are supported through the numerical works. The simple method of our class (10)-(11) is compared with the sixth-order scheme of Khattri and Argyros (2), the sixth-order method of Soleymani and Hosseinabadi (3) and the optimal eighth-order derivative-free family of Kung-Traub (4) with $\beta = 1$. All the computations reported here were done using MATLAB 7.6, where for convergence we have selected that $|f(xn)|\leq 10^{-5000}$. Scientific computations in many branches of science and technology demand high degree of numerical precision. The minimum number of precision digits chosen as 5000, being large enough to minimize round-off errors as well as to clearly observe the computed asymptotic error constants requiring small number of divisions.

The test nonlinear scalar functions are listed in Table 2. The results of comparisons for the test functions are provided in Tables 3-6. It can be seen that the resulted method from our class is accurate and efficient in terms of number of accurate decimal places to find the roots after each iteration. In terms of computational cost, our class is much better than the compared methods. The class includes four evaluations of the function per full iteration to reach the efficiency index 1.682.

Under the same order of convergence, one should note that the speed of local convergence of $|x_n-\alpha|$ is dependent on c_j, namely f(x) and α. In general, computational accuracy strongly depends on the structures of the iterative methods, the sought zeros and the test functions as well as good starting points. One should be aware that no iterative method always shows best accuracy for all the nonlinear functions. Each initial guess x_0 close to a was used not only to mostly guarantee the convergence but also to observe the asymptotic error constants as well as the convergence order. Note that more experimental results for our class show that for small positive value of $\beta\in R-\{0\}$, the numerical results will be more promising and the output error equation will be confined as well.

Table 2: The examples considered in this study

Test functions	Zeros	Guess
$f_1=(1+x^3)\cos(\frac{\pi x}{2})+\sqrt{1-x^2}-\frac{2(9\sqrt{2}+7\sqrt{3})}{27}$	$\alpha_1=1/3$	0.8
$f_2=(\sin x)^2-x^2+1$	$\alpha_2\approx 1.404491648215341$	2.0
$f_3=\sin^{-1}(x^2-1)-\frac{x}{2}+1$	$\alpha_3\approx 0.594810968398369$	0.3
$f_4=\sin^{-1}(x^2-1)-\frac{x}{2}+\tan^{-1}(x)+1$	$\alpha_4\approx 0.300980060061363$	0.5

Table 3: Convergence study for the test function f_1

Methods	$\|f_1(x_1)\|$	$\|f_1(x_2)\|$	$\|f_1(x_3)\|$	$\|f_1(x_4)\|$
(2)	0.1	0.1e-2	0.3e-13	0.3e-77
(3)	0.2e-1	0.9e-11	0.1e-66	0.2e-402
(4)	0.9e-1	0.9e-14	0.2e-113	0.1e-910
(10)	0.1e-3	0.5e-31	0.1e-249	0.8e-1997

Table 4: Convergence study for the test function f_2

Methods	$\lvert f_2(x_1)\rvert$	$\lvert f_2(x_2)\rvert$	$\lvert f_2(x_3)\rvert$	$\lvert f_2(x_4)\rvert$
(2)	0.8e-1	0.1e-5	0.8e-34	0.2e-203
(3)	Div.	-	-	-
(4)	Div.	-	-	-
(10)	0.3	0.8e-6	0.1e-50	0.1e-407

Table 5: Convergence study for the test function f_3

Methods	$\lvert f_3(x_1)\rvert$	$\lvert f_3(x_2)\rvert$	$\lvert f_3(x_3)\rvert$	$\lvert f_3(x_4)\rvert$
(2)	0.1e-8	0.1e-56	0.1e-344	0.1e-2072
(3)	0.2e-5	0.2e-35	0.2e-215	0.5e-1295
(4)	0.1e-6	0.9e-58	0.3e-466	0.5e-3734
(10)	0.1e-7	0.1e-64	0.7e-520	0.5e-4163

Table 6: Convergence study for the test function f_4

Methods	$\lvert f_4(x_1)\rvert$	$\lvert f_4(x_2)\rvert$	$\lvert f_4(x_3)\rvert$	$\lvert f_4(x_4)\rvert$
(2)	0.2e-8	0.1e-56	0.1e-346	0.7e-2086
(3)	0.1e-8	0.2e-57	0.8e-350	0.2e-2104
(4)	0.2e-8	0.1e-72	0.2e-588	0.4e-4713
(10)	0.1e-8	0.2e-75	0.7e-609	0.2e-4877

CONCLUSION

It is widely known that many problems in different scientific fields of study are reduced to solve single valued nonlinear equations. On the other hand, the construction of iterative without memory methods for approximating the solution of nonlinear equations or systems is an interesting task in numerical analysis. During the last years, numerous papers, devoted to the mentioned iterative methods, have appeared in several journals, [17, 18, 20]. The existence of an extensive literature on these iterative methods reveals that this topic is a dynamic branch of the numerical and nonlinear studies with interesting and promising applications (the study of dynamical models of chemical reactors, radioactive transfer, preliminary orbit determination, etc). For these reasons, we have constructed an efficient class of derivative-free without memory methods in which there are four function evaluations per full cycle. Taking into consideration of the efficiency index of multi-point iterations, we have attained that our proposed class possesses 1.682 as its index of efficiency which is greater than that of the newly published works (2) and (3). The convergence rate of the presented contribution was established theoretically and its performance was tested through numerical examples. Our contribution is promising when the calculation of derivatives of the function takes up a great deal of time or impossible. Hence, each method of our class is very effective and can be considered as an alternative to the existing methods available in literature.

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