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*Research article*

## Numerical simulation of multiple roots of van der Waals and CSTR problems with a derivative-free technique

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**Abstract:** In this paper, a derivative-free one-point iterative technique is proposed, with memory for finding multiple roots of practical problems, such as van der Waals and continuous stirred tank reactor problems, whose multiplicity is unknown in the literature. The new technique has an order of convergence of 1.84 and requires two function evaluations. It can be used as a seed to produce higher-order methods with similar properties, and it increases the efficiency of a similar procedure without memory due to Schröder. After studying its order of convergence, its stability is checked by applying it to the considered problems and comparing with the technique of the same nature for finding multiple roots. The geometrical behavior of the numerical results of the techniques is also studied.

**Keywords:** nonlinear equations; multiple roots; derivative-free method; convergence

**Mathematics Subject Classification:** 41A25, 49M15, 65H05

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### 1. Introduction

One of the fundamental one-point techniques, which has quadratic convergence and requires one function and one derivative evaluation of every iteration, is Newton's technique [1, 2] in literature, which may diverge if the derivative is very small or zero. Researchers have also suggested a few derivative-free one-point techniques to solve this issue, among which are the Secant technique [2], the Jarratt and Nudds technique [3], the Muller technique [4, 5], the Sharma techniques [6, 7] and the Traub technique [2]. Newton's technique is a one-point technique without memory, whereas the other techniques are classified as one-point techniques with memory. Except for Secant, which has an order

of 1.62, all of the aforementioned one-point techniques with memory require one function evaluation each iteration and have orders of convergence of 1.84.

In the literature, Behl et al. [8] presented an optimal derivative-free method with a two-step scheme, Kumar et al. [9, 10] developed two-step optimal derivative-free methods, and in [10], the authors used a weight function. Zafar et al. [11] developed optimal two-step methods that require a derivative of the function and used a weight function, Sharma and Arora [12] developed non-optimal two step fifth order methods that require a derivative of the functions and Akram et al. [13] developed three-step eighth-order methods that require a derivative of the function. All methods were developed in order to obtain the multiple roots of a nonlinear equation  $\phi(z) = 0$ . However, they are known for the multiplicity  $m$  of these roots.

The most common and simple technique, which is independent of knowledge of the multiplicity of the roots of the functions is Schröder's technique [14], given by

$$z_{j+1} = z_j - \frac{\phi(z_j)\phi'(z_j)}{\phi'(z_j)^2 - \phi(z_j)\phi''(z_j)}, \quad j = 0, 1, 2, \dots \quad (1.1)$$

This scheme (1.1) has quadratic convergence and it requires three function evaluations per iteration. The scheme (1.1) was originally developed from Newton's scheme [1, 2] and applied to the quotient  $\chi(z) = \frac{\phi(z)}{\phi'(z)}$ :

$$z_{j+1} = z_j - \frac{\chi(z_j)}{\chi'(z_j)}, \quad j = 0, 1, 2, \dots \quad (1.2)$$

In the recent years in literature, Cordero et al. [15] presented a derivative-free technique with the memory of order 1.84 for finding multiple roots. The scheme is given by

$$z_{j+1} = z_j - \frac{\chi(z_j)}{\chi[z_{j-2}, z_j] - \chi[z_{j-2}, z_{j-1}] + \chi[z_{j-1}, z_j]}, \quad j = 2, 3, 4, \dots \quad (1.3)$$

where  $\chi(z) = \frac{\phi(z)}{\phi'(z)}$ ,  $\chi[z_{j-1}, z_j] = \frac{\chi(z_{j-1}) - \chi(z_j)}{z_{j-1} - z_j}$  and  $\chi[z_{j-1}, z_j]$  is also called the first-order divided difference. Equation (1.3) will be denoted hereon by CM (from Cordero's Method). This scheme requires only two function evaluations per iteration. As the authors discussed in [15], that scheme is more efficient than Schröder's technique (1.1). The scheme developed in CM is the first known scheme in mathematics literature, and was written in [15]. The aim of this study is to develop a derivative-free technique with memory for solving nonlinear equations. Here, the study's aim is double: first, this new approach strives to be similar to the CM scheme; second, the goal is for this new scheme to be more stable than the existing scheme given by CM.

To check the stability and applications of the new technique, van der Waals and continuous stirred tank reactor (CSTR) problems were considered. Van der Waals and CSTR problems are classic examples in the field of chemical engineering. They involve the simulation of multi roots, which are challenging to solve due to their non-differentiable and multi-modal nature. To tackle these problems, derivative-free iterative techniques have been developed, which rely on function evaluations instead of derivatives in order to find the solution. Derivative-free methods have gained popularity in recent years due to their ability to handle complex functions, where traditional gradient-based methods may fail. These techniques have been successfully applied to various fields, including chemical engineering, where they have been used to solve the van der Waals and CSTR problems with great success.

The new technique was compared with the existing ones, and the techniques' behavior when applied to the considered problems (numerically and geometrically) was studied. The geometrical representation of techniques is one kind of analysis named visual analysis, meaning that the behavior of techniques can be seen at any point. The main advantage of the new technique over the existing one is that the new technique will be more consistent and stable.

The proposed work is divided into four sections. Section 2 includes the construction of a new technique and the study of convergence analysis. Some real-life problems are studied in Section 3, and stability is also verified in this section, viz. numerically and geometrically. Lastly, the conclusion is discussed in Section 4.

## 2. Design of technique

Please consider a derivative-free technique with memory, developed by Sharma et al. [7]:

$$z_{j+1} = z_j - \frac{\phi[z_{j-2}, z_{j-1}]}{\phi[z_{j-1}, z_j]\phi[z_{j-2}, z_j]}\phi(z_j), \quad j = 2, 3, 4, \dots \quad (2.1)$$

for the simple root of the function. The technique defined in (2.1) is also applicable for solving the system of equations. To solve the system of Eq (2.1), one proceeds as such:

$$z_{j+1} = z_j - \Phi[z_{j-1}, z_j]^{-1}\Phi[z_{j-2}, z_{j-1}]\Phi[z_{j-2}, z_j]^{-1}\Phi(z_j), \quad (2.2)$$

where  $z_0$ ,  $z_1$  and  $z_2$  are their initial approximations. The orders of convergence of (2.1) and (2.2) are 1.84. In the [7] technique, (2.1) is not applied to find the multiple zeros of the function. In order to find the multiple zeros of  $\phi(z) = 0$ , one defines the function  $\chi(z) = \frac{\phi(z)}{\phi'(z)}$ , and then applies the Sharma et al. method (2.1) with  $\chi(z) = 0$ , obtaining

$$z_{j+1} = z_j - \frac{\chi[z_{j-2}, z_{j-1}]}{\chi[z_{j-1}, z_j]\chi[z_{j-2}, z_j]}\chi(z_j). \quad (2.3)$$

In this situation, the technique (2.3) is not required for the derivative and multiplicity of the zeros of the function  $\phi$ . The technique (2.3) has been shown to converge the same order of convergence as the one proven in [7] and requires two function evaluations per iteration.

The order of convergence of (2.3) shall be determined in the subsequent theorem. The concept of Ortega and Rheinboldt [16] is to be used for the R-order of convergence. Assume that sequence  $z_j$  is an output of an iterative method and  $\varepsilon_j = z_j - \alpha$ . Then, the sequence is written as such:

$$\varepsilon_{j+1} \sim \varepsilon_j^r, \quad (2.4)$$

if it converges to a zero  $\alpha$  of  $\phi$  with R-order  $\geq r$ .

**Theorem 1.** Let  $\phi : \mathbb{C} \rightarrow \mathbb{C}$  represent an analytical function in the vicinity of a multiple zero (say,  $\alpha$ ) with multiplicity  $m \geq 2$ . Consider that initial guesses  $z_0$ ,  $z_1$  and  $z_2$  are sufficiently close to  $\alpha$ ; then, the scheme defined by (2.3) has R-order of convergence, which is 1.84, with its error equation:

$$\varepsilon_{j+1} = \frac{2a_2 - a_1^2}{m}\varepsilon_j\varepsilon_{j-1}\varepsilon_{j-2} + O(\varepsilon_j, \varepsilon_{j-1}, \varepsilon_{j-2}),$$

where  $a_n = \frac{m}{(m+n)!} \frac{\phi^{(m+n)}(\alpha)}{\phi^m(\alpha)}$ ,  $n = 1, 2, 3, \dots$  and  $O(\varepsilon_j, \varepsilon_{j-1}, \varepsilon_{j-2})$  represents the higher power of  $\varepsilon_j$ ,  $\varepsilon_{j-1}$ , and  $\varepsilon_{j-2}$ .

*Proof.* Using Taylor's expansion of  $\phi(z_j)$  and  $\phi'(z_j)$  about  $\alpha$ , the result is

$$\phi(z_j) = \frac{\phi^m(\alpha)}{m!} \varepsilon_j^m (1 + a_1 \varepsilon_j + a_2 \varepsilon_j^2 + a_3 \varepsilon_j^3 + \dots), \quad (2.5)$$

$$\phi'(z_j) = \frac{\phi^m(\alpha)}{m!} \varepsilon_j^{m-1} (1 + (m+1)a_1 \varepsilon_j + (m+2)a_2 \varepsilon_j^2 + \dots), \quad (2.6)$$

where  $a_n = \frac{m}{(m+n)!} \frac{\phi^{(m+n)}(\alpha)}{\phi^m(\alpha)}$ ,  $n = 1, 2, 3, \dots$

Using Eqs (2.5) and (2.6), the result is

$$\chi(z_j) = \frac{\varepsilon_j}{m} - \frac{a_1}{m^2} \varepsilon_j^2 + \frac{(1+m)a_1^2 - 2ma_2}{m^3} \varepsilon_j^3 + O(\varepsilon_j^4). \quad (2.7)$$

In similar way, it can be written as such

$$\chi(z_{j-1}) = \frac{\varepsilon_{j-1}}{m} - \frac{a_1}{m^2} \varepsilon_{j-1}^2 + \frac{(1+m)a_1^2 - 2ma_2}{m^3} \varepsilon_{j-1}^3 + O(\varepsilon_{j-1}^4). \quad (2.8)$$

$$\chi(z_{j-2}) = \frac{\varepsilon_{j-2}}{m} - \frac{a_1}{m^2} \varepsilon_{j-2}^2 + \frac{(1+m)a_1^2 - 2ma_2}{m^3} \varepsilon_{j-2}^3 + O(\varepsilon_{j-2}^4). \quad (2.9)$$

By inserting Eqs (2.7), (2.8) and (2.9) in (2.3), the result is

$$\varepsilon_{j+1} = \frac{2a_2 - a_1^2}{m} \varepsilon_j \varepsilon_{j-1} \varepsilon_{j-2} + O(\varepsilon_j, \varepsilon_{j-1}, \varepsilon_{j-2}), \quad (2.10)$$

that is,

$$\varepsilon_{j+1} \sim \varepsilon_j \varepsilon_{j-1} \varepsilon_{j-2}. \quad (2.11)$$

From (2.4), the results are

$$\varepsilon_j \sim \varepsilon_{j+1}^{\frac{1}{r}}, \quad (2.12)$$

$$\varepsilon_{j-1} \sim \varepsilon_j^{\frac{1}{r}} \quad (2.13)$$

and

$$\varepsilon_{j-2} \sim \varepsilon_{j-1}^{\frac{1}{r}} \sim \varepsilon_j^{\frac{1}{r^2}}. \quad (2.14)$$

Combining (2.11), (2.13) and (2.14), it follows that

$$\varepsilon_{j+1} \sim \varepsilon_j \varepsilon_j^{\frac{1}{r}} \varepsilon_j^{\frac{1}{r^2}} = \varepsilon_j^{1 + \frac{1}{r} + \frac{1}{r^2}}. \quad (2.15)$$

Upon the comparison of (2.4) and (2.15), it follows that

$$r^3 - r^2 - r - 1 = 0;$$

it has a positive real root 1.84. This means that the technique (2.3) has a convergence order 1.84.

### 3. Application of technique

In this section, the existing technique (CM) and new technique (2.3), denoted by NM, are compared. Neither technique requires the multiplicity of the root, but they both require two function evaluations per iteration. Here, van der Waals [17] and CSTR [17] problems have been considered. These problems are defined as

**Problem 1.** First, van der Waals equation-of-state is considered:

$$\left(P + \frac{b_1 n^2}{V^2}\right)(V - nb_2) = nRT,$$

which explains the behavior of a real gas by adding two parameters,  $b_1$  and  $b_2$ , that are unique to each gas in the ideal gas equations. A nonlinear equation in volume must be solved in order to calculate the volume of gas  $V$  in terms of the other parameters.

$$PV^3 - (nb_2P + nRT)V^2 + b_1n^2V = b_1b_2n^3.$$

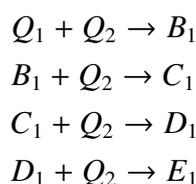
One can find values for  $n$ ,  $P$  and  $T$  such that this equation has three real zeros given the parameters  $b_1$  and  $b_2$  of a certain gas. The following nonlinear equation is obtained by utilizing the specific parameters (see [17] for details):

$$z^3 - 5.22z^2 + 9.0825z - 5.2675 = 0, \quad (3.1)$$

where  $z = V$ . For numerical work, (3.1) is written as

$$\phi_1(z) = z^3 - 5.22z^2 + 9.0825z - 5.2675. \quad (3.2)$$

**Problem 2.** Second, CSTR problems are assumed. Consider the components  $Q_1$  and  $Q_2$ , which represent the feed rates to reactors  $B_1$  and  $B_2 - B_1$ , respectively. The following reaction scheme is therefore obtained in the reactor (for further information, see [17]):



Douglas [18] analyzed the aforementioned model when he was developing a straightforward model for feedback control systems. He derived the following mathematical expression from the aforementioned model:

$$T_{C_1} \frac{2.98(z + 2.25)}{(z + 1.45)(z + 2.85)^2(z + 4.35)} = -1,$$

where the proportional controller gain is  $T_{C_1}$ . For values of  $T_{C_1}$  which produce roots of the transfer function with a negative real portion, the control system is stable. The roots of the nonlinear equation are the poles of the open-loop transfer function if  $T_{C_1} = 0$  is selected:

$$\phi_2(z) = z^4 + 11.50z^3 + 47.49z^2 + 83.06325z + 51.23266875.$$

The multiplicity of the above considered two problems is computed by the following formula:

$$m = \frac{z_{j+1} - z_j}{\chi(z_{j+1}) - \chi(z_j)},$$

where  $\chi(z) = \frac{\phi(z)}{\phi'(z)}$ . This scheme was applied in this study's technique (NM) and the existing technique (CM), and, afterward, the multiplicity of the problems was calculated. The results are displayed in Table 1. To find the particular roots of the considered problems which were discussed, two sets of initial guesses and performance are displayed in Tables 2 and 3. Displayed also are graphs of the root versus iterations and error versus iterations of the two techniques.

The numerical performance shown in Tables 2 and 3 show the required iterations  $j$ , estimated error  $|z_j - z_{j-1}|$  of the techniques in the last five iterations, speed of convergence (SOC) of the techniques, time consumed in the execution of the program denoted as CPU-time, and time calculated in seconds. The SOC is calculated by using the formula [19]

$$\text{SOC} = \frac{\ln(|z_{j+1} - z_j|/|z_j - z_{j-1}|)}{\ln(|z_j - z_{j-1}|/|z_{j-1} - z_{j-2}|)}.$$

**Table 1.** Computed results of the techniques.

Problem	Root	Multiplicity	Initial guess
Problem 1 (van der Waals, [17])	1.75	2	2.4,1,1.7
	1.75	2	0,3,1.5
Problem 2 (CSTR, [17, 18])	-2.85	2	-4,-2.6,-3.3
	-2.85	2	-4.4,-3,-3.7

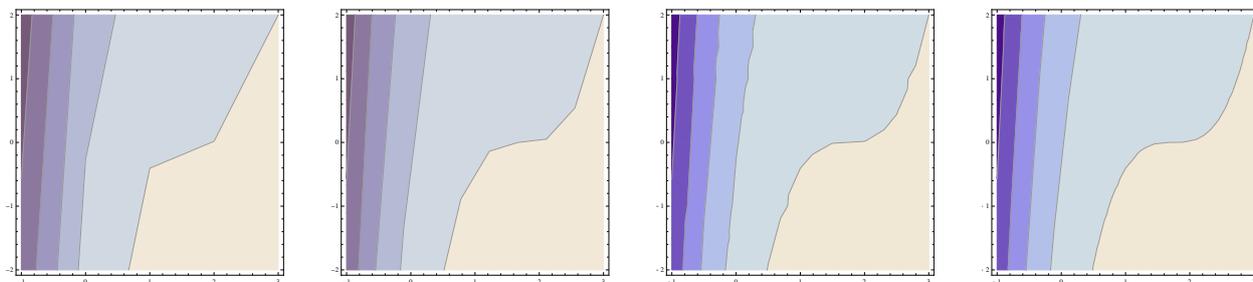
**Table 2.** Performance of techniques for Problem 1.

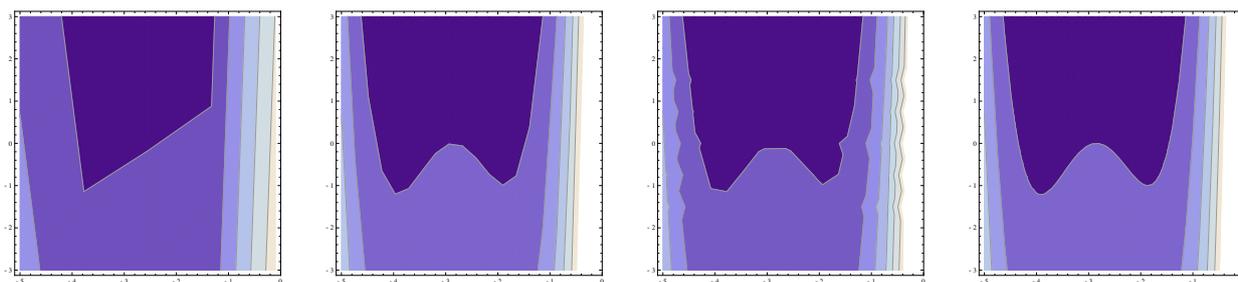
Methods	$j$	$ z_{j-4} - z_{j-5} $	$ z_{j-3} - z_{j-4} $	$ z_{j-2} - z_{j-3} $	$ z_{j-1} - z_{j-2} $	$ z_j - z_{j-1} $	SOC	CPU-time
$z_0 = 2.4, z_1 = 1,$								
$z_2 = 1.7$								
CM	16	5.57(-8)	1.11(-12)	1.45(-21)	7.50(-38)	1.01(-67)	1.83	0.1721
NM	15	6.98(-10)	1.58(-16)	1.85(-28)	1.13(-50)	1.83(-91)	1.86	0.1412
$z_0 = 0, z_1 = 3,$								
$z_2 = 1.5$								
CM	11	2.78(-9)	2.95(-15)	3.71(-26)	2.54(-46)	2.31(-83)	1.85	0.1563
NM	11	2.46(-10)	2.05(-17)	4.74(-30)	1.32(-53)	7.14(-97)	1.86	0.1316

**Table 3.** Performance of techniques for Problem 2.

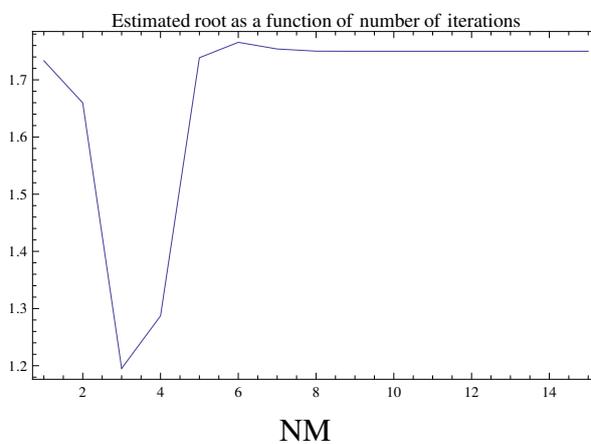
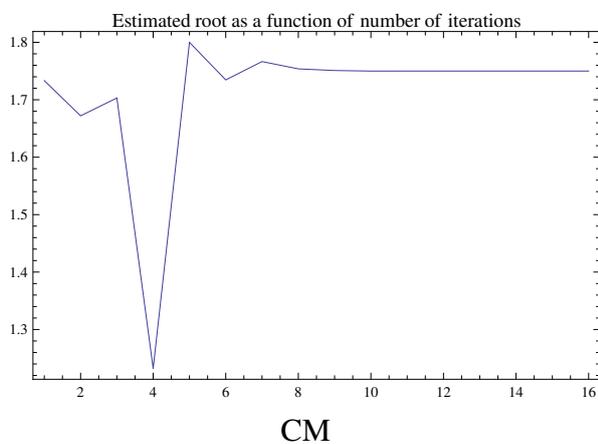
Methods	$j$	$ z_{j-4} - z_{j-5} $	$ z_{j-3} - z_{j-4} $	$ z_{j-2} - z_{j-3} $	$ z_{j-1} - z_{j-2} $	$ z_j - z_{j-1} $	SOC	CPU-time
$z_0 = -4, z_1 = -2.6,$								
$z_2 = -3.3$								
CM	11	1.25(-8)	4.08(-15)	1.53(-27)	3.73(-50)	1.12(-91)	1.81	0.16981
NM	9	7.54(-6)	1.93(-10)	1.21(-18)	8.41(-34)	9.37(-62)	1.85	0.1399
$z_0 = -4.4, z_1 = -3,$								
$z_2 = -3.7$								
CM	D	D	D	D	D	D	D	D
NM	11	9.22(-6)	5.09(-10)	6.36(-18)	1.42(-32)	2.20(-59)	1.85	0.1427

Figures 1 and 2 show the contour graph of the considered functions. The contour graph is a representation of the functions in which the values of the functions are represented by contour lines or isocurves. These lines connect points of equal value, creating a visual representation of the functions that helps show the shape and structure of the functions. The necessary iterations ( $j$ ) in the above Tables 2 and 3 are calculated so as to satisfy the criterion  $(|z_{j+1} - z_j| + |\chi(z_j)|) < 10^{-100}$ . Here, the first two initial approximations,  $z_0$  and  $z_1$ , are obtained by the intermediate value property of continuous functions, and the third  $z_2$  is merely an average of  $z_0$  and  $z_1$ . Now, based on the results shown in Tables 2 and 3 and Figures 3–8, one can say that the accuracy and stability of the new technique (NM) is better than the CM technique. In the van der Waals problem, NM has performed better in terms of error and time. The error versus iteration graph of Problem 1 was also presented, and it is visible that NM satisfies the stopping criterion in minimum time. Therefore, the new technique is more efficient. In a CSTR problem, the CM technique is not consistent. In Table 3, D represents the divergence behavior of the technique. For this particular set of initial values, the CM technique is not converging to the desired root, as it can be seen in Figure 7. Whereas, the new technique proposed in this paper converges to the root. So, in Problem 2 the new technique is more efficient and stable than CM. NM has also been applied to many various problems, and the stability and consistency were checked. The new method presented in the paper follows a scheme presented by Cordero et al. [15] and thus cannot be of use for systems of equations as it is now, as it was designed (in Cordero et al. [15]) only for finding multiple roots of a nonlinear equation. However, the desired development is to extend the method for inclusion of other cases of interest, and possibly to extend it to systems of equations, such as for the cases given in [20] (Tables 2 and 5 in [20]).

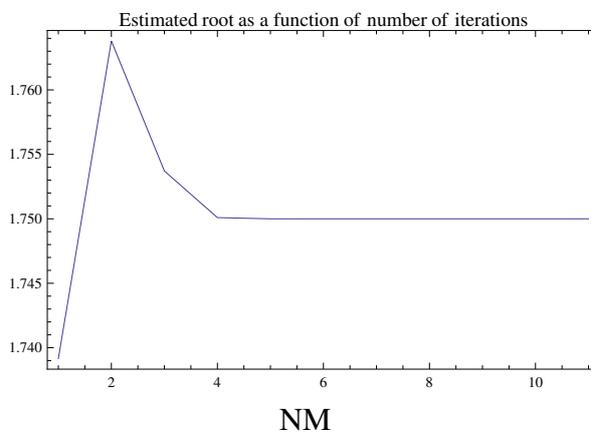
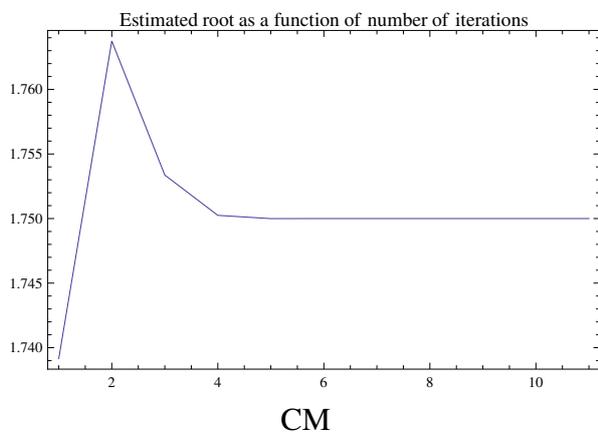
**Figure 1.** Contour graph of problem  $\phi_1(z)$ .



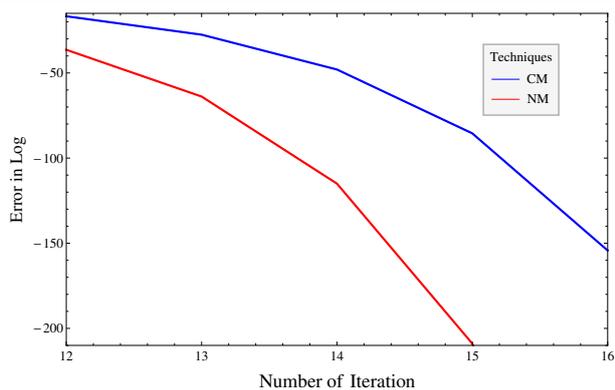
**Figure 2.** Contour graph of problem  $\phi_2(z)$ .



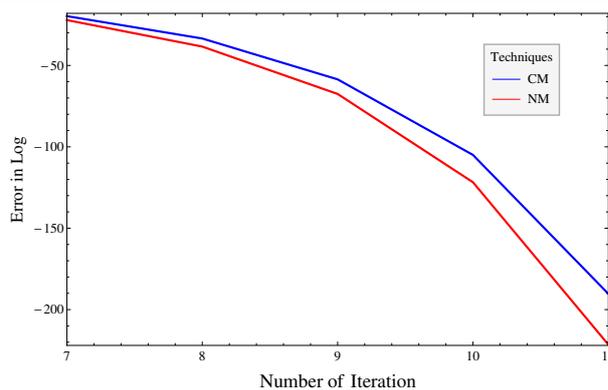
**Figure 3.** Graph of root versus iteration of  $\phi_1(z)$  for  $z_0 = 2.4, z_1 = 1, z_2 = 1.7$ .



**Figure 4.** Graph of root versus iteration of  $\phi_1(z)$  for  $z_0 = 0, z_1 = 3, z_2 = 1.5$ .

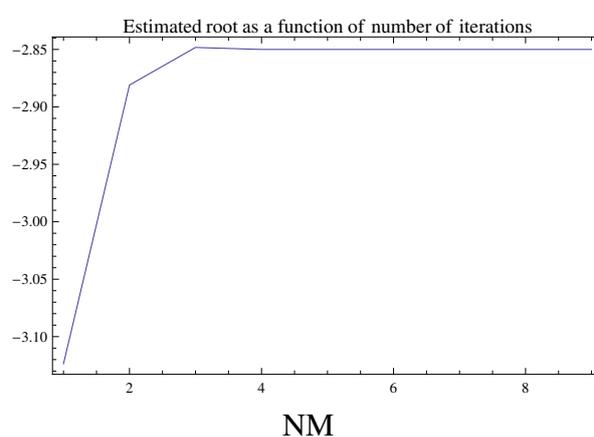
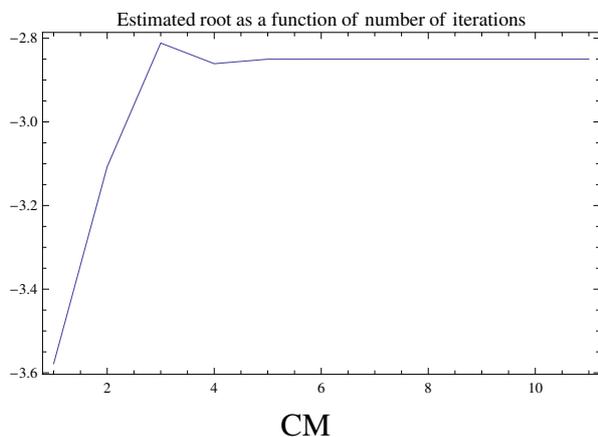


For  $z_0 = 2.4, z_1 = 1, z_2 = 1.7$

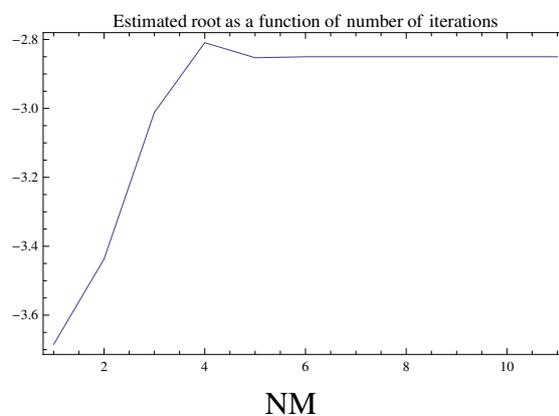
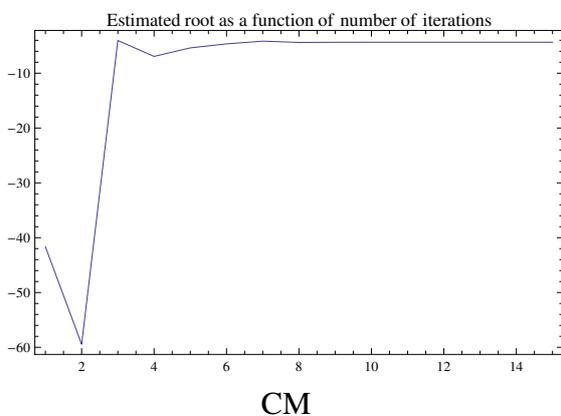


For  $z_0 = 0, z_1 = 3, z_2 = 1.5$

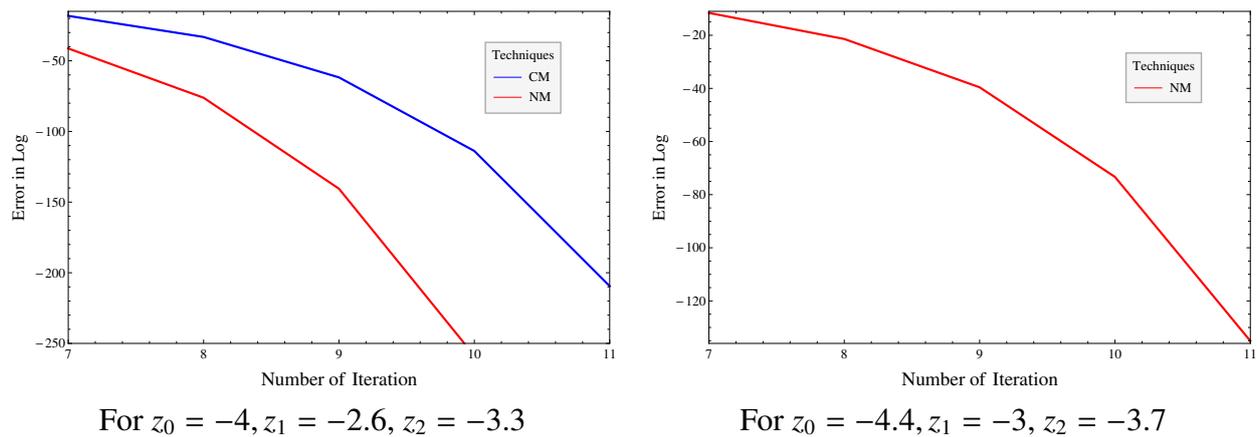
**Figure 5.** Graph of error versus iteration of  $\phi_1(z)$ .



**Figure 6.** Graph of root versus iteration of  $\phi_2(z)$  for  $z_0 = -4, z_1 = -2.6, z_2 = -3.3$ .



**Figure 7.** Graph of root versus iteration of  $\phi_2(z)$  for  $z_0 = -4.4, z_1 = -3, z_2 = -3.7$ .



**Figure 8.** Graph of error versus iteration of  $\phi_2(z)$ .

The method proposed in this paper presents a significant contribution to the field of numerical methods by providing a novel approach to finding multiple roots of nonlinear equations. The with-memory method of order 1.84 presented in this paper is an innovative solution that improves upon existing methods. It is worth noting that any advancement in numerical methods, regardless of how small it may seem, is worth studying, as it contributes to the collective knowledge of the field and may lead to further advancements in the future. Here, one can also agree that there are large amounts of derivative-free methods for simple roots but not for multiple roots. Derivative-free methods for multiple roots are very rare in the literature. Derivative-free methods are a highly demanding research area in numerical methods at present.

#### 4. Conclusions

A new derivative-free iterative technique with memory and the ability to find multiple roots without knowing the multiplicity of the function has been developed. It is the second known technique in mathematics with these properties. The new technique (NM) requires two function evaluations per iteration. The first technique (CM) of the same nature is developed in the literature. The stability of the new technique (NM), and also of the existing technique (CM), was studied in the last section. In the last section, the CM and NM techniques were applied to van der Waals and CSTR problems and their behavior was analyzed in both ways, i.e., numerically and geometrically. The analysis of the new technique (NM), and of the existing technique (CM), concludes this study, demonstrating that the performance of NM is better than that of CM in terms of time consumption and the error and stability of the technique.

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## Conflict of interest

The authors declare no conflict of interest.

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