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A Family of Optimal Methods for Solving Nonlinear Equations

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Abstract

In this paper we show a family of iterative schemes for solving nonlinear equations with order of convergence 2^n, by using $n+1$ functional evaluations per step, so these methods are optimal in the sense of the Kung-Traub's conjecture. The family is obtained by composing n Newton's steps and approximating the derivative by using Hermite's interpolation polynomial.

Some numerical examples are provided to confirm the theoretical results and to show the good performance of the new methods, comparing them with a well known family of similar characteristics.

Keywords: nonlinear equation, iterative method, order of convergence, optimality, Hermite polynomial, efficiency index.

1 Introduction

Finding iterative methods for solving nonlinear equations is an important area of research in numerical analysis and it has interesting applications in different branches of Science and Engineering. In this study, we analyze new iterative schemes to find a simple root α of a nonlinear equation $f(x) = 0$, where $f : I \subseteq \mathbb{R} \longrightarrow \mathbb{R}$ is a scalar function on an open interval I.

In this case, one tries to obtain high convergence speed at the lowest possible computational cost. Convergence speed is measured by the convergence order and the computational cost by the number of functional evaluations per iteration. In order to compare different methods, Ostrowski, [1], introduced the efficiency index, defined as $I = p^{1/d}$, where p is the order of convergence and d is the total number of functional evaluations. In [2], Kung and Traub conjectured that an iterative method, without memory, that uses $n+1$ functional evaluations per iteration can have at most convergence order $p = 2^n$. If this bound is reached, the method is said to be optimal. Thus, the optimal order for methods with four or five functional evaluations per step would be eight or sixteen, respectively.

In recent years, different optimal iterative methods have been published, trying to increase the order of convergence. For instance, for $n = 3$, optimal eighth order methods can be found in [3, 4, 5, 6, 7, 8]. For $n = 4$, optimal sixteenth order methods have been published in [9].

General procedures to obtain families of optimal multipoint iterative methods for every n were given in [2, 10]. Here we introduce a new procedure and compare it with the previous one, showing that the new family is competitive in terms of simplicity of the computations and convergence speed.

The outline of the paper is as follows. In Section 2 we describe the procedure to generate the new family of optimal iterative schemes of arbitrary order 2^n, giving an explicit expression for the iterates. In Section 3 we establish the convergence order showing its optimality. Finally, in Section 4, different numerical tests confirm the theoretical results and allow us to compare our optimal iterative methods with a classical family introduced in [2].

2 The design of the family

The best known iterative method for solving a nonlinear equation $f(x) = 0$ is Newton's method which is optimal, because it only needs 2 functional evaluations per step and has order of convergence two, under some conditions. The composition of n Newton's steps

$$\begin{aligned} y_1 &= x_k - \frac{f(x_k)}{f'(x_k)}, \\ y_{i+1} &= y_i - \frac{f(y_i)}{f'(y_i)}, \quad i = 1, 2, \ldots, n-1 \end{aligned}$$

produces a method $x_{k+1} = y_n = y_n(x_k)$ of order 2^n, (see [12], Theorem 2.4), but it is not optimal because uses $2n$ instead of $n + 1$ functional evaluations.

In order to get optimality, the value of $f'(y_i),\ i = 1, \ldots, n-1$ is approximated by the derivative $h_i'(y_i)$ of a polynomial that is obtained using already computed function values, namely, the Hermite's interpolation polynomial $h_i(t)$ of degree $i + 1$, for $i = 1, \ldots, n-1$, satisfying the following conditions:

$$\begin{aligned} h_i(y_j) &= f(y_j), \quad j = 0, 1, \ldots, i \\ h_i'(y_0) &= f'(y_0), \end{aligned}$$

where $y_0 = x_k$.

Writing this polynomial as

$$h_i(t) = a_0^{(i)} + a_1^{(i)}(t - y_i) + a_2^{(i)}(t - y_i)^2 + \ldots + a_{i+1}^{(i)}(t - y_i)^{i+1},$$

one has $h_i'(y_i) = a_1^{(i)}$. We will obtain this value from the following linear system, with $i+2$ equations and $i+2$ unknowns.

$$\left.\begin{array}{r} a_1^{(i)} + 2a_2^{(i)}(y_0 - y_i) + \ldots + (i+1)a_{i+1}^{(i)}(y_0 - y_i)^i = f'(y_0) \\ a_0^{(i)} + a_1^{(i)}(y_j - y_i) + a_2^{(i)}(y_j - y_i)^2 + \ldots + a_{i+1}^{(i)}(y_j - y_i)^{i+1} = f(y_j) \\ j = 0, 1, \ldots, i \end{array}\right\} \quad (1)$$

The last equation of (1) gives the value of $a_0^{(i)} = h_i(y_i) = f(y_i)$ and so, the system (1) can be written as

$$\left.\begin{array}{r} a_1^{(i)} + 2a_2^{(i)}(y_0 - y_i) + 3a_3^{(i)}(y_0 - y_i)^2 + \ldots + (i+1)a_{i+1}^{(i)}(y_0 - y_i)^i = f'(y_0) \\ a_1^{(i)} + a_2^{(i)}(y_j - y_i) + a_3^{(i)}(y_j - y_i)^2 + \ldots + a_{i+1}^{(i)}(y_j - y_i)^i = f[y_j, y_i] \\ j = 0, 1, \ldots, i-1 \end{array}\right\}$$

where $f[y_j, y_i]$ denotes the divided difference of order 1, $\dfrac{f(y_j) - f(y_i)}{y_j - y_i}$.

The coefficient $a_1^{(i)}$ can be obtained applying Cramer's rule

$$a_1^{(i)} = \frac{\Delta_1}{\Delta}, \quad (2)$$

where,

$$\Delta = \begin{vmatrix} 1 & 2(y_0 - y_i) & 3(y_0 - y_i)^2 & \ldots & (i+1)(y_0 - y_i)^i \\ 1 & (y_0 - y_i) & (y_0 - y_i)^2 & \ldots & (y_0 - y_i)^i \\ 1 & (y_1 - y_i) & (y_1 - y_i)^2 & \ldots & (y_1 - y_i)^i \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & (y_{i-1} - y_i) & (y_{i-1} - y_i)^2 & \ldots & (y_{i-1} - y_i)^i \end{vmatrix} \quad (3)$$

and

$$\Delta_1 = \begin{vmatrix} f'(y_0) & 2(y_0 - y_i) & 3(y_0 - y_i)^2 & \ldots & (i+1)(y_0 - y_i)^i \\ f[y_0, y_i] & (y_0 - y_i) & (y_0 - y_i)^2 & \ldots & (y_0 - y_i)^i \\ f[y_1, y_i] & (y_1 - y_i) & (y_1 - y_i)^2 & \ldots & (y_1 - y_i)^i \\ \vdots & \vdots & \vdots & & \vdots \\ f[y_{i-1}, y_i] & (y_{i-1} - y_i) & (y_{i-1} - y_i)^2 & ldots & (y_{i-1} - y_i)^i \end{vmatrix}.$$

Both determinants can be explicitly expressed in terms of the points y_j and of already computed values of f in these points. The first determinant is easily computed:

$$\Delta = \prod_{j=1}^{i}(y_j - y_0) V(y_0, y_1, \ldots, y_{i-1}),$$

where $V(y_0, y_1, \ldots, y_{i-1})$ stands for the Vandermonde determinant. The other determinant can be computed by cofactors of its first column,

$$\Delta_1 = f'(y_0)C + \sum_{u=0}^{i-1}(-1)^{u+1} f[y_u, y_i] C_u.$$

It is not difficult to see that

$$C = \prod_{j=0}^{i-1}(y_j - y_i)V(y_0, y_1, \ldots, y_{i-1}),$$

$$C_0 = \prod_{j=0}^{i-1}(y_j - y_i)\left(2V(y_0, y_1, \ldots, y_{i-1}) + \prod_{j=1}^{i}(y_j - y_0)\sum_{u=1}^{i-1}(-1)^{u+1}\frac{V_u(y_0, y_1, \ldots, y_{i-1})}{y_u - y_0}\right),$$

and

$$C_u = (y_0 - y_i)\frac{\prod_{j=0}^{i-1}(y_j - y_i)}{y_u - y_i}\frac{\prod_{j=1}^{i}(y_j - y_0)}{y_u - y_0}V_u(y_0, y_1, \ldots, y_{i-1}),$$

for $u = 1, \ldots, i-1$, where $V_u(y_0, y_1, \ldots, y_{i-1})$ is the Vandermonde determinant of the list of arguments where y_u is missing.

Then, we have defined a new family of methods, $M_{2^n}, \;\; n = 1, 2, \ldots$, that starting from an initial approximation x_0 perform the iterations

$$x_{k+1} = y_n(x_k), \;\; k = 0, 1, \ldots$$

where

$$y_1(x) \;=\; x - \frac{f(x)}{f'(x)}, \tag{4}$$

$$y_{i+1}(x) \;=\; y_i(x) - \frac{f(y_i(x))}{h_i'(y_i(x))}, \quad i = 1, \ldots, n-1, \tag{5}$$

and h_i' is obtained from (2).

In each of the steps, $i = 1, \ldots, n-1$, we only compute one functional value $f(y_i(x))$ and use it and the previous functional values to obtain the polynomial $h_i(t)$, what gives a total of $n+1$ functional evaluations, so that the method will be optimal if we show that its convergence order is 2^n.

3 Convergence results

Theorem 1 *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_{2^n} defined by (4-5) has optimal convergence order 2^n.*

Proof: The expression for the error of the Hermite interpolation polinomial (see [12], p.244) gives us:

$$f(t) - h_i(t) = \frac{f^{(i+2)}(\xi(t))}{(i+2)!}(t - y_0)^2(t - y_1)\ldots(t - y_i),$$

for $i = 1, 2, \ldots, n$, where $\xi(t) \in I$. Assuming $\xi(t)$ differentiable and setting $t = y_i$, we have

$$f'(y_i) - h_i'(y_i) = \frac{f^{(i+2)}(\xi)}{(i+2)!}(y_i - y_0)^2(y_i - y_1)\ldots(y_i - y_{i-1}). \tag{6}$$

We proceed by induction on n. First of all, we prove that M_{2^2} is an optimal method of order 2^2.

Let $\epsilon_{m,k}$ be the error in x_k, that is $\epsilon_{m,k} = y_m(x_k) - \alpha$, $m = 1, 2, \ldots, n$; $k = 0, 1, \ldots$ Then, by the assumption in the iterative method we have:

$$\begin{aligned} \epsilon_{0,k} &= \epsilon_k = x_k - \alpha, \\ \epsilon_{1,k} &= y_1(x_k) - \alpha = O(\epsilon_k^2), \quad \text{Newton's method.} \end{aligned} \tag{7}$$

Thus, for obtaining the approximation $h_1'(y_1)$ in M_{2^2} the polynomial is of degree 2 and the error equation (6) is:

$$f'(y_1) - h_1'(y_1) = \frac{f^{(3)}(\xi)}{3!}(y_1 - y_0)^2,$$

by substituting (7) here one gets

$$\begin{aligned} f'(y_1) - h_1'(y_1) &= \frac{f^{(3)}(\xi)}{3!}((y_1 - \alpha) - (y_0 - \alpha))^2 \\ &= \frac{f^{(3)}(\xi)}{3!}(O(\epsilon_k^2) - \epsilon_k)^2 = O(\epsilon_k^2). \end{aligned}$$

Thereby

$$f'(y_1) = h_1'(y_1)(1 + O(\epsilon_k^2)), \tag{8}$$

and so, the order of M_{2^2} can be established by:

$$\epsilon_{2,k} = y_2(x_k) - \alpha = y_1(x_k) - \alpha - \frac{f(y_1(x_k))}{h_1'(y_1(x_k))}.$$

By using (8), we have

$$\begin{aligned} \epsilon_{2,k} &= y_2(x_k) - \alpha = y_1(x_k) - \alpha - \frac{f(y_1(x_k))(1 + O(\epsilon_k^2))}{f'(y_1(x_k))} \\ &= y_1(x_k) - \alpha - \frac{f(y_1(x_k))}{f'(y_1(x_k))} - \frac{f(y_1(x_k))}{f'(y_1(x_k))}O(\epsilon_k^2). \end{aligned} \tag{9}$$

Now, by dividing the Taylor's expansions of $f(y_1)$ and $f'(y_1)$ in $x_k = \alpha$, we obtain

$$\frac{f(y_1(x_k))}{f'(y_1(x_k))} = (y_1(x_k) - \alpha) - \frac{c_2}{c_1}(y_1(x_k) - \alpha)^2 + \ldots, \tag{10}$$

with $c_1 = f'(\alpha)$ and $c_2 = \dfrac{f''(\alpha)}{2!}$.

By substituting (10) in (9) and using that Newton's method has quadratic convergence we get

$$\epsilon_{2,k} \;=\; -\frac{c_2}{c_1}(y_1(x_k)-\alpha)^2+\ldots+(y_1(x_k)-\alpha)O(\epsilon_k^2)+\ldots=O(\epsilon_k^4). \quad (11)$$

That gives us order 2^2 for the iterative method M_{2^2} and so, Theorem 1 is proved for $n=2$. We suppose by induction hypothesis that the assertion is valid for $3,4,5,\ldots,n-1$, that is

$$\epsilon_{i,k} \;=O(\epsilon_k^{2^i}),\;\; i=3,4,5,\ldots,n-1 \quad (12)$$

and we have to prove it for n.

In this case, the error equation (6) is:

$$f'(y_n)-h_n'(y_n)=\frac{f^{(n+2)}(\xi)}{(n+2)!}(y_n-y_0)^2(y_n-y_1)\ldots(y_n-y_{n-1}).$$

By using (7) and (12), we have

$$f'(y_n)-h_n'(y_n) \;=\; \frac{f^{(n+2)}(\xi)}{(n+2)!}O(\epsilon_k^2)O(\epsilon_k^2)O(\epsilon_k^4)\ldots O(\epsilon_k^{2^{n-2}})=O(\epsilon_k^{2^{n-1}}).$$

Then

$$f'(y_n)=h_n'(y_n)(1+O(\epsilon_k^{2^{n-1}})),$$

and so, with the same computations as in (9-11), we show that the order of convergence of scheme M_{2^n} is 2^n. □

4 Numerical results

In this section we check the effectiveness of the new optimal iterative methods M_q comparing them with the optimal family K_q, for $q = 2,4,8$ and 16 introduced by Kung and Traub in [2].

As we have already said, M_2 is Newton's method,

$$y_1=y_0-\frac{f(y_0)}{f'(y_0)},$$

the fourth-order method, M_4, is obtained by adding the following step

$$y_2=y_1-\frac{f(y_1)}{2f[y_0,y_1]-f'(y_0)},$$

the scheme of order 8 results from adding

$$y_3=y_2-\frac{f(y_2)(y_0-y_1)^2}{f[y_1,y_2](y_0-y_2)^2+(y_1-y_2)^2(f'(y_0)(y_0-y_1)+f[y_0,y_2](2y_1+y_2-3y_0))}$$

and, finally, method M_{16} has as last step

$$y_4 = y_3 - \frac{f(y_3)(y_0 - y_1)^2(y_0 - y_3)^2(y_1 - y_3)}{w(y_0, y_1, y_2, y_3)},$$

where

$$\begin{aligned} w(y_0, y_1, y_2, y_3) &= f[y_3, y_2](y_0 - y_1)^2(y_0 - y_2)^2(y_1 - y_2) \\ &- (y_3 - y_2)(f[y_1, y_2](y_0 - y_3)^2(y_0 - y_2)^2 \\ &+ (y_1 - y_3)(y_1 - y_2)(f'(y_0)(y_0 - y_1)(y_0 - y_3) \\ &- f[y_0, y_2](4y_0^2 + 2y_1y_3 + y_1y_2 + y_3y_2 - y_0(3y_1 + 3y_3 + 2y_2)))). \end{aligned}$$

To test the different iterative methods, we use the following examples:

a) $f(x) = xe^{x^2} - \sin^2(x) + 3\cos(x) + 5; \quad \alpha \approx -1.207647827130918927$

b) $f(x) = x^3 - 10; \quad \alpha \approx 2.1544346900318837218$

c) $f(x) = \sin^2(x) - x^2 + 1; \quad \alpha \approx 1.4044916482153412260$

d) $f(x) = (x + 2)e^x - 1; \quad \alpha \approx -0.44285440100238858$

e) $f(x) = (x - 1)^3 - 2; \quad \alpha \approx 2.2599210498948731648$

f) Let us consider Kepler's equation $f(x) = x - e\sin(x) - M$; where $0 \le e < 1$ and $0 \le M \le \pi$. A numerical study, for different values of M and e has been performed in [14]. We take values $M = 0.01$ and $e = 0.9995$. In this case the solution is $\alpha \approx 0.3899777749463621$.

Numerical computations have been carried out using variable precision arithmetic in MATLAB R2010b with 10000 significant digits. The iterations stop when the difference between two consecutive iterates is less than $1e - 200$.

The convergence order is estimated without using the solution value according to this formula, [13],

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

The behavior of the methods is summarized in Table 1. For each test equation we compare the methods of the same order of Kung-Traub an ours. The values shown in the table correspond to the increment in the last iteration before convergence, the estimated convergence order and the number of iterations.

In the order 2 case, both methods coincide with Newton's method. The results are given for comparison with higher order methods.

Observe that the estimated convergence order agrees very well with its theoretical value. The number of iterations required by our methods to reach convergence is always less than or equal to that of the reference methods. When both families perform the same number of iterations, our methods have lesser increments. Then, our methods show a good performance, comparable to that of Kung-Traub's family.

		$\lvert x_{k+1}-x_k\rvert$	ρ	k		$\lvert x_{k+1}-x_k\rvert$	ρ	k
a) $x_0=-1$	M_2	5.31e−256	2	10	K_2	5.31e−256	2	10
	M_4	4.34e−224	4	5	K_4	7.86e−495	4	6
	M_8	3.82e−358	7.93	4	K_8	2.51e−246	8	4
	M_{16}	4.64e−2918	15.94	4	K_{16}	1.94e−1963	16.02	4
b) $x_0=2$	M_2	4.53e−288	2	9	K_2	4.53e−288	2	9
	M_4	9.22e−303	4	5	K_4	7.87e−268	4	5
	M_8	9.32e−603	8.02	4	K_8	7.84e−518	8.03	4
	M_{16}	1.08e−300	16.02	3	K_{16}	5.08e−255	16.03	3
c) $x_0=1$	M_2	1.51e−202	2	10	K_2	1.51e−202	2	10
	M_4	1.25e−438	4	6	K_4	1.46e−289	4	6
	M_8	2.34e−226	8	4	K_8	8.22e−981	8	5
	M_{16}	5.61e−1786	16.25	4	K_{16}	3.36e−903	16.69	4
d) $x_0=-1$	M_2	3.08e−366	2	11	K_2	3.08e−366	2	11
	M_4	1.99e−520	4	6	K_4	2.39e−303	4	6
	M_8	8.32e−237	8	4	K_8	6.72e−1103	8	5
	M_{16}	7.55e−1884	16.08	4	K_{16}	3.11e−1052	16.32	4
e) $x_0=2$	M_2	5.68e−321	2	10	K_2	5.68e−321	2	10
	M_4	5.71e−708	4	6	K_4	1.68e−549	4	6
	M_8	5.42e−350	8.09	4	K_8	2.83e−256	8	4
	M_{16}	3.55e−2782	16.08	4	K_{16}	1.26e−1974	16.18	4
f) $x_0=1$	M_2	1.04e−341	2	10	K_2	1.04e−341	2	12
	M_4	1.64e−771	4	7	K_4	4.36e−566	4	7
	M_8	1.11e−760	7.99	5	K_8	1.86e−518	7.96	5
	M_{16}	4.59e−746	14.32	4	K_{16}	1.92e−493	12.96	4

Table 1: Numerical results

5 Conclusion

We have design and study a family of optimal order iterative methods for solving nonlinear equations, alternative to the family described by Kung and Traub in [2], proving a convergence result that shows the optimality of the methods. We have also derived an explicit formula for the computation of the approximated derivative that avoids the solution of linear systems in each step of the iteration. The numerical results show that the new family has a slightly better performance than the classical one, so it can be competitive.

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