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Algorithm for forming derivative-free optimal methods

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Abstract We develop a simple yet effective and applicable scheme for constructing derivative free optimal iterative methods, consisting of one parameter, for solving nonlinear equations. According to the, still unproved, Kung-Traub conjecture an optimal iterative method based on k+1 evaluations could achieve a maximum convergence order of 2^k . Through the scheme, we construct derivative free optimal iterative methods of orders two, four and eight which request evaluations of two, three and four functions, respectively. The scheme can be further applied to develop iterative methods of even higher orders. An optimal value of the free-parameter is obtained through optimization and this optimal value is applied adaptively to enhance the convergence order without increasing the functional evaluations. Computational results demonstrate that the developed methods are efficient and robust as compared with many well known methods.

Keywords Iterative methods \cdot Fourth order \cdot Eighth order \cdot Newton \cdot Convergence \cdot Nonlinear \cdot Optimal \cdot Optimization \cdot Adaptivity

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1 Introduction

Many problems, in science and engineering, result in solving nonlinear equation f(x) = 0. The Newton method is the best known, and probably the most used method, for solving nonlinear equation which is given as (**NM**)

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \qquad n = 0, 1, 2, 3, \dots, \text{ and } |f'(x_n)| \neq 0.$$
 (1)

It is well-known that the Newton method converges quadratically in some neighborhood of the solution. There exists numerous modifications of the Newton method which improve the rate of convergence (see [4, 10, 17, 20–23, 25, 32] and references therein). For fourth order methods we refer to [4, 11, 16, 18, 32], for eighth order convergent methods we refer to [8, 12, 30] and references therein and for sixteenth order iterative method we refer to the literature [10, 12, 17, 20–24]. We notice that if the derivative of the function vanishes, that is $|f'(x_n)| = 0$, during the iterative process then the sequence generated by the Newton (1) or the methods that require computation of derivatives, e.g., see [8, 16, 18, 24] are not defined. Accordingly we are interested in derivative free methods. One of the purposes of this paper is to illustrate the asymptotic behavior of different derivative free methods for solving nonlinear equations.

In most test problems for nonlinear equations computing derivatives are an easy exercise. However, for many practical problems computing the derivative might be a cumbersome task and we have to relay on methods free of derivatives or tools for automatic differentiation [see [14] Chap. 6]. In the derivative free method of Steffensen [31] the derivative $f'(x_n)$ in Newton's method (1) is replaced by the finite difference $(f(x_n + f(x_n)) - f(x_n))/f(x_n)$ or $(f(x_n + \alpha_n f(x_n)) - f(x_n))/(\alpha_n f(x_n))$ where $\{\alpha_n\}$ is a bounded sequence. The Steffensen's method will have local and quadratic rate of convergence. The parameter α_n can be chosen to improve the rate of convergence [32] or the stability [3] of the family of methods. However one drawback of the derivative free methods, based upon the Steffensen scheme, is huge cancelation of significant digits in the expression $f(x + \alpha f(x)) - f(x)$. Therefore, to study the asymptotic behavior one needs to use arithmetic with much higher precision than it would be necessary for methods that use derivatives instead of finite differences. For this purpose, we use the ARPREC library which supports arbitrarily high level of numeric precision [5].

An attractive feature of the Steffensen's method is that it generalizes to function $f : X \mapsto X$ on a Banach space X [1, 9]. The finite difference operator for Steffensen's method will now be the bounded linear operator [x, x + f(x); f] where the finite difference operator [u, v; f] satisfies [u, v; f](v - u) = f(v) - f(u) and the method can be written as

$$x_{n+1} = x_n - [x_n, x_n + \alpha_n f(x_n); f]^{-1} f(x_n), \qquad n = 0, 1, 2, 3, \dots$$
(2)

The central difference operator $[x_n - \alpha_n f(x_n), x_n + \alpha_n f(x_n); f]$ [3] will require one extra function evaluation for each iteration but will give higher order approximation of $f'(x_n)$ than using the the operator $[x_n, x_n + \alpha_n f(x_n); f]$. A further generalization of Steffensen's method can be found by replacing the finite difference [x, x + f(x); f] by using [x, g(x); f] where g is a smooth function [26] or a 'central difference operator' $[g_1(x), g_2(x); f]$ [2].

In this work, we contribute a scheme for constructing derivative free optimal iterative methods. According to the Kung-Traub conjecture an iterative method based upon k + 1 evaluations in each iteration could achieve an optimal convergence order of 2^k [19]. We construct optimal iterative methods of order two, four and eight which request two, three and four functional evaluations in each iteration, respectively. From this derivation, the construction of optimal convergence order 2^k follows directly. Kung and Traub [19] derive an optimal method based on inverse interpolation. Optimal methods with convergence order 2^k can be based on different interpolations [12, 34].

The constructed iterative methods have one free parameter. We propose value of the free parameter and apply it adaptively to achieve higher convergence order without increasing the functional evaluations. The Section 2 presents our construction of methods up to order eight and formally proves the rate of convergence and gives the asymptotic error constant. The section is ended with a conjecture on the order and error constant for iterative methods using k + 1, $k \ge 1$, function evaluations based on this construction. In Section 3 we make a numerical comparison with other well known methods using derivatives and in the last part of the testing we make a numerical comparison with derivative free methods. We also indicate the robustness of the developed methods by showing convergence with different starting points.

2 Scheme for constructing optimal derivative free iterative methods

Our motivation is to develop a scheme for constructing optimal derivative free iterative methods. Let us approximate the derivative in the Newton's method (1) as follows

$$f'(x_n) \approx \eta_1 f(x_n) + \eta_2 f(x_n + \alpha f(x_n)).$$
(3)

To determine the real constants η_1 and η_2 in the preceding equation, we consider the equation is valid with equality for the two functions: f(t) = 1 and f(t) = t. This yields the equations

Solving the preceding equations and substituting the constants η_1 , η_2 in the (3), we obtain

$$f'(x_n) \approx \frac{f(x_n + \alpha f(x_n)) - f(x_n)}{\alpha f(x_n)}.$$
(5)

Combining the Newton method (1) and preceding approximation for the derivative, we propose the method (**M-2**)

$$x_{n+1} = x_n - \alpha \, \frac{f(x_n)^2}{f(x_n + \alpha \, f(x_n)) - f(x_n)}.$$
(6)

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This is the well known Steffensen's method for $\alpha = 1$. To construct higher order method from the Newton's method (1), we use the following generalization of the Traub's theorem (see [32, Theorem 2.4] and [28, Theorem 3.1]).

Theorem 1 Let $g_1(x), g_2(x), \ldots, g_s(x)$ be iterative functions with orders r_1, r_2, \ldots, r_s , respectively. Then the composite iterative functions

$$g(x) = g_1(g_2(\cdots(g_s(x))\cdots))$$

define the iterative method of the order $\prod_{i=1}^{s} r_i$.

From the preceding theorem, combination of the Newton method (1) and the second order method (6) produces the following fourth order iterative method

$$\begin{cases} y_n = x_n - \alpha \frac{f(x_n)^2}{f(x_n + \alpha f(x_n)) - f(x_n)}, \\ x_{n+1} = y_n - \frac{f(y_n)}{f'(y_n)}. \end{cases}$$
(7)

The convergence order of the preceding method is four and it requires four evaluations during each step. Therefore according to the Kung and Traub conjecture, for the preceding method to be optimal it must require only three function evaluations. To construct derivative free optimal fourth order method, we approximate the derivative in the preceding method as follows

$$f'(y_n) \approx \omega_1 f(x_n) + \omega_2 f(x_n + \alpha f(x_n)) + \omega_3 f(y_n)$$
(8)

We assume the (8) is valid with equality for the three functions: f(t) = 1, f(t) = tand $f(t) = t^2$ to determine the real constants ω_1, ω_2 and ω_3 . This yields the equations

$$\begin{array}{l}
\omega_{1} + \omega_{2} + \omega_{3} = 0, \\
\omega_{1} x_{n} + \omega_{2} (x_{n} + \alpha f(x_{n})) + \omega_{3} y_{n} = 1, \\
\omega_{1} x_{n}^{2} + \omega_{2} (x_{n} + \alpha f(x_{n}))^{2} + \omega_{3} y_{n}^{2} = 2 y_{n}.
\end{array}$$
(9)

Solving the preceding equations and substituting the values in the (8), we obtain

$$f'(y_n) \approx \frac{x_n - y_n + \alpha f(x_n)}{(x_n - y_n)\alpha} - \frac{(x_n - y_n) f(x_n + \alpha f(x_n))}{(x_n - y_n + \alpha f(x_n)) \alpha f(x_n)} - \frac{(2 x_n - 2 y_n + \alpha f(x_n)) f(y_n)}{(x_n - y_n) (x_n - y_n + \alpha f(x_n))}.$$
(10)

By putting the (9) in matrix notation

$$\begin{bmatrix} 1 & 1 & 1 \\ x_n & x_n + \alpha & f(x_n) & y_n \\ x_n^2 & (x_n + \alpha & f(x_n))^2 & y_n^2 \end{bmatrix} \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 2y_n \end{pmatrix}$$
(11)

the coefficient matrix will be the Vandermonde matrix. The coefficient matrix is nonsingular provided the three points x_n , $x_n + \alpha f(x_n)$, and y_n are different and if the method is well defined the Vandermonde matrix will be nonsingular if $f(x_n) \neq 0$ and

 $f(x_n + \alpha f(x_n)) \neq 0$. Combining the method (7) and the preceding approximation for the derivative, we propose the method (**M-4**)

$$\begin{cases} y_n = x_n - \alpha \frac{f(x_n)^2}{f(x_n + \alpha f(x_n)) - f(x_n)}, \\ x_{n+1} = y_n - \frac{x_n - y_n + \alpha f(x_n)}{(x_n - y_n)\alpha} - \frac{(x_n - y_n)f(x_n + \alpha f(x_n))}{(x_n - y_n + \alpha f(x_n))\alpha f(x_n)} - \frac{(2x_n - 2y_n + \alpha f(x_n))f(y_n)}{(x_n - y_n)(x_n - y_n + \alpha f(x_n))}. \end{cases}$$
(12)

The method (**M-4**) is totally free of derivatives. It requests only three evaluations and it will be shown that the method (**M-4**) is fourth order convergent. It is an optimal method according to the Kung-Traub conjecture.

From the Theorem 1, combination of the Newton method (1) and the fourth order method (12) produces the following eighth order iterative method

$$\begin{cases} y_n = x_n - \alpha \frac{f(x_n)^2}{f(x_n + \alpha f(x_n)) - f(x_n)}, \\ z_n = y_n - \frac{f(y_n)}{\frac{x_n - y_n + \alpha f(x_n)}{(x_n - y_n)\alpha} - \frac{(x_n - y_n)f(x_n + \alpha f(x_n))}{(x_n - y_n + \alpha f(x_n))\alpha f(x_n)} - \frac{(2x_n - 2y_n + \alpha f(x_n))f(y_n)}{(x_n - y_n)(x_n - y_n + \alpha f(x_n))}, \end{cases}$$
(13)
$$x_{n+1} = z_n - \frac{f(z_n)}{f'(z_n)}.$$

To construct derivative free optimal eighth order method, we approximate the derivative as follows

$$f'(z_n) \approx \nu_1 f(x_n) + \nu_2 f(x_n + \alpha f(x_n)) + \nu_3 f(y_n) + \nu_4 f(z_n).$$
(14)

To determine the real constants v_1 , v_2 , v_3 and v_4 in the preceding equation, we consider the equation is valid with equality for the four functions: f(t) = 1, f(t) = t, $f(t) = t^2$ and $f(t) = t^3$. Which yields the equations

$$\begin{array}{l} \nu_{1} + \nu_{2} + \nu_{3} + \nu_{4} &= 0, \\ \nu_{1} x_{n} + \nu_{2} (x_{n} + \alpha f(x_{n})) + \nu_{3} y_{n} + \nu_{4} z_{n} &= 1, \\ \nu_{1} x_{n}^{2} + \nu_{2} (x_{n} + \alpha f(x_{n}))^{2} + \nu_{3} y_{n}^{2} + \nu_{4} z_{n}^{2} = 2 z_{n}, \\ \nu_{1} x_{n}^{3} + \nu_{2} (x_{n} + \alpha f(x_{n}))^{3} + \nu_{3} y_{n}^{3} + \nu_{4} z_{n}^{3} = 3 z_{n}^{2}. \end{array} \right\}$$

$$(15)$$

The preceding equations have a unique solution if $f(x_n) \neq 0 \neq f(x_n + \alpha f(x_n))$ and $f(y_n) \neq 0$, i.e. the method is not terminating with the solution after a finite number of steps. Substituting the values in the (14), we obtain the approximation for the derivative at the point z_n

$$f'(z_n) \approx -\frac{(y_n - z_n)(x_n + \alpha f(x_n) - z_n)}{(x_n - z_n)\alpha(x_n - y_n)} + \frac{(y_n - z_n)(x_n - z_n)f(x_n + \alpha f(x_n))}{(x_n + \alpha f(x_n) - z_n)(x_n + \alpha f(x_n) - y_n)\alpha f(x_n)} \\ + \frac{(x_n - z_n)(x_n + \alpha f(x_n) - z_n)f(y_n)}{(y_n - z_n)(x_n - y_n + \alpha f(x_n))(x_n - y_n)} \\ + \frac{(x_n \alpha - 2\alpha z_n + \alpha y_n)f(x_n) + x_n^2 + (-4z_n + 2y_n)x_n + 3z_n^2 - 2y_n z_n}{(y_n - z_n)(x_n - z_n)(x_n - z_n + \alpha f(x_n))} f(z_n).$$
(16)

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Combining the method (13) and the preceding approximation for the derivative, we propose the method (**M-8**)

$$\begin{cases} y_n = x_n - \alpha \frac{f(x_n)^2}{f(x_n + \alpha f(x_n)) - f(x_n)}, \\ z_n = y_n - \frac{x_n - y_n + \alpha f(x_n)}{(x_n - y_n)\alpha} - \frac{(x_n - y_n)f(x_n + \alpha f(x_n))}{(x_n - y_n + \alpha f(x_n))\alpha f(x_n)} - \frac{(2x_n - 2y_n + \alpha f(x_n))f(y_n)}{(x_n - y_n)(x_n - y_n + \alpha f(x_n))}, \end{cases}$$
(17)

$$x_{n+1} = z_n - \frac{f(z_n)}{\mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_3 + \mathcal{H}_4}.$$

Here,

$$\mathcal{H}_{1} = -\frac{(y_{n} - z_{n})(x_{n} + \alpha f(x_{n}) - z_{n})}{(x_{n} - z_{n})\alpha(x_{n} - y_{n})},$$

$$\mathcal{H}_{2} = \frac{(y_{n} - z_{n})(x_{n} - z_{n})f(x_{n} + \alpha f(x_{n}))}{(x_{n} + \alpha f(x_{n}) - z_{n})(x_{n} + \alpha f(x_{n}) - y_{n})\alpha f(x_{n})},$$

$$\mathcal{H}_{3} = \frac{(x_{n} - z_{n})(x_{n} + \alpha f(x_{n}) - z_{n})f(y_{n})}{(y_{n} - z_{n})(x_{n} - y_{n} + \alpha f(x_{n}))(x_{n} - y_{n})},$$

$$\mathcal{H}_{4} = \frac{(x_{n}\alpha - 2\alpha z_{n} + \alpha y_{n})f(x_{n}) + x_{n}^{2} + (-4z_{n} + 2y_{n})x_{n} + 3z_{n}^{2} - 2y_{n}z_{n}}{(y_{n} - z_{n})(x_{n} - z_{n})(x_{n} - z_{n} + \alpha f(x_{n}))} f(z_{n}).$$

The contributed methods (6), (12) and (17) are totally free of derivatives. We prove the convergence of the iterative methods (6), (12) and (17) through the following theorem.

Theorem 2 Let γ be a simple zero of a sufficiently differentiable function $f : \mathbf{D} \subset \mathbf{R} \mapsto \mathbf{R}$ in an open interval \mathbf{D} . If x_0 is sufficiently close to γ , the convergence order of the method (6) is 2 and the error equation for the method is given as

$$e_{n+1} = \frac{c_2 \left(1 + \alpha \, c_1\right)}{c_1} \, e_n^2 + O\left(e_n^3\right),\tag{18}$$

the convergence order of the method (12) is 4 and the error equation for the method is given as

$$e_{n+1} = \frac{c_2 \left(1 + \alpha \, c_1\right)^2 \left(c_2^2 - c_1 \, c_3\right)}{c_1^3} e_n^4 + O\left(e_n^5\right),\tag{19}$$

and the convergence order of the method (17) is 8 and the error equation for the method is given as

$$e_{n+1} = \frac{c_2^2 (1 + \alpha c_1)^3 \left(c_2^3 - c_1 c_3 c_4\right) \left(c_4^2 - c_1 c_2\right)}{c_1^7} e_n^8 + O\left(e_n^9\right).$$
(20)

Here, $e_n = x_n - \gamma$, $c_m = f^m(\gamma)/m!$ with $m \ge 1$.

Proof The Taylor's expansion of f(x) around the solution γ is given as

$$f(x_n) = c_1 e_n + c_2 e_n^2 + c_3 e_n^3 + c_4 e_n^4 + O\left(e_n^5\right),$$
(21)

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similarly the Taylor expansion of $f(x_n + \alpha f(x_n))$ around γ

$$f(x_n + \alpha f(x_n)) = \sum_{i=1}^{\infty} c_i (x_n - \gamma + \alpha f(x_n))^i,$$

substituting from the (21) into the previous equation, we have

$$f(x_n + \alpha f(x_n)) = c_1(1 + \alpha c_1)e_n + c_2\left(1 + 3c_1\alpha + \alpha^2 c_1^2\right)e_n^2 + O(e_n^3).$$
(22)

Here, we have accounted for $f(\gamma) = 0$. Substituting (21) and (22) into the first step of the method (**M-4**) (12), we obtain

$$y_{n} = \gamma + \frac{c_{2}(1 + \alpha c_{1})e_{n}^{2}}{c_{1}} + \frac{\left(c_{3}c_{1}\left(\alpha c_{1} + 2\right)\left(1 + \alpha c_{1}\right) + \left(-\alpha^{2}c_{1}^{2} - 2\alpha c_{1} - 2\right)c_{2}^{2}\right)e_{n}^{3}}{c_{1}^{2}} + O\left(e_{n}^{4}\right).$$
(23)

In the preceding equation, we notice that the method (M-2) is second order with the error (18). By the Taylor's expansion of $f(y_n)$ around the solution γ

$$f(y_n) = \sum_{k=0}^{\infty} c_k (y_n - \gamma)^k \left(-\frac{f(x_n)}{f'(x_n)} \right)^2 + \dots,$$

substituting from the (23) into the preceding equation yields

$$f(y_n) = c_2(1 + \alpha c_1)e_n^2 + \frac{(c_3c_1(\alpha c_1 + 2)(1 + \alpha c_1) + c_2^2(-\alpha^2 c_1^2 - 2\alpha c_1 - 2))e_n^3}{c_1} + O(e_n^4).$$
(24)

Substituting from (21), (22) and (24) into the second step of the method (M-4) (17), we get the error equation for the method (M-4)

$$z_{n} = \gamma - \frac{c_{2}(1 + \alpha c_{1})^{2} \left(-c_{2}^{2} + c_{1}c_{3}\right) e_{n}^{4}}{c_{1}^{3}} - \frac{1}{c_{1}^{4}} \left[\left(1 + \alpha c_{1}\right) \left(\left(2 c_{1}^{2} \alpha^{2} + 4 + 4 \alpha c_{1}\right) c_{2}^{4} + \left(-4 c_{3} \alpha^{2} c_{1}^{3} - 10 c_{3} \alpha c_{1}^{2} - 8 c_{1} c_{3}\right) c_{2}^{2} \right. \left. + \left(2 c_{4} c_{1}^{2} + c_{1}^{4} c_{4} \alpha^{2} + 3 c_{4} \alpha c_{1}^{3}\right) c_{2} + 2 c_{1}^{2} c_{3}^{2} + c_{1}^{4} \alpha^{2} c_{3}^{2} + 3 c_{3}^{2} \alpha c_{1}^{3}\right) e_{n}^{5} \right] \times O\left(e_{n}^{6}\right).$$
(25)

In the preceding equation, we notice that the method (M-4) is fourth order with the error (19). By the Taylor's expansion of $f(z_n)$ around the solution γ

$$f(z_n) = \sum_{k=0}^{\infty} c_k (z_n - \gamma)^k,$$

substituting from the (25) into the preceding equation, we get

$$f(z_n) = -\frac{(1+\alpha c_1)^2 (c_1 c_3 - c_2^2) e_n^4}{c_1^2} -\frac{1}{c_1^3} \Big[\Big(2 c_1^2 c_2^4 - 4 c_2^2 c_3 c_1^3 + (c_3^2 + c_2 c_4) c_1^4 \Big) \alpha^2 + \Big(\Big(3 c_2 c_4 + 3 c_3^2 \Big) c_1^3 - 10 c_2^2 c_3 c_1^2 + 4 c_1 c_2^4 \Big) \alpha + 4 c_2^4 - 8 c_1 c_2^2 c_3 + (2 c_2 c_4 + 2 c_3^2) c_1^2 \Big] + (1+\alpha c_1) e_n^5 + O\left(e_n^6\right).$$
(26)

Finally substituting from the (21), (22), (23), (24), (25) and (26) into the third step of the method (17), we obtain the error equation for the method

$$e_{n+1} = \frac{c_2^2 (1 + \alpha c_1)^3 \left(c_2^3 - c_1 c_3 c_4\right) \left(c_4^2 - c_1 c_2\right)}{c_1^7} e_n^8 + O\left(e_n^9\right).$$
(27)

Therefore the contributed method (17) is eighth order convergent. This completes our proof.

In this work, we have contributed the methods (6), (12), (17). For the parameter $\alpha = 1$, the method (6) produces the well known second order Steffensen method [4].

To find the optimal value of the free parameter α , in the contributed methods (6), (12) and (17), we minimize the absolute value of the asymptotic error constant. For $\alpha = -c_1^{-1}$ asymptotic error constant vanishes (see the (18), (19) and (20)) and thereby the convergence order of the methods (6), (12) and (17) increases to three, five and nine, respectively. Since c_1 is not known a priori, we define the parameter α adaptively as follows

$$\alpha_{n+1} = -\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}, \quad n \ge 1.$$
(28)

For the first iterate, we choose a small α_1 . For evaluating, α_n through the preceding equation, we are using two previous iterates and it does not increase functional evaluations. However, the methods will now have memory [32]. A similar adaptive choice of a free parameter in a fourth order derivative free method is proposed by Peng et al [29]. However, the main reason for their choice is the stability of the method and not speed. Other adaptive choices are discussed in [13, 32].

In [27] a rich family of fourth order methods is introduced using three function evaluation. Methods of this family will be optimal in the sense of Kung and Traub and have an asymptotic error constant on the form

$$C_4(\alpha) = (1 + \alpha f'(\gamma))\Psi, \qquad (29)$$

where Ψ is a nonzero constant. It follows from Theorem 2 that the asymptotic error constant for method (M-4) is

$$\tilde{C}_4(\alpha) = (1 + \alpha f'(\gamma))^2 \tilde{\Psi}.$$
(30)

The constants Ψ and $\tilde{\Psi}$ depend on c_1 , c_2 and c_3 . The different asymptotic error constants play an important role with an adaptive choice of the parameter α where the method (**M-4**) with the adaptive choices (28) will have a higher rate of convergence than the corresponding Method(II) in [27]. A family of optimal fourth order derivative free methods with the same asymptotic error constant as (19) for $\alpha = 1$ is presented in [11]. However, these methods are not equivalent to (**M-4**).

The obtained three-point method (**M-8**) given by (17) is similar to the already known derivative free three-point methods proposed in [11, 13, 33, 34], however, they are not the same methods. Doing the same analysis as for (**M-4**) and the methods in the [27] it is interesting to note that the asymptotic rate of convergence for the three point method (**M-8**) with the adaptive choice (28) will be slightly lower than the family of three point methods in [13] with the same adaptive choice.

We conjecture that, for a 2^k - order iterative method formed by the scheme developed at the beginning of the §2, the error constant will behave like

$$e_{n+1} = \mathbf{C} \frac{(1+lpha c_1)^k}{c_1^{2^k-1}} e_n^{2^k}.$$

Here, k = 1, 2, 3, ... and **C** is a constant that depends upon $c_m = f^m(\gamma)/m!$ with m = 1, 2, ..., k+1. The general construction for higher order method devised in this paper shows that it is possible to construct derivative free optimal methods for any 2^k order with a constant α and with an adaptive choice the rate can be super 2^k -order.

3 Numerical examples

Let us review some optimal iterative methods for numerical comparison. Peng et al. [29] introduced an adaptive fourth order derivative free method.

$$\begin{cases} y_n = x_n - \alpha_n \frac{f(x_n)^2}{f(x_n) - f(x_n - \alpha_n f(x_n))}, \\ x_{n+1} = x_n - \alpha_n \frac{f(x_n)^2}{f(x_n) - f(x_n - \alpha_n f(x_n))} \\ \left\{ 1 + \frac{f(y_n)}{f(x_n)} + \left(1 + \frac{f(x_n)}{f(x_n - \alpha_n f(x_n))}\right) \left(\frac{f(y_n)}{f(x_n)}\right)^2 \right\} \end{cases}$$
(31)

where the adaptive parameter is chosen as

$$\alpha_{n+1} = \begin{cases} -\operatorname{sign}(f(x_n) - f(x_n - \alpha_n f(x_n))) \text{ provided } |\epsilon_n| < 10^{-3} \\ \frac{1}{\epsilon_n} & \text{otherwise} \end{cases}$$

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where $\epsilon_n = \frac{f(x) - f(x_n - \alpha_n f(x_n))}{\alpha_n f(x_n)}$ and the initial $\alpha_0 = 1$. The classical Kung-Traub optimal eight order method is given as

$$\begin{aligned} y_n &= x_n - \alpha \frac{f(x_n)^2}{f(w_n) - f(x_n)}, \\ z_n &= y_n - \frac{f(x_n)f(w_n)}{f(y_n) - f(x_n)} \quad \left\{ \frac{1}{[w_n, x_n; f]} - \frac{1}{[w_n, y_n; f]} \right\} \\ x_{n+1} &= z_n - \frac{f(x_n)f(w_n)f(y_n)}{f(z_n) - f(x_n)} \quad \left\{ \left(\frac{1}{f(z_n) - f(w_n)} \right) \left(\frac{1}{[y_n, z_n; f]} - \frac{1}{[w_n, y_n; f]} \right) \right\} \\ &- \left(\frac{1}{f(y_n) - f(x_n)} \right) \left(\frac{1}{[w_n, y_n; f]} - \frac{1}{[w_n, x_n; f]} \right) \right\} \end{aligned}$$
(32)

Here, $[s, t; f] = \frac{f(s) - f(t)}{s - t}$ for $s \neq t$ and $w_n = x_n + \alpha f(x_n)$. The eighth order derivative free method of Thukral [33] is given by

$$\begin{cases} y_n = x_n - \alpha \frac{f(x_n)^2}{f(w_n) - f(x_n)}, \\ z_n = y_n - \frac{[w_n, x_n; f]f(y_n)}{[x_n, y_n; f][w_n, y_n; f]} \\ x_{n+1} = z_n - \widehat{\mathcal{H}}_0 \frac{f(z_n)}{[y_n, z_n; f] - [x_n, y_n; f] + [x_n, z_n; f]} \end{cases}$$
(33)

where

$$\widehat{\mathcal{H}}_0 = \left(1 - \frac{f(z_n)}{f(w_n)}\right)^{-1} \left(1 + \frac{2f(y_n)^3}{f(w_n)^2 f(x_n)}\right)^{-1}.$$

The convergence order $\xi \in [1, \infty)$ of an iterative method is defined as

$$\lim_{n \to \infty} \frac{|e_{n+1}|}{|e_n|^{\xi}} = C \neq 0,$$

and furthermore this leads to the following approximation of the computational order of convergence (COC) (see [15] and the references therein):

$$\rho \approx \frac{\ln |(x_{n+1} - \gamma)/(x_n - \gamma)|}{\ln |(x_n - \gamma)/(x_{n-1} - \gamma)|}.$$
(34)

Computations are done in the programming language C⁺⁺. Scientific computations in many areas of science and engineering, for example climate modeling, planetary orbit calculations, Colomb *n*-body atomic systems, scattering amplitudes of quarks, nonlinear oscillator theory, Ising theory, quantum field theory, demand very high degree of numerical precision [5, 24]. For applications of high precision computations in experimental mathematics and physics, we refer to [7, and references therein]. Many applications of real-number computation require to evaluate elementary functions such as $\exp(x)$, $\tan^{-1}(x)$ to high precision (see for example [6]).

f(x)	<i>x</i> ₀	Method (31)	Method (32)	Method (33)	NM	M-2	M-4	M-8
$f_1(x)$	1.2	(6,4.24)	(16,8)	(16,8)	(20,2)	(16,2.4)	(15,4.5)	(16,8.5)
$f_2(x)$	-1.0	(7,4.24)	(20,8)	(20,8)	(22,2)	(18,2.4)	(18,4.4)	(16,8.5)
$f_3(x)$	1.5	(6,4.24)	(16,8)	(16,8)	(20,2)	(16,2.4)	(15,4.5)	(16,8.5)
$f_4(x)$	0.5	(5,5.69)	(16,11)	(16,11)	(18,2)	(14,3.5)	(15,5.7)	(16,11.6)
$f_5(x)$	1.3	(6,4.24)	(24,3)	(16,8)	(16,8)	(16,4.4)	(15,4.5)	(16,8.5)
$f_6(x)$	1.2	(7,4.24)	(20,8)	(20,8)	(26,2)	(18,2.4)	(18,4.5)	(20,8.5)

Table 1 Number of functional evaluations, COC for various iterative methods

For performing high precision computation, we are using the high precision C⁺⁺ library ARPREC [5]. The ARPREC library supports arbitrarily high level of numeric precision [5]. In the program, the precision in decimal digits is set with the command "mp::mp init(2005)"[5]. For convergence it is required: $|x_{n+1} - x_n| < \epsilon$ and $|f(x_n)| < \epsilon$. Here, $\epsilon = 10^{-320}$. We test the methods for the following functions

$f_1(x) = x^3 + 4x^2 - 10,$	$\gamma \approx 1.365.$
$f_2(x) = x \exp(x^2) - \sin^2(x) + 3\cos(x) + 5,$	$\gamma \approx -1.207$
$f_3(x) = \sin^2(x) - x^2 + 1,$	$\gamma \approx \pm 1.404$
$f_4(x) = \tan^{-1}(x)$	$\gamma = 0.$
$f_5(x) = x^4 + \sin\left(\pi/x^2\right) - 5,$	$\gamma = \sqrt{2}.$
$f_6(x) = e^{(-x^2 + x + 2)} - 1,$	$\gamma = 2.$

Computational results are reported in Tables 1, 2, 3, 4, 5 and 6. Table 1 presents pairs of numbers where the first element is the number of functional evaluations to reach the desired accuracy and the second element is COC – given in (34) – during the second last iterative step for various methods. While the Tables 2, 3, 4, 5 and 6 reports $|x_{n+1} - x_n|$, respectively, for the method (**M-4**), the method (**M-8**), (32), (33) and (31). In the method (32) and (33), $\alpha = 0.01$.

Table 2 Generated $|x_{n+1} - x_n|$ with $n \ge 0$ by the method (M-4). For x_0 see the Table 1

$f_1(x_n)$	$f_2(x_n)$	$f_3(x_n)$	$f_4(x_n)$	$f_5(x_n)$	$f_6(x_n)$
$1.6 \times 10^{-1} \\ 8.3 \times 10^{-5} \\ 3.1 \times 10^{-20} \\ 1.3 \times 10^{-88} \\ 7.1 \times 10^{-393} \\ \end{cases}$	2.0×10^{-1} 4.4×10^{-4} 1.5×10^{-15} 8.9×10^{-67} 1.2×10^{-294} 1.7×10^{-1308}	$9.5 \times 10^{-2} 2.7 \times 10^{-5} 1.2 \times 10^{-21} 4.5 \times 10^{-94} 1.6 \times 10^{-416} $	$5.0 \times 10^{-1} 5.6 \times 10^{-3} 3.4 \times 10^{-15} 6.5 \times 10^{-84} 2.1 \times 10^{-476} $	$\begin{array}{c} 1.1 \times 10^{-1} \\ 7.1 \times 10^{-5} \\ 6.8 \times 10^{-20} \\ 2.0 \times 10^{-86} \\ 1.3 \times 10^{-382} \end{array}$	$7.3 \times 10^{-1} 6.4 \times 10^{-2} 3.5 \times 10^{-6} 8.5 \times 10^{-25} 9.3 \times 10^{-108} 7.4 \times 10^{-477} $

$f_1(x_n)$	$f_2(x_n)$	$f_3(x_n)$	$f_4(x_n)$	$f_5(x_n)$	$f_6(x_n)$
1.6×10^{-1}	$2.0 imes 10^{-1}$	$9.5 imes 10^{-2}$	$4.9 imes 10^{-1}$	1.1×10^{-1}	$7.9 imes 10^{-1}$
3.3×10^{-9}	2.5×10^{-6}	4.0×10^{-10}	1.4×10^{-5}	1.1×10^{-8}	$8.6 imes 10^{-4}$
3.5×10^{-75}	$2.0 imes 10^{-47}$	$1.5 imes 10^{-81}$	1.1×10^{-60}	1.9×10^{-69}	1.8×10^{-26}
7.6×10^{-634}	1.0×10^{-395}	$3.0 imes 10^{-686}$	9.5×10^{-703}	1.6×10^{-583}	1.5×10^{-218}
*****	*****	****	****	*****	7.1×10^{-1846}

Table 3 Generated $|x_{n+1} - x_n|$ with $n \ge 0$ by the method (M-8). For x_0 see Table 1

An optimal iterative method for solving nonlinear equations must require least number of functional evaluations. In the Table 1, we notice that the developed methods are performing at least as good as existing optimal methods. Comparison among Tables 2, 3, 4, 5 and 6 reveal that the developed method are more efficient at reducing the error $|x_{n+1} - x_n|$ (the distance between two iterates – a measure of the residual). Thus developed methods are not only taking less iterations but they are also producing less residuals compared to the existing optimal methods.

3.1 Robustness of iterative methods with respect to initialization

It is known that iterative methods are locally convergent [4]. An iterative method may not converge if the initial guess is far from the zero of the function or if the derivative of the function vanishes during the iterative processes. Therefore we perform numerical tests to examine the robustness of iterative methods for several initialization. We find the zeros of the function

$$f(x) = \cos^2(x) - x/5,$$
(35)

for various initializations. Computational results are reported in the Table 7. In the proposed methods (6), (12) and (17), for the first iterate $\alpha = 1.0$ while for the successive iterates α is computed using the (28). Computational results are reported in the Table 7. We notice that the developed methods do display a robustness with respect to initialization.

$f_1(x_n)$	$f_2(x_n)$	$f_3(x_n)$	$f_4(x_n)$	$f_5(x_n)$	$f_6(x_n)$
$1.6 imes 10^{-1}$	$2.0 imes 10^{-1}$	$9.5 imes 10^{-2}$	$5.0 imes 10^{-1}$	1.1×10^{-1}	$7.9 imes 10^{-1}$
$8.9 imes 10^{-8}$	1.6×10^{-4}	$4.5 imes 10^{-9}$	1.7×10^{-5}	1.2×10^{-8}	$6.6 imes 10^{-3}$
$3.3 imes 10^{-58}$	2.8×10^{-29}	2.1×10^{-67}	$1.7 imes 10^{-54}$	$3.5 imes 10^{-64}$	4.5×10^{-17}
1.25×10^{-461}	1.9×10^{-227}	5.6×10^{-534}	$1.5 imes 10^{-593}$	1.8×10^{-508}	2.2×10^{-130}
*****	1.8×10^{-1812}	****	*****	*****	8.4×10^{-1037}

Table 4 Generated $|x_{n+1} - x_n|$ with $n \ge 0$ by the method (32). For x_0 see the Table 1

$f_1(x_n)$	$f_2(x_n)$	$f_3(x_n)$	$f_4(x_n)$	$f_5(x_n)$	$f_6(x_n)$
1.6×10^{-1} 1.5×10^{-7} 3.3×10^{-56} 1.5×10^{-445}	2.0×10^{-1} 2.8×10^{-3} 8.3×10^{-19} 4.2×10^{-143} 1.9×10^{-1137}	9.5×10^{-2} 3.5×10^{-9} 2.9×10^{-68} 6.6×10^{-541}	4.9×10^{-1} 4.3×10^{-5} 4.3×10^{-50} 4.5×10^{-545}	$1.1 \times 10^{-1} \\ 1.5 \times 10^{-8} \\ 6.4 \times 10^{-63} \\ 6.2 \times 10^{-498} \\ ***********************************$	7.9×10^{-1} 2.7 × 10 ⁻³ 5.6 × 10 ⁻²⁰ 2.0 × 10 ⁻¹⁵³ 4.8 × 10 ⁻¹²²¹

Table 5 Generated $|x_{n+1} - x_n|$ with $n \ge 0$ by the method (33). For x_0 see the Table 1

3.2 Numerical results for nonsmooth function

Here, we compare the methods **M-2**, **M-4** and **M-8** with the corresponding optimal second, fourth and eighth order methods proposed in the enriching work [12] by Cordero et al. for the following nonsmooth function

$$f(x) = |x^2 - 9|.$$

The above function is of special interest because it has severe stability problems near the nonsmoothness [12, cf.]. Optimal derivative free methods of order 2^n developed by Cordero et al. [12] are

$$\begin{cases} y_0 = x_k, \\ y_1 = y_0 + f(y_0), \\ y_{j+1} = y_j - \frac{f(y_j)}{a^j} \\ x_{k+1} = y_{n+1}, \end{cases} \text{ for } j = 1, 2, 3, \dots, n,$$

where

$$a_{j} = \sum_{i=0}^{j-1} \left(\prod_{k=0, k \neq i}^{j-1} \frac{y_{k} - y_{j}}{y_{k} - y_{i}} \right) [y_{i}, y_{j}; f].$$

Table 6 Generated $|x_{n+1} - x_n|$ with $n \ge 0$ by the method (31). For x_0 see the Table 1

$f_1(x_n)$	$f_2(x_n)$	$f_3(x_n)$	$f_4(x_n)$	$f_5(x_n)$	$f_6(x_n)$
1.3×10^{-1} 3.6 × 10 ⁻² 3.7 × 10 ⁻⁷ 5.0 10 ⁻²⁹	1.6×10^{-7} 2.7×10^{-1} 6.3×10^{-2}	9.4×10^{-2} 1.4×10^{-3} 9.0×10^{-13}	5.0×10^{-1} 4.3×10^{-5} 1.0×10^{-25}	8.4×10^{-2} 2.9×10^{-2} 6.8×10^{-7} $4.0 - 10^{-27}$	2.5×10^{0} 3.0×10^{-1} 3.9×10^{-3}
5.8×10^{-29} 2.3×10^{-121} 9.8×10^{-513} *********	2.3×10^{-6} 1.4×10^{-24} 5.1×10^{-101} 4.9×10^{-425}	4.5×10^{-32} 1.4×10^{-218} 6.6×10^{-924} $************************************$	$4.9e - 145$ 4.4×10^{-824} $************************************$	4.9×10^{-27} 1.9×10^{-112} 3.4×10^{-474} $************************************$	2.2×10^{-11} 1.5×10^{-45} 1.9×10^{-190} 4.2×10^{-804}

<i>x</i> ₀	NM	M-2	M-4	M-8
-0.1	div	(18, 2.4)	(24, 4.4)	(32, 8.4)
0.0	(75, 1)	(20, 2.4)	(21, 4.4)	(24, 8.4)
-10000	div	(24, 2.4)	(24, 4.4)	(24, 2.4)
10000	div	(24, 4.5)	(24, 4.4)	(24, 2.4)

Table 7 Performance of methods NM (1), M-2, M-4 and M-8 for initializations for the function (35)

Here, $[y_i, y_j; f]$ denotes the divided difference $(f(y_i) - f(y_j))/(y_i - y_j)$. Using n = 1, 2, 3 - in the above algorithm – will produce, respectively, second, fourth and eighth order methods. Let us represent these methods by **C-2**, **C-4** and **C-8**. Table 8 reports our numerical work.

In the Table 8, we see that the developed methods are performing at least as well as the recently developed methods by Cordero et al. [12].

Initialization	Methods	$ f(x_{n+1}) $	$ x_{n+1} - x_n $	n	ρ	γ
$x_0 = 2$	M-2	$1.7 imes 10^{-878}$	3.5×10^{-364}	12	2.4	3.0
	M-4	0.0	$5.8 imes 10^{-874}$	7	4.5	3.0
	M-8	0.0	5.0×10^{-324}	5	8.4	3.0
	C-2			$> \times 10^4$		
	C-4			$> \times 10^4$		
	C-8	0.0	2.4×10^{-982}	5	8.0	3.0
$x_0 = 2.8$	M-2	9.3×10^{-847}	4.9×10^{-351}	9	2.4	3.0
	M-4	0.0	2.8×10^{-1416}	7	4.5	3.0
	M-8	0.0	6.7×10^{-1923}	5	8.5	3.0
	C-2	7.7×10^{-1172}	1.1×10^{-586}	31	2.0	3.0
	C-4	9.6×10^{-321}	9.6×10^{-322}	1567	1.4	3.0
	C-8	0.0	6.1×10^{-1270}	5	8.0	3.0
$x_0 = -2.8$	M-2	4.8×10^{-1773}	1.0×10^{-734}	9	2.4	-3.0
	M-4	0.0	1.1×10^{-947}	7	4.5	-3.0
	M-8	0.0	6.7×10^{-1923}	5	8.5	-3.0
	C-2			$> \times 10^4$		
	C-4	$7.5 imes 10^{-321}$	7.5×10^{-322}	1572	1.4	-3.0
	C-8	1.3×10^{-890}	1.3×10^{-889}	12	$3.4 \times 10^{+02}$	-3.0
$x_0 = -10.0$	M-2	$9.5 imes 10^{-827}$	9.2×10^{-343}	10	2.4	-3.0
	M-4	0.0	4.2×10^{-941}	7	4.5	-3.0
	M-8	0.0	6.5×10^{-1312}	5	8.5	-3.0
	C-2			$> \times 10^4$		
	C-4			$> \times 10^4$		
	C-8	2.0×10^{-373}	1.9×10^{-372}	13	$1.4\times10^{+02}$	-3.0

Table 8 Numerical results for nonsmooth function

4 Conclusions

In this work, we have developed a scheme to generate families of higher order derivative free methods. By choosing the parameter adaptively the methods show a higher rate of convergence than the corresponding method for a fixed value of the parameter. Computational results demonstrate that family of methods are efficient and exhibit better performance compared with other well known methods using derivatives and derivative free methods.

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