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Optimal derivative-free root finding methods based on the Hermite interpolation

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Abstract

We develop n-point optimal derivative-free root finding methods of order 2^n, based on the Hermite interpolation, by applying a first-order derivative transformation. Analysis of convergence confirms that the optimal order of convergence of the transformed methods is preserved, according to the conjecture of Kung and Traub. To check the effectiveness and reliability of the newly presented methods, different type of nonlinear functions are taken and compared. ©2016 all rights reserved.

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1. Introduction

Nonlinear problems frequently arise in real life situations. Commonly, mathematical models arise in modeling of the problems of electrical, mechanical, civil, and chemical engineering, which ends up with a nonlinear equation or a system of nonlinear equations. Moreover, nonlinear problems are commonly found in number theory, modeling and simulation, and cryptography. Therefore, the development of efficient methods for finding the solution of nonlinear equations has been of great importance. Various one-point and multipoint root finding methods, were developed in recent past (see for example [1–3, 5, 7, 12]). A significant one-point method is Newton's method, which bears a second order of convergence and is optimal according to the conjecture of Kung and Traub [10]. Newton's method requires one functional and one derivative

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evaluation for the completion of one computational cycle. But the method is very sensitive regarding the choice of initial guess. One more drawback of it is frequent unavailability of the first derivative of the function, so we have another attraction, which is to develop iterative schemes without requiring any derivatives. For comparison of root finding methods, Ostrowski [4] coined the concept of efficiency index: "the efficiency index of an iterative method is $\theta^{1/\nu}$ where θ represents the order of convergence of an iterative method and ν is the number of functional evaluations per iteration". We say that an iterative method is more efficient if it takes less time and evaluations to provide fast and accurate approximations. The development of highly efficient multipoint root finding methods has been focused by many researchers in the last decade.

Steffensen [9] approximate the first derivative arising in the Newton's method by

$$f'(x_n) \approx \frac{f(x_n) - f(w_n)}{x_n - w_n} = f[x_n, w_n] \tag{1.1}$$

and obtain the following iterative scheme

$$x_{n+1} = x_n - \frac{f(x_n)}{f[w_n, x_n]}, \quad n \geq 0 \tag{1.2}$$

with second order convergence, where $w_n = x_n + f(x_n)$. Recently Cordero and Torregrosa in [1] used the following approximation of the first derivative

$$f'(x_n) \approx f[x_n, w_n], w_n = x_n + \gamma f(x_n)^m, m \geq q, \gamma \in \mathbb{R} - \{0\} \tag{1.3}$$

to transform a three point eighth order with-derivative method, to a derivative-free method by preserving the order of convergence. We generalize transformation (1.3) to transform n-point optimal methods involving first derivative, based on the Hermite interpolation.

In Section 2, we present 2-point, 3-point, 4-point and n-point optimal derivative-free methods based on the Hermite interpolation. We wish that the first derivative at each successive iterate is approximated using the Hermite interpolation. Hence first we construct a two-point with-derivative iterative method, then transform this newly developed two-point iterative method to derivative-free. The 3-point, 4-point and $n-$point methods are transformed forms of existing optimal with-derivative methods based on the Hermite interpolation. We apply the transformation (1.3) in such a way that the optimal order of convergence of newly developed Hermite interpolation based schemes is preserved. Analysis of convergence of the newly developed schemes are also given. In Section 3, we give numerical comparison of the presented methods with the existing methods of same domain.

2. Transforming with-derivative methods based on the Hermite interpolation into derivative-free methods

In this section, first we develop two, three, four, and n-point with-derivative methods based on the Hermite interpolation and then use (1.3) to transform the with-derivative optimal methods based on the Hermite interpolation to derivative-free ones.

2.1. *Optimal two-point fourth-order method*

For a construction of an optimal fourth-order two-point method using three function evaluations, we use the following quadratic polynomial,

$$f(t) = H_2(t) = a_0 + a_1(t - x) + a_2(t - x)^2, \tag{2.1}$$

satisfying

$$f(x) = H_2(x), f'(x) = H_2'(x), f(y) = H_2(y). \tag{2.2}$$

By using (2.2) we get

$$a_0 = f(x), \tag{2.3}$$

$$a_1 = f'(x) = H_2'(x), \tag{2.4}$$

$$a_2 = \frac{f[y,x] - f'(x)}{(y-x)}. \tag{2.5}$$

Hence, by using the values of a_1 and a_2, we obtain

$$H_2'(y_n) = 2f[y_n, x_n] - f'(x_n). \tag{2.6}$$

By using (2.6), we obtain the following two-point optimal with-derivative method:

$$\begin{aligned} y_n =& x_n - \frac{f(x_n)}{f'(x_n)}, n \geq 0, \\ x_{n+1} =& y_n - \frac{f(y_n)}{2f[y_n, x_n] - f'(x_n)}. \end{aligned} \tag{2.7}$$

Theorem 2.1. *Let $f : D \subseteq \mathbb{R} \to \mathbb{R}$ be a sufficiently differentiable function in an open interval D and α a simple root of f. If x_0 is close enough to α, then the iterative scheme defined by (2.7) is of optimal order 4 and has the following error equation:*

$$e_{n+1} = c_2(-c_3 + c_2^2)e_n^4 + O(e_n^5), \tag{2.8}$$

where, $c_j = \frac{f^{(j)}(\alpha)}{j!f'(\alpha)}, j \geq 2$ and $e_n = x_n - \alpha$.

Proof. By using Taylor's expansions about α, we have

$$f(x_n) = f'(\alpha)[e_n + c_2e_n^2 + c_3e_n^3 + c_4e_n^4] + O(e_n^5)$$

and

$$f'(x_n) = f'(\alpha)[1 + 2c_2e_n + 3c_3e_n^2 + 4c_4e_n^3] + O(e_n^4).$$

By substituting above expressions in the first step of (2.7), we get

$$y_n - \alpha = c_2e_n^2 + (2c_3 - 2c_2^2)e_n^3 + (3c_4 - 7c_3c_2 + 4c_2^3)e_n^4 + O(e_n^5).$$

Again by using Taylor's expansion we have

$$f(y_n) = c_2f'(\alpha)e_n^2 + (2c_3 - 2c_2^2)f'(\alpha)e_n^3 + (3c_4 - 7c_3c_2 + 4c_2^3)f'(\alpha)e_n^4 + O(e_n^5).$$

Hence, by using the above expressions in the second step of (2.7), we get the following error equation:

$$e_{n+1} = c_2(-c_3 + c_2^2)e_n^4 + O(e_n^5).$$

Thus the proof is complete. □

Now, we intend to transform the optimal two-point method (2.7) into a derivative free one by using (1.3) so that the optimal order is preserved.

By using the approximation given in (1.3), the scheme (2.7) transforms into

$$\begin{aligned} y_n =& x_n - \frac{f(x_n)}{f[w_n, x_n]}, w_n = x_n + f(x_n)^2, n \geq 0, \\ x_{n+1} =& y_n - \frac{f(x_n)}{2f[y_n, x_n] - f[w_n, x_n]}, \end{aligned} \tag{2.9}$$

where $H_2'(y_n)$ is given by (2.6). Similar to Theorem 2.1, it can be easily shown that the scheme (2.9) has optimal order four with the following error equation:

$$e_{n+1} = -c_2(c_3 + f'(\alpha)^2c_2 - 2c_2^2)e_n^4 + O(e_n^5).$$

2.2. Optimal three-point eighth-order method

Petković in [6] proposed a three-point method, based on the Hermite interpolation, which is given by

$$\begin{aligned} y_n =& x_n - \frac{f(x_n)}{f'(x_n)}, n \geq 0, \\ z_n =& \varphi_f(x_n, y_n), \varphi_f \; \epsilon \psi_4, \\ x_{n+1} =& z_n - \frac{f(z_n)}{H_3'(z_n)}, \end{aligned} \tag{2.10}$$

where, ψ_4 is a real function chosen in such a way that it requires already computed values $f(x_n), f'(x_n)$ and $f(y_n)$ and it provides the fourth-order convergence of the sequence $\{x_n\}$. The scheme (2.9) is an example of such a function. The value of $H_3'(z_n)$ in [6] is given by

$$H_3'(z_n) = f[z_n, x_n](2 + \frac{z_n - x_n}{z_n - y_n}) - \frac{(z_n - x_n)^2}{(y_n - x_n)(z_n - y_n)} f[y_n, x_n] + f'(x_n)\frac{z_n - y_n}{y_n - x_n}. \tag{2.11}$$

By applying the transformation (1.3) to the three-point scheme (2.10) and using the scheme (2.9) at the second step, we obtain a new optimal three-point method given by

$$\begin{aligned} y_n =& x_n - \frac{f(x_n)}{f[w_n, x_n]}, w_n = x_n + f(x_n)^3, n \geq 0, \\ z_n =& y_n - \frac{f(y_n)}{2f[y_n, x_n] - f[w_n, x_n]}, \\ x_{n+1} =& z_n - \frac{f(z_n)}{K_3'(z_n)}, \end{aligned} \tag{2.12}$$

where

$$K_3'(z_n) = f[z_n, x_n](2 + \frac{z_n - x_n}{z_n - y_n}) - \frac{(z_n - x_n)^2}{(y_n - x_n)(z_n - y_n)} f[y_n, x_n] + f[w_n, x_n]\frac{z_n - y_n}{y_n - x_n}.$$

Theorem 2.2. *Let $f : D \subseteq \mathbb{R} \to \mathbb{R}$ be a sufficiently differentiable function in an open interval D and α a simple root of f. If x_0 is close enough to α, then the iterative scheme defined by* (2.12) *is of optimal order* 8 *and has the following error equation:*

$$e_{n+1} = e_{n+1} = c_2^2(c_2c_3^2 - 2c_2^3c_3 + c_4c_2^2 + c_2^5 - c_4c_3)e_n^8 + O(e_n^9), \tag{2.13}$$

where, $c_j = \frac{f^{(j)}(\alpha)}{j!f'(\alpha)}, j \geq 2$, *and* $e_n = x_n - \alpha$.

Proof. By using Taylor's expansions, the proof would be similar to Theorem 2.1 and those already taken in [6, 12]. Hence it is omitted. □

2.3. Optimal four-point sixteenth-order method

Fiza et al. in [11] developed an optimal sixteenth-order four-point scheme based on the Hermite interpolation. We add the fourth step of their scheme to (2.12) and obtain a new derivative-free optimal four-point method, using the transformation (1.3) as follows:

$$\begin{aligned} y_n =& x_n - \frac{f(x_n)}{f[w_n, x_n]}, w_n = x_n + f(x_n)^4, n \geq 0, \\ z_n =& y_n - \frac{f(y_n)}{2f[y_n, x_n] - f[w_n, x_n]}, \\ t_n =& z_n - \frac{f(z_n)}{K_3'(z_n)}, \\ x_{n+1} =& t_n - \frac{f(t_n)}{K_4'(t_n)}, \end{aligned} \tag{2.14}$$

where

$$\begin{aligned} K_3'(z) =& f[z,x](2+\frac{z-x}{z-y}) - \frac{(z-x)^2}{(y-x)(z-y)} f[y,x] + f[w,x]\frac{(z-y)}{(y-x)}, \\ K_4'(t) =& f[t,z] + (t-z)f[t,z,y] + (t-z)(t-y)f[t,z,y,x] + (t-z)(t-y)(t-x)f[t,z,y,x,2] \end{aligned} \tag{2.15}$$

and $f[t,z,y,x,2]$ is defined by

$$\begin{aligned} f[t,z,y,x,2] =& \frac{1}{(t-x)^2(t-y)}(f[t,z]-f[z,y]) - \frac{1}{(t-x)^2(z-x)}(f[z,y]-f[y,x]) \\ & - \frac{1}{(t-x)(z-x)^2}(f[z,y]-f[y,x]) + \frac{1}{(t-x)(z-x)(y-x)}(f[y,x]-f[w,x]). \end{aligned}$$

Theorem 2.3. *Let $f : D \subseteq \mathbb{R} \to \mathbb{R}$ be a sufficiently differentiable function in an open interval D and α a simple root of f. If x_0 is close enough to α, then the iterative scheme defined by (2.14) is of optimal order 16 and has the following error equation:*

$$e_{n+1} = -c_2^4(-c_3+c_2^2)^2(c_2^3-c_3c_2+c_4)(-c_2^4+c_3c_2^2+c_1^4c_2-c_4c_2+c_5)e^{16}+O(e^{17}),$$

where, $c_j = \frac{f^{(j)}(\alpha)}{j!f'(\alpha)}, j \geq 2$ and $e_n = x_n - \alpha$.

Proof. By using Taylor's expansions, the proof would be similar to those already taken in [11]. Hence it is skipped over. □

2.4. Optimal n-point method of order 2^n

In [6], Petković et al. designed an n-point n-step method of order 2^n requiring n evaluations of function and one evaluation of the first derivative $f'(x_n)$ at each step. By applying the transformation (1.3), we obtain the following derivative-free n-point n-step method:

$$\begin{aligned} \phi_1(x_k) &= x_k - \frac{f(x_k)}{f[z_k,x_k]}, z_k = x_k + f(x_k)^m, m \geq n \geq 0, \\ \phi_2(x_k) &= \Psi_f(x,\phi_1(x_k)), \Psi_f \in \Psi_4, \\ \phi_3(x_k) &= \phi_2 - \frac{f(\phi_2(x_k))}{K_3'(\phi_2(x_k))}, \\ &\vdots \\ x_{k+1} = \phi_n(x_k) &= \phi_{(n-1)}(x_k) - \frac{f(\phi_{(n-1)}(x_k))}{K_n'(\phi_{(n-1)}(x_k))}, \end{aligned} \tag{2.16}$$

where, Ψ_4 is any fourth-order iterative method and K_n is the Hermite interpolating polynomial of degree n given by

$$K_n(x) = f(x) = a_0 + a_1(f(x)-f(x_k)) + a_2(f(x)-f(x_k))^2 + \cdots + a_n(f(x)-f(x_k))^n, \tag{2.17}$$

with the conditions

$$\begin{aligned} f(x_k) =& K_n(x_k), f'(x_k) = K_n'(x_k), \\ f(\phi_1)) =& K_n(\phi_1), ..., f(\phi_n) = K_n(\phi_n). \end{aligned} \tag{2.18}$$

By the use of conditions (2.18) and implementing scheme (2.9) at the second step, the coefficients $a_0, a_1, ..., a_n$ can be determined easily, and hence we obtain an n-point derivative-free method of the following form:

$$
\begin{aligned}
\phi_1(x_k) =& x_k - \frac{f(x_k)}{f[w_k, x_k]}, w_k = x_k + f(x_k)^m, m \geq n \geq 0, \\
\phi_2(x_k) =& \phi_1 - \frac{f(\phi_1(x_k))}{K_2'(\phi_1(x_k))}, \\
\phi_3(x_k) =& \phi_2 - \frac{f(\phi_2(x_k))}{K_3'(\phi_2(x_k))}, \\
&\vdots \\
x_{k+1} =& \phi_n(x_k) = \phi_{(n-1)}(x_k) - \frac{f(\phi_{(n-1)}(x_k))}{K_n'(\phi_{(n-1)}(x_k))},
\end{aligned}
\tag{2.19}
$$

where, K_n is defined by (2.17).

Theorem 2.4. *Let $f : D \subseteq \mathbb{R} \to \mathbb{R}$ be a sufficiently differentiable function in an open interval D and α a simple root of f. If x_0 is close enough to α, then the n- point iterative scheme defined by* (2.19) *is of optimal order 2^n.*

3. Numerical results

In this section, we first transform an optimal four-point method of Sharifi et al. [7], denoted by SL16, which is given by

$$
\begin{aligned}
y_n =& x_n - \frac{f(x_n)}{f'(x_n)}, n \geq 0, \\
r_n =& y_n - L_1(u_n)\frac{f(y_n)}{f'(x_n)}, \\
s_n =& r_n - L_2(u_n, v_n, w_n)\frac{f(r_n)}{f'(x_n)}, \\
x_{n+1} =& s_n - L_3(u_n, v_n, w_n, p_n, q_n, t_n)\frac{f(s_n)}{f'(x_n)},
\end{aligned}
\tag{3.1}
$$

where,

$$
\begin{aligned}
L_1(u_n) =& 1 + 2u_n + 5u_n^2 - 6u_n^3, \\
L_2(u_n, v_n, w_n) =& 1 + 2u_n + 4w_n + 6u_n^2 + v_n, \\
L_3(u_n, v_n, w_n, p_n, q_n, t_n) =& 1 + 6u_n^2 + 2u_n - v_n^3 + v_n + 4w_n - 4w_n^2 + u_n w_n \\
&+ 6u_n^2 w_n + 2u_n^3 w_n - 10u_n w_n^2 + t_n + 2q_n + 8p_n \\
&+ 2u_n t_n + 2v_n w_n + 6u_n^2 t_n - 4v_n^2 w_n + 24u_n^4 w_n,
\end{aligned}
$$

are weight functions, where

$$
u_n = \frac{f(y_n)}{f(x_n)}, v_n = \frac{f(r_n)}{f(y_n)}, w_n = \frac{f(r_n)}{f(x_n)}, p_n = \frac{f(s_n)}{f(x_n)}, q_n = \frac{f(s_n)}{f(y_n)}, t_n = \frac{f(s_n)}{f(r_n)} \tag{3.2}
$$

and the modified form of which is denoted by MSL16, given by

$$
\begin{aligned}
y_n =& x_n - \frac{f(x_n)}{f[w_n, x_n]}, \\
w_n =& x_n + f(x_n)^4, n \geq 0,
\end{aligned}
$$

$$\begin{aligned} r_n =& y_n - L_1(u_n)\frac{f(y_n)}{f[w_n,x_n]},\\ s_n =& r_n - L_2(u_n,v_n,w_n)\frac{f(r_n)}{f[w_n,x_n]},\\ x_{n+1} =& s_n - L_3(u_n,v_n,w_n,p_n,q_n,t_n)\frac{f(s_n)}{f[w_n,x_n]}. \end{aligned}$$

We now test all the discussed methods using a number of nonlinear equations. We employ multiprecision arithmetic with 4000 significant decimal digits in the programming package Maple 16 to obtain a high accuracy and avoid loss of significant digits. We compare the convergence behavior of the modified methods MSL16 and (2.14), denoted by MFM16, with their with-derivative versions, i.e., SL16 and the optimal four-point method by Fiza et al. (FM16) [11] and optimal sixteenth-order class of Soleymani (SSS16) et al. [8] respectively using the nonlinear functions given in Table 1. Table 1 also includes the exact root α and initial approximation x_0, which are calculated using Maple 16. The error $|x_n - \alpha|$ and the computational order of convergence (coc) for the first three iterations of various methods are displayed in Tables 2–6 which supports the theoretical order of convergence. The formula to compute the computational order of convergence (coc) is given by

$$coc \approx \frac{\log|(x_{n+1}-\alpha)/(x_n-\alpha)|}{\log|(x_n-\alpha)/(x_{n-1}-\alpha)|}.$$

It can be seen from Tables 1–6 that for the presented examples, the modified four-point methods MSL16, MFM16 and MSSS16 are comparable and competitive to the methods SL16, FM16 and SSS16.

Table 1: Test functions

Example	Test Functions	Exact root α	x_0
1	$f_1(x) = (2+x^3)\cos(\frac{\pi x}{2}) + \log(x^2+2x+2)$	-1	-0.93
2	$f_2(x) = x^2e^x + x\cos\frac{1}{x^3} + 1$	$-1.5650602...$	-2.0
3	$f_3(x) = xe^x + \log(1+x+x^4)$	0	-0.5
4	$f_4(x) = e^{\sin(8x)} - 4x$	$0.34985721...$	7.0
5	$f_5(x) = -20x^5 - \frac{x}{2} + \frac{1}{2}$	$0.42767729...$	0.38

Table 2: Numerical results of example 1

$f_1(x) = (2+x^3)\cos(\frac{\pi x}{2}) + \log(x^2+2x+2), x_0 = -0.93$						
	SL16	FM16	SSS16	MSL16	MFM16	MSSS16
$\lvert x_1-\alpha\rvert$	2.63(-9)	2.60(-12)	4.97(-11)	2.59(-9)	1.86(-12)	4.35(-11)
$\lvert x_2-\alpha\rvert$	1.61(-127)	2.75(-177)	1.18 (-154)	1.23(-127)	1.15(-179)	1.36(-155)
$\lvert x_3-\alpha\rvert$	6.48(-2019)	6.94(-2817)	1.23 (-2452)	8.22(-2021)	4.91(-2855)	1.17(-2467)
coc	16.00	16.00	16.00	16.00	16.00	16.00

Table 3: Numerical results of example 2

$f_2(x) = x^2e^x + x\cos\frac{1}{x^3} + 1, x_0 = -2.0$						
	SL16	FM16	SSS16	MSL16	MFM16	MSSS16
$\lvert x_1-\alpha\rvert$	9.71(-15)	8.50(-15)	5.80 (-15)	4.34(-15)	2.86(-15)	7.33 (-15)
$\lvert x_2-\alpha\rvert$	1.08(-228)	8.63(-231)	6.47 (-234)	2.89(-234)	2.95(-238)	1.11(-232)
$\lvert x_3-\alpha\rvert$	5.76(-3652)	1.11(-3686)	3.77 (-3737)	4.42(-3714)	4.91(-3806)	9.19(-3718)
coc	16.00	16.00	16.00	16.00	16.00	16.00

Table 4: Numerical results of example 3

$f_3(x) = xe^x + \log(1 + x + x^4), x_0 = -0.5$						
	SL16	FM16	SSS16	MSL16	MFM16	MSSS16
$\lvert x_1 - \alpha\rvert$	2.97	6.04(-6)	3.80(-4)	1.52(-7)	4.12(-10)	1.83(-10)
$\lvert x_2 - \alpha\rvert$	7.70(-1)	2.67(-88)	8.79(-60)	1.24(-112)	4.37(-154)	2.29(-160)
$\lvert x_3 - \alpha\rvert$	4.59(-6)	5.85(-1406)	5.72(-950)	4.90(-1794)	1.16(-2457)	7.91(-2559)
coc	8.94	16.00	16.00	16.00	16.00	16.00

Table 5: Numerical results of example 4

$f_4(x) = e^{(\sin 8x)} - 4x, x_0 = 7$						
	SL16	FM16	SSS16	MSL16	MFM16	MSSS16
$\lvert x_1 - \alpha\rvert$	D*	33.22	D	3.00(-2)	2.42(-3)	3.04(-3)
$\lvert x_2 - \alpha\rvert$	D	3.26(-4)	D	5.71(-11)	2.06(-32)	3.79(-30)
$\lvert x_3 - \alpha\rvert$	D	5.75(-51)	D	8.21(-155)	3.90(-498)	1.38(-461)
coc	D	9.33	D	16.49	16.02	16.03

Table 6: Numerical results of example 5

$f_5(x) = -20x^5 - \frac{x}{2} + \frac{1}{2}, x_0 = 0.38$						
	SL16	FM16	SSS16	MSL16	MFM16	MSSS16
$\lvert x_1 - \alpha\rvert$	1.28(-3)	1.11(-13)	2.19(-9)	1.05(-3)	4.86(-14)	1.51(-9)
$\lvert x_2 - \alpha\rvert$	2.68(-34)	4.53(-200)	6.00(-128)	1.05(-35)	3.87(-205)	1.65(-131)
$\lvert x_3 - \alpha\rvert$	5.39(-525)	2.70(-3182)	6.02(-2025)	1.60(-547)	1.01(-3262)	7.74(-2083)
coc	16.00	16.00	16.00	16.00	16.00	16.00

*D stands for divergence

3.1. Conclusions

We applied the well-known conjecture of Cordero and Torregrosa [1] to transform an n-point optimal method based on the Hermite interpolation to derivative-free optimal methods. Some existing derivative-based methods are also modified using this transformation. Convergence analysis is performed for the transformed methods. Finally, numerical examples is supplied and a comparison is provided, which supports the theoretical results. It can be seen that the modified derivative-free methods can compete, and work better than their with-derivative versions. Specially in the case of example 5, it can be seen that derivative-involved methods SL16 and SSS16 fail to converge to any root, while their transformed derivative-free forms converge even when the initial guess is taken far from the required root.

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