An optimal scheme for finding multiple roots free of derivatives

J.H. Jerezano$^{\natural}$ [1], F.I. Chicharro$^{\flat}$ and N. Garrido$^{\flat}$

($\flat$) I.U. de Matemática Multidisciplinar, Universitat Politècnica de València
Camí de Vera s/n, València, Spain.

($\natural$) Escuela de Doctorado, Universitat Politècnica de València
Camí de Vera s/n, València, Spain.

1 Introduction

The problem of finding the roots of a non-linear equation $g(x) = 0$, where $g : D \subseteq \mathbb{R} \longrightarrow \mathbb{R}$, is one of the oldest problems in numerical approximation. The most common method for solving non-linear equations is the well-known Newton's method, whose convergence is quadratic. Sometimes it is necessary to solve nonlinear equations that have one or more multiple roots. In these cases the iterative methods with good properties to find simple roots present convergence problems. It is therefore necessary to use iterative methods specifically designed to find multiple roots. An example of this issue is Newton's scheme, whose convergence is reduced to linear when used for solving non-linear equations with multiple roots, as Lagrange realised in 1808. One modification on Newton's method was proposed by Schröder [1] in 1870, where the convergence remains quadratic by using the iterative expression

$$x_{n+1} = x_n - m\frac{g(x_n)}{g'(x_n)}, \quad n = 0, 1, \ldots$$

Multiple roots α of multiplicity m satisfy $g(\alpha) = g'(\alpha) = g''(\alpha) = \cdots = g^{(m-1)}(\alpha) = 0$, and $g^{(m)}(\alpha) \neq 0$. In this work we consider iterative methods to approximate this kind of roots.

There are many methods in the literature of different order of convergence to find the multiple roots of $g(x) = 0$, many of them designed from the combination of multiple-root methods or combinations of multiple-root methods with single-root methods. Most of these methods require the evaluation of first-order or first and second-order derivatives. It is well known that the presence of derivatives in the iterative expression reduces the applicability of the method to certain problems, so we focus on designing derivative-free methods.

Another objective in the design is the optimality in the sense of the Kung-Traub conjecture [2]. It points that the order of convergence p of a method without memory that performs d different functional evaluations per iteration meets $p \leq 2^{d-1}$; the method is called optimal when $p = 2^{d-1}$. According to the conjecture, there are few optimal iterative methods for multiple roots in the literature.

[1] jhjerull@doctor.upv.es

Focusing on the design of derivative-free schemes, one of the derivative-free techniques is the Traub–Steffensen [3] type scheme, which replaces g' in Newton's iterative method by an approximation of the form

$$g'(x_n) \approx \frac{g(x_n + \beta g(x_n)) - g(x_n)}{\beta g(x_n)} = g[w_n, x_n],$$

where $w_n = x_n + \beta g(x_n)$, $\beta \in \mathbb{R} - \{0\}$, and $g[w_n, x_n] = \dfrac{g(w_n) - g(x_n)}{w_n - x_n}$ denotes the first-order divided difference operator.

Recently, Kumar et al. [4] presented the second-order optimal scheme defined as:

$$x_{n+1} = x_n - G(\theta_n), \quad n = 0, 1, \ldots, \tag{1}$$

where $G(\theta) : D \subset \mathbb{C} \longrightarrow \mathbb{C}$ is a weight function and $\theta = \dfrac{g(x)}{g[w, x]}$. Let us remark that Traub-Steffensen method is the particular case $G(\theta) = \theta$ of (1).

In this work, a new scheme of optimal iterative derivative-free methods is proposed to find multiple roots. The two-step procedure is designed starting from Traub-Steffensen method and using the technique of weight functions. The complete design process is shown in Section 2. Section 3 covers a numerical analysis, presented by applying some members of the proposed scheme to different non-linear functions and comparing the results with other existing methods in the literature. Finally, the conclusions of this work are shown in Section 4.

2 Iterative scheme with weight function

Taking as a starting point the iterative scheme with a weight function (1) but using a different divided difference based on $w = x + \beta g(x)^2$, the proposed multipoint iterative scheme with two steps is

$$\begin{aligned} y_n &= x_n - m\frac{g(x_n)}{g[w_n, x_n]}, \\ x_{n+1} &= x_n - m\frac{g(x_n)}{g[w_n, x_n]}H(t_n), \end{aligned} \qquad n = 0, 1, \ldots, \tag{2}$$

where $t = \left(\dfrac{g(y_n)}{g(x_n)}\right)^{1/m}$.

It is observed that the iterative family (2) is obtained from the composition of the Traub-Steffensen method modified twice, including in the second step of the algorithm a weight function H dependent on the variable t. Using Taylor series expansions, it can be shown that family of iterative schemes (2) has order of convergence 4 whenever $H(0) = H'(0) = 1$, $H''(0) = 4$ and $|H''(0)| < \infty$. Let us remark that the number of functional evaluations per iteration in such scheme is three, resulting in an optimal class. In addition, a family of iterative schemes free of derivatives is proposed, resulting in a different iterative method for each value of the selected parameter and the weight function used.

3 Numerical experiments

This section is devoted to the performance of some members of the iterative scheme (2). These members are tested to verify their functionality when solving non-linear equations.

Two members of family (2) are considered. We denote by M1 the method obtained using the polynomial weight function $H(t) = 2t^2 + t + 1$ and by M2 the method corresponding to the rational weight function $H(t) = \dfrac{-t + 1}{-2t + 1}$.

In order to evaluate the proposed methods M1 and M2, their results are compared with existing methods in the literature that include derivatives. The first one is the iterative scheme proposed by Sharma [5], based on Jarratt scheme for simple roots and denoted in this work by Ss. Also, the one described by Behl et al. [6], denoted by Bh, designed from the arithmetic mean of Chebyshev's method [3] for simple zeros and Schröder's method. Moreover, the performance is also compared with two derivative-free methods. The first one was developed by Kumar et al. [7]. The first step y_n is the Traub-Steffensen method setting $\beta = \frac{1}{100}$ and the second step is

$$x_{n+1} = y_n - H(t_n)\frac{g(x_n)}{g[w_n, x_n] + 2g[w_n, y_n]}, n = 0, 1, \ldots, \tag{3}$$

where $t = \left(\dfrac{g(y)}{g(x)}\right)^{\frac{1}{m}}$ and $H(t) = (m+2)\frac{t}{1-2t}$. Method (3) has been denoted by KK. The second method for the comparison was presented by Behl et al. [8]. The first step y_n is the Traub-Steffensen method setting $\beta = \frac{1}{100}$ and the second step is

$$x_{n+1} = x_n - H(t_n)\frac{g(x_n)}{g[w_n, x_n]}, \quad n = 0, 1, \ldots, \tag{4}$$

where $t = \left(\dfrac{g(y)}{g(x)}\right)^{\frac{1}{m}}$, $s = \left(\dfrac{g(y)}{g(w)}\right)^{\frac{1}{m}}$ and $H(t) = (1+t)\left(\frac{t}{2} - 1 - \frac{s}{2} - 2s^2\right)$. Method (4) has been denoted by BB.

The non-linear functions selected for the numerical tests are

- $g_1(x) = x^3 - 5.22x^2 + 9.0825x - 5.2675$, with a double root $\alpha_1 = 1.75$ and a single root $\alpha_2 = 1.72$.
- $g_2(x) = \left(e^{-x} - 1 + \frac{x}{5}\right)^3$, with a root of multiplicity three $\alpha \approx 4.96511423174428$.

Numerical experiments have been carried out using Matlab R2023a software and variable precision arithmetic with 10000 digits. Despite the expressions of w differ from our method with respect to the others, we also have selected $\beta = \frac{1}{100}$. Furthermore, since it is an iterative process, we use $|x_{n+1} - x_n| + |g(x_n)| < 10^{-200}$ as a stopping criterion with a maximum of 50 iterations. If after this amount of iterations the method has not converged will be denoted by –.

Table 1 shows the numerical performances for comparing the methods. The table shows the number of iterations necessary to obtain the root (iter) from the initial condition x_0, the estimated errors $|x_{n+1} - x_n|$, residual errors of the considered function $|g(x_n)|$ and the approximate order of computational convergence ACOC [9].

Numerical results evidence the competitiveness of the proposed methods with respect with those present in the literature. Specifically, for function $g_1(x)$, all methods achieve convergence with few iterations and with high accuracy for any initial guess. Also, the ACOC obtained is the same as the theoretical order of convergence for each method. Regarding function $g_2(x)$, iterative methods with derivatives do not always converge, and the proposed methods are the least iterate-consuming to reach the solution. It is observed that for the initial estimate $x_0 = 4.4$ the ACOC is not a good estimate of the order of convergence of the methods due to the difference between the last iterations of each algorithm. However, the last column reveals that good accuracy is still obtained with few iterations. The results improve greatly with $x_0 = 5.2$, obtaining for the derivative-free methods very close approximations to the solution of the non-linear function. Therefore, we can consider that M1 and M2 iterative schemes selected in this numerical experiments provide good approximations to the multiple roots of both problems in an efficient way.

Table 1: Numerical results for solving non-linear problems.

Function	x_0	Method	Iter	ACOC	$\|x_{n+1} - x_n\|$	$\|g(x_{n+1})\|$
g_1	1.9	Ss	7	4.0	3.63e–615	3.95e–1231
		Bh	7	4.0	8.19e–562	2.01e–1124
		KK	6	4.0	4.81e–209	6.94e–419
		BB	7	4.0	1.40e–604	5.87e–1210
		M1	7	4.0	9.52e–537	2.72e–1074
		M2	7	4.0	1.38e–776	5.70e–1554
	3	Ss	8	4.0	2.39e–556	1.71e–1113
		Bh	8	4.0	9.85e–487	2.91e–974
		KK	7	4.0	3.25e–216	3.17e–433
		BB	8	4.0	5.44e–530	8.89e–1061
		M1	8	4.0	2.52e–450	1.90e–901
		M2	7	4.0	4.10e–204	5.05e–409
g_2	4.4	Ss	–	–	–	–
		Bh	12	2.0	1.92e–255	3.65e–765
		KK	7	5.99	1.76e–405	3.92e–1217
		BB	7	5.99	4.05e–404	4.77e–1213
		M1	7	5.99	1.09e–402	9.36–1209
		M2	7	5.99	2.27e–405	8.46e–1217
	5.2	Ss	–	–	–	–
		Bh	–	–	–	–
		KK	5	4.0	8.73e–505	4.79e–1515
		BB	5	4.0	9.36e–502	5.89e–1506
		M1	5	4.0	1.03e–498	7.79e–1497
		M2	5	4.0	1.02e–504	7.58e–1515

4 Conclusions

In this work, a fourth-order family of optimal and derivative-free iterative schemes is presented. To design the proposed class, the modified Traub–Steffensen type scheme has been taken as the first step and in the second step a weight function has been incorporated. To check the efficiency of the iterative family, two weight functions are selected, one polynomial and the other rational, giving rise to iterative methods M1 and M2. The performance of these two members of the family are analysed in comparison with other existing methods in the literature for solving non-linear equations with multiple roots. The numerical implementation shows that the methods M1 and M2 selected from the proposed scheme are competitive compared to existing robust methods in the literature in terms of absolute error difference between two iterations, absolute residual error and computational order of convergence.

Acknowledgments

This study has been funded by "Ayuda a Primeros Proyectos de Investigación (PAID-06-23), Vicerrectorado de Investigación de la Universitat Politècnica de València (UPV)", in the framework of project MERLIN.

References

[1] Schöder, E.O., On infinitely many algorithms for solving equations. *Math. Ann.*, 2:317–365, 1870.

[2] Kung, H.T., Traub, J.F. Optimal order of one-point and multipoint iteration *Journal of the Association for Computing Machinery*, 21:643–651, 1974.

[3] Traub, J.F., Iterative Methods for the Solution of Equations. New York, USA, Chelsea Publishing Company, 1982.

[4] Kumar, D., Sharma, J.R., Argyros, I.K., Optimal one-point iterative function free from derivatives for multiple roots. *Mathematics*, 8(709), 2020.

[5] Sharma, J.R., Sharma, R., Modified Jarratt method for computing multiple roots. *Applied Mathematics and Computation*, 217(2):878–881, 2010.

[6] Behl, R., Cordero, A., Motsa, S.S., Torregrosa, J.R., An optimal fourth-order family of methods for multiple roots and its dynamics. *Numerical Algorithms*, 271:775–796, 2016.

[7] Kumar, S., Kumar, D., Sharma, J.R., Cesarano, C., Agarwal, P., Chu, Y.M., An Optimal Fourth Order Derivative-Free Numerical Algorithm for Multiple roots. *Symmetry*, 12(1038), 2020.

[8] Behl, R., Bhalla, S., Magreñán, Á.A., Moysi, A., An Optimal Derivative Free Family of Chebyshev-Halley's Method for Multiple Zeros. *Mathematics*, 9(546), 2021.

[9] Cordero, A., Torregrosa, J.R., Variants of Newton's method using fifth order quadrature formulas. *Applied Mathematics and Computation*, 190:686–698, 2007.