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A new technique to obtain derivative-free optimal iterative methods for solving nonlinear equations[☆]

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ABSTRACT

A new technique to obtain derivative-free methods with optimal order of convergence in the sense of the Kung–Traub conjecture for solving nonlinear smooth equations is described. The procedure uses Steffensen-like methods and Padé approximants. Some numerical examples are provided to show the good performance of the new methods.

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1. Introduction

A variety of problems in different fields of science and technology require to find the solution of a nonlinear equation. Iterative methods for approximating solutions are the most used technique. The efficiency index, introduced by Ostrowski in [1], establishes the effectiveness of the iterative method. In this sense, Kung and Traub conjectured in [2] that a method is optimal if it reaches an order of convergence $p = 2^{n-1}$, where n is the number of functional evaluations per step.

Newton's method is optimal for $n = 2$, but it uses the derivative, which can be a drawback in some applications. Steffensen's method (SM), (see [3]) is not only optimal but also derivative free,

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

where $z_n = x_n + f(x_n)$.

In this work, we introduce a technique to obtain optimal order methods for $n = 3, 4, \dots$. The idea is to compose an optimal derivative-free method with a modified Newton's step in which the derivative is estimated using a Padé approximant.

The paper is organized as follows. In Section 2 we apply the technique to Steffensen's method, obtaining an optimal fourth order method and prove a convergence result. In the next section, the technique is generalized for getting higher order derivative-free optimal methods. Finally, different numerical tests confirm the theoretical results. In this numerical section, we also analyze the behavior of the new schemes on nonsmooth equations.

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2. Fourth order optimal method

We first compose the well-known Steffensen method, defined by (1), with Newton's method obtaining the fourth order scheme

$$\begin{aligned} y_n &= x_n - \frac{f(x_n)^2}{f(z_n) - f(x_n)}, \\ x_{n+1} &= y_n - \frac{f(y_n)}{f'(y_n)}, \end{aligned} \quad (2)$$

where $z_n = x_n + f(x_n)$. Now, in order to avoid the evaluation of $f'(y_n)$, we approximate it by the derivative $m'(y_n)$ of the following first degree Padé approximant

$$m(t) = \frac{a_1 + a_2(t - y_n)}{1 + a_3(t - y_n)},$$

where a_1 , a_2 and a_3 are real parameters to be determined satisfying the following conditions:

$$m(x_n) = f(x_n), \quad (3)$$

$$m(y_n) = f(y_n), \quad (4)$$

and

$$m(z_n) = f(z_n). \quad (5)$$

From (4) one immediately obtains

$$a_1 = f(y_n).$$

Conditions (3) and (5), give, respectively,

$$a_2 - f(x_n)a_3 = f[x_n, y_n]$$

and

$$a_2 - f(z_n)a_3 = f[z_n, y_n],$$

where $f[x_n, y_n]$ denotes the divided difference $\frac{f(x_n) - f(y_n)}{x_n - y_n}$. After some algebraic manipulations, the following values are obtained for the parameters:

$$a_2 = f[y_n, z_n] - \frac{f(z_n)f[x_n, y_n, z_n]}{f[z_n, x_n]}$$

and

$$a_3 = -\frac{f[x_n, y_n, z_n]}{f[x_n, z_n]},$$

where $f[x_n, y_n, z_n] = \frac{f[x_n, y_n] - f[y_n, z_n]}{x_n - z_n}$ is a second order divided difference.

The derivative of the Padé approximant evaluated in y_n can be expressed as

$$m'(y_n) = \frac{f[x_n, y_n]f[y_n, z_n]}{f[x_n, z_n]}. \quad (6)$$

Substituting (6) in the second equation of (2), we obtain a new iterative method denoted by M_4 , whose expression is:

$$y_n = x_n - \frac{f(x_n)^2}{f(z_n) - f(x_n)}, \quad (7)$$

$$x_{n+1} = y_n - \frac{f(y_n)f[x_n, z_n]}{f[x_n, y_n]f[y_n, z_n]}. \quad (8)$$

Let us note that in each iteration we only evaluate $f(x_n)$, $f(y_n)$ and $f(z_n)$, so that the method will be optimal in the sense of Kung–Traub's conjecture if we show that its convergence order is 4.

Theorem 1. Let $\alpha \in I$ be a simple zero of a sufficiently differentiable function $f : I \subseteq \mathbb{R} \rightarrow \mathbb{R}$ in an open interval I . If x_0 is sufficiently close to α , then the method M_4 defined by (7)–(8) has optimal convergence order 4.

Proof. Let e_n be the error in x_n , that is $e_n = x_n - \alpha$. By using Taylor's expansion around $x = \alpha$, we write

$$f(x_n) = c_1 e_n + c_2 e_n^2 + c_3 e_n^3 + c_4 e_n^4 + O(e_n^5), \quad (9)$$

where $c_k = f^{(k)}(\alpha)/k!$, $k = 1, 2, \dots$

Using that $z_n = x_n + f(x_n)$, we write

$$\begin{aligned} f(z_n) &= c_1 (1 + c_1) e_n + (c_1 + (1 + c_1)^2) c_2 e_n^2 + (2(1 + c_1) c_2^2 + c_1 c_3 + (1 + c_1)^3 + c_3) e_n^3 \\ &\quad + (3(1 + c_1)^2 c_2 c_3 + c_2 (c_2^2 + 2(1 + c_1) c_3) + c_1 c_4 + (1 + c_1)^4 c_4) e_n^4 + O(e_n^5). \end{aligned} \quad (10)$$

Substituting (9) and (10) in (7) we have

$$\begin{aligned} y_n - \alpha &= \left(1 + \frac{1}{c_1}\right) c_2 e_n^2 + \frac{-(2 + 2c_1 + c_1^2) c_2^2 + c_1 (2 + 3c_1 + c_1^2) c_3}{c_1^2} e_n^3 \\ &\quad + \frac{(4 + 5c_1 + 3c_1^2 + c_1^3) c_2^3 - c_1 (7 + 10c_1 + 7c_1^2 + 2c_1^3) c_2 c_3}{c_1^3} e_n^4 \\ &\quad + \frac{c_1^2 (3 + 6c_1 + 4c_1^2 + c_1^3) c_4}{c_1^3} e_n^4 + O(e_n^5). \end{aligned} \quad (11)$$

Then,

$$\begin{aligned} f(y_n) &= (1 + c_1) c_2 e_n^2 + \frac{-(2 + 2c_1 + c_1^2) c_2^2 + c_1 (2 + 3c_1 + c_1^2) c_3}{c_1} e_n^3 \\ &\quad + \frac{(5 + 7c_1 + 4c_1^2 + c_1^3) c_2^3 - c_1 (7 + 10c_1 + 7c_1^2 + 2c_1^3) c_2 c_3}{c_1^2} e_n^4 \\ &\quad + \frac{c_1^2 (3 + 6c_1 + 4c_1^2 + c_1^3) c_4}{c_1^2} e_n^4 + O(e_n^5). \end{aligned} \quad (12)$$

Using (8) we obtain

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

showing that the method is of fourth order. \square

3. Higher order optimal methods

This technique can be applied to a higher order multistep method using higher degree Padé's approximations for the derivative that appears when adding a Newton's step.

Recently, in [4] Ren et al. derive a one-parameter class of fourth order methods with three functional evaluations per step. In these methods, an interpolation polynomial of order three is used to get a better approximation to the derivative of the given function. Other Steffensen type methods and their applications are also discussed by Liu et al. in [5] and by Zheng et al. in [6] and by Feng and He in [7].

In [8], Cordero and Torregrosa obtain a family of optimal fourth-order methods, that we will denote by CT_4 and is given by:

$$x_{n+1} = y_n - \frac{f(y_n)}{\frac{f(y_n) - b f(z_n)}{y_n - z_n} + \frac{f(y_n) - d f(x_n)}{y_n - x_n}}, \quad (13)$$

where y_n is the approximation of the Steffensen's method (1) and $b, d \in \mathbb{R}$ are parameters such as $b + d = 1$.

Our aim now is to obtain optimal order derivative free methods for $n = 4$, starting from any optimal fourth order method.

So, let us consider ψ_4 a function that defines an optimal fourth order derivative free iterative method, which we compose with Newton's scheme. If a Padé approximant of degree two is applied to the estimation of the derivative in the last step, the resulting method will appear as:

$$\begin{aligned} y_n &= x_n - \frac{f(x_n)^2}{f(z_n) - f(x_n)}, \\ u_n &= \psi_f(x_n, y_n, z_n), \\ x_{n+1} &= u_n - \frac{f(u_n)}{\tilde{m}'(u_n)}, \end{aligned} \quad (14)$$

where $\bar{m}(t) = \frac{b_1 + b_2(t-u_n) + b_3(t-u_n)^2}{1 + b_4(t-u_n)}$, and the parameters b_1, b_2, b_3 and b_4 satisfy the following conditions:

$$\bar{m}(x_n) = f(x_n), \quad (15)$$

$$\bar{m}(y_n) = f(y_n), \quad (16)$$

$$\bar{m}(z_n) = f(z_n), \quad (17)$$

and

$$\bar{m}(u_n) = f(u_n). \quad (18)$$

Again, from (18) one obtains

$$b_1 = f(u_n),$$

and, by solving the system described by (15)–(17) in a similar way as before, the following values are obtained for the parameter b_4 :

$$b_4 = \frac{f[y_n, u_n, x_n] - f[y_n, u_n, z_n]}{f[y_n, z_n] - f[y_n, x_n]}$$

and also b_3 :

$$b_3 = f[y_n, u_n, z_n] + b_4 f[y_n, z_n]$$

and b_2 :

$$b_2 = f[y_n, u_n] - b_3(y_n - u_n) + f(y_n)b_4.$$

Therefore the derivative of the second-degree Padé approximant can be expressed as

$$\bar{m}'(u_n) = b_2 - b_1 b_4. \quad (19)$$

Substituting (19) in (14), we obtain a new scheme, denoted by $M\psi_8$, whose iterative expression is:

$$y_n = x_n - \frac{f(x_n)^2}{f(z_n) - f(x_n)}, \quad (20)$$

$$u_n = \psi_4(x_n, y_n, z_n), \quad (21)$$

$$x_{n+1} = u_n - \frac{f(u_n)}{b_2 - b_1 b_4}. \quad (22)$$

Let us notice that in each iteration we evaluate $f(x_n), f(y_n), f(z_n)$ and $f(u_n)$, so that the method will be optimal, if we show that its convergence order is 8.

Theorem 2. Let $\alpha \in I$ be a simple zero of a sufficiently differentiable function $f : I \subseteq \mathbb{R} \longrightarrow \mathbb{R}$ in an open interval I . If x_0 is sufficiently close to α , then the method $M\psi_8$ defined by (20)–(22) has optimal convergence order 8.

Proof. Let e_n be the error of x_n , that is, $e_n = x_n - \alpha$. Taylor's expansion of $f(x)$ around α gives

$$f(x_n) = c_1 e_n + c_2 e_n^2 + c_3 e_n^3 + c_4 e_n^4 + \cdots + c_7 e_n^7 + c_8 e_n^8 + O(e_n^9), \quad (23)$$

where $c_k = \frac{f^{(k)}(\alpha)}{k!}$, $k = 1, 2, \dots$. Using that $z_n = x_n + f(x_n)$, we write

$$f(z_n) = c_1 (1 + c_1) e_n + (c_1 + (1 + c_1)^2) c_2 e_n^2 + (2(1 + c_1) c_2^2 + c_1 c_3 + (1 + c_1)^3 + c_3) e_n^3 + O(e_n^4). \quad (24)$$

Substituting (23) and (24) in (20) we have

$$\begin{aligned} y_n - \alpha &= \left(1 + \frac{1}{c_1}\right) c_2 e_n^2 + \frac{(2 + 2c_1 + c_1^2) c_2^2 + c_1 (2 + 3c_1 + c_1^2) c_3}{c_1^2} e_n^3 \\ &\quad + \frac{(4 + 5c_1 + 3c_1^2 + c_1^3) c_2^3 - c_1 (7 + 10c_1 + 7c_1^2 + 2c_1^3) c_2 c_3}{c_1^3} e_n^4 \\ &\quad + \frac{c_1^2 (3 + 6c_1 + 4c_1^2 + c_1^3) c_4}{c_1^3} e_n^4 + O(e_n^5) \end{aligned} \quad (25)$$

and

$$\begin{aligned} f(y_n) = & (1 + c_1) c_2 e_n^2 + \frac{-(2 + 2c_1 + c_1^2) c_2^2 + c_1 (2 + 3c_1 + c_1^2) c_3}{c_1} e_n^3 \\ & + \frac{(5 + 7c_1 + 4c_1^2 + c_1^3) c_2^3 - c_1 (7 + 10c_1 + 7c_1^2 + 2c_1^3) c_2 c_3}{c_1^2} e_n^4 \\ & + \frac{c_1^2 (3 + 6c_1 + 4c_1^2 + c_1^3) c_4}{c_1^2} e_n^4 + O(e_n^5). \end{aligned} \quad (26)$$

Assume that u_n is obtained by means of a fourth order method. Then

$$u_n - \alpha = h_4 e_n^4 + h_5 e_n^5 + h_6 e_n^6 + h_7 e_n^7 + h_8 e_n^8 + O(e_n^9), \quad (27)$$

and so,

$$f(u_n) = c_1 h_4 e_n^4 + c_1 h_5 e_n^5 + c_1 h_6 e_n^6 + c_1 h_7 e_n^7 + (c_2 h_4^2 + c_1 h_8) e_n^8 + O(e_n^9). \quad (28)$$

By computing (19) and substituting in (22) we obtain

$$x_{n+1} - \alpha = \frac{-(1 + c_1)^2 c_3^2 + c_2 ((1 + c_1)^2 c_4 + c_1 h_4)}{c_1^2} h_4 e_n^8 + O(e_n^9), \quad (29)$$

showing that the method is of eighth order. \square

This result has been just obtained independently by Soleymani et al. in [9].

The same procedure can be applied to obtain higher-order optimal methods. In this case, we can write

$$\begin{aligned} y_n &= x_n - \frac{f(x_n)^2}{f(z_n) - f(x_n)}, \\ u_n &= \psi_4(x_n, y_n, z_n), \\ v_n &= \varphi_8(x_n, y_n, z_n, u_n), \\ x_{n+1} &= v_n - \frac{f(v_n)}{\bar{m}'(v_n)}, \end{aligned} \quad (30)$$

where ψ_4 and φ_8 are the iteration functions of optimal iterative methods of orders 4 and 8, respectively. Now, the Pade's approximant is of third degree

$$\bar{m}(t) = \frac{b_1 + b_2(t - v_n) + b_3(t - v_n)^2 + b_4(t - v_n)^3}{1 + b_5(t - v_n)},$$

and the parameters b_1, b_2, b_3, b_4 and b_5 can be determined analogously to the previous cases. Then, by substituting the approximation of the derivative $\bar{m}'(v_n) = b_2 - b_1 b_5$, in (30) a new method is defined. We give the following result for the error equation in this case.

Theorem 3. Let $\alpha \in I$ be a simple zero of a sufficiently differentiable function $f : I \subseteq \mathbb{R} \rightarrow \mathbb{R}$ in an open interval I . If x_0 is sufficiently close to α , then the method $M\psi\varphi_{16}$ defined by (30) has optimal convergence order 16, and satisfies the following relation:

$$e_{n+1} = \frac{c_2 j_9 ((1 + c_1)^2 c_4^2 h_4 - c_3 ((1 + c_1)^2 c_5 h_4 - c_1 j_9))}{c_1^2 c_3} e_n^{16} + O(e_n^{17})$$

where $c_k = \frac{f^{(k)}(\alpha)}{k! f'(\alpha)}$, $k = 1, 2, \dots, 16$, and h_k, j_k , $k = 1, 2, \dots, 16$ are the generic coefficients of the error equation for methods of fourth and eighth orders given by ψ_4 and φ_8 , that is:

$$\begin{aligned} u_n - \alpha &= h_4 e_n^4 + h_5 e_n^5 + \dots + h_{16} e_n^{16} + O(e_n^{17}), \\ v_n - \alpha &= j_8 e_n^8 + j_9 e_n^9 + \dots + j_{16} e_n^{16} + O(e_n^{17}). \end{aligned}$$

Table 1
Numerical results for function (32).

	SM		M_4		M_8		M_{16}	
	Iter	Error	Iter	Error	Iter	Error	Iter	Error
$x_0 = 0.1$								
$\alpha = 0$	1	4.52e-2	1	1.98e-2	1	6.74e-3	1	2.96e-3
	2	4.60e-3	2	7.23e-3	2	6.18e-5	2	1.18e-011
	⋮		⋮		⋮		⋮	
incr1	8	9.98e-124	7	6.50e-92	7	5.82e-130	4	5.01e-091
	9	2.99e-246	8	8.45e-183	8	5.08e-259	5	7.54e-182
	incr2	9.98e-124	6.50e-92	5.82e-130	5.01e-091			
ρ	2.99e-246	8.45e-183	1.02e-258	7.54e-182				
ρ	2.0058	2.0000	2.0000					
$x_0 = 5$								
$\alpha = 1$	1	2.70	1	1.42	1	3.83e-1	1	8.32e-2
	2	1.21	2	0.57	2	3.25e-1	2	3.61e-16
	⋮		⋮		⋮		3	1.32e-246
incr1	11	1	6	2.28e-081	4	4.76e-36		
	12	1	7	5.43e-323	5	1.08e-282		
	incr2	2.76e-080	2.28e-081	4.78e-36	3.61e-16			
ρ	3.05e-159	1.09e-322	2.17e-282	2.64e-246				
ρ	2.0000	4.0000	7.7025	8.5860				
$x_0 = -10$								
$\alpha = -1$	1	8.36	1	4.13	1	1.73	1	6.72e-1
	2	7.71	2	1.64	2	8.08e-1	2	2.40e-3
	⋮		⋮		⋮		3	2.07e-62
incr1	15	9.08e-130	11	6.06e-37	9	1	4	0
	16	0	12	9.88e-218	10	1		
	incr2	9.04e-130	6.06e-037	1.115e-142	2.07e-062			
ρ	0.0000	9.88e-218	4.90e-285	0				
ρ	3.0000	–	2.0000	–				

4. Numerical results

In this section we check the effectiveness of the new optimal methods comparing them with Steffensen's method and also with the method of which they are derived. Specifically, we consider the new fourth-order method M_4 introduced in (7) and the method CT_4 given by (13). Applying (20), we obtain the new optimal methods M_8 and CT_8 and using (30), we derive methods M_{16} and CT_{16} .

Nowadays, high-order methods are important because numerical applications use high precision in their computations; for this reason numerical tests have been carried out using variable precision arithmetic in MATLAB 7.1. with 2000 significant digits.

Tables 1 and 2 show for each initial estimation and every method, the exact absolute error at first and last iterations, the number of iterations required to obtain $\text{incr1} = |x_{k+1} - x_k| < 10^{-150}$ or $\text{incr2} = |f(x_{k+1})| < 10^{-150}$ and the corresponding computational order of convergence ρ (usually called ACOC), defined by Cordero and Torregrosa in [10]:

$$p \approx \rho = \frac{\ln(|x_{k+1} - x_k|/|x_k - x_{k-1}|)}{\ln(|x_k - x_{k-1}|/|x_{k-1} - x_{k-2}|)}. \quad (31)$$

The value of ρ appearing in Tables 1 and 2 is the last component of the vector defined by (31), when it is stable. In other cases we will denote it by '-'. The tests have been made on the nonsmooth function:

$$f(x) = \begin{cases} x(x+1), & \text{if } x < 0, \\ -2x(x-1), & \text{if } x \geq 0, \end{cases} \quad (32)$$

that can be found in [11]. We use three initial estimations in order to approximate the three different roots of the equation, $\{-1, 0, 1\}$. From Table 1 it can be inferred that, as every root is close to each other, the initial estimation must be quite good

Table 2

More numerical results for function (32).

	CT_4		CT_8		CT_{16}	
	Iter	Error	Iter	Error	Iter	Error
$x_0 = 0.1$						
$\alpha = 0$	1	1.93e-2	1	6.73e-3	1	2.93e-3
	2	6.95e-4	2	6.18e-5	2	1.14e-11
	⋮		⋮		⋮	
	8	6.45e-184	8	5.68e-130	4	3.76e-91
	9	0	9	4.85e-259	5	4.25e-182
incr1	6.45e-184		5.68e-130		3.76e-91	
incr2	0		9.69e-259		4.25e-182	
ρ	2.0000		2.0000		-	
$x_0 = 5$						
$\alpha = 1$	1	1.44	1	3.97e-1	1	8.79e-2
	2	5.25e-1	2	3.27e-1	2	5.66e-17
	⋮		⋮		3	1.10e-260
	6	2.87e-197	5	1.34e-137		
	7	0	6	0		
incr1	2.87e-197		1.34e-137		5.66e-17	
incr2	0		0		2.21e-260	
ρ	4.0000		8.0017		9.2156	
$x_0 = -10$						
$\alpha = -1$	1	4.29	1	1.82	1	7.15e-1
	2	1.82	2	5.30e-1	2	1.32e-3
	⋮		⋮		3	8.33e-70
	7	1.98e-323	4	1.08e-17	4	0
	8	0	5	2.53e-204		
incr1	1.98e-323		1.08e-17		8.33e-70	
incr2	0		2.53e-204		0	
ρ	5.9990		-		-	

if convergence to the central root is looked for. In fact, for $x_0 = 5$, Steffensen's method converges to 0 (instead of 1) and, for $x_0 = -10$, method M_8 converges to 0, instead of the closest root, -1 .

Moreover, when $x_0 = 0.1$, the nonsmoothness of the function (32) in 0 is the reason why the estimated order of convergence is 2 for all the methods, except in the case of M_{16} and CT_{16} in which, although ρ is not stable, a visible reduction of the number of iterations shows the better behavior of these methods. In this case, the stability problems do not allow the order of convergence to reach the theoretical one (let us remember that these orders of convergence have been calculated under the assumption of the smoothness of the nonlinear function).

When the initial approximation is near 1 or -1 , the behavior of the methods is stable and the ACOC is near the theoretical order of convergence. High-order methods are shown to be more efficient when the root is far enough; for $x_0 = -10$, the number of iterations needed have been reduced in a reason of 1/4 from Steffensen's method. It must be also taken into account that, for (32), it is verified that $c_1 = 1$, so the theoretical order of convergence for all the methods involved, from SM to CT_{16} , are higher than in the standard case. The specific order of convergence will depend on each method.

5. Conclusions

We have introduced a new technique which applied to optimal derivative-free methods of order 2, 4 and 8 provides new optimal derivative-free methods of order 4, 8 and 16. We think that this behavior will remain for higher order methods. The procedure uses Steffensen-like methods and Padé approximant. Some numerical tests are provided on a nonsmooth function to show the good performance of the new methods.

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