A Special Interval Newton Step for Solving Nonlinear Equations

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Abstract: The problem of finding the zeros of a nonlinear equation has been extensively and thoroughly studied. Point methods constitute a significant and extensive category of techniques, allowing for the efficient finding of zeros with arbitrary precision under specific conditions. However, the limitation of these methods is that they typically yield a single zero. An alternative approach employs Interval Analysis, leveraging its properties to provide reliable and with certainty inclusions of all zeros within a given search interval. Interval methods, such as the Interval Newton method, exhibit quadratic convergence to the corresponding inclusions when monotonicity and simple zeros exist. Nonetheless, there exist pathological cases, like the existence of multiple zeros, where the obtained inclusions cannot be bounded with arbitrary precision, necessitating the adoption of bisection schemes to refine the search interval. These schemes not only increase computational time and cost but also result in a higher number of enclosures, enclosing sometimes the same zero more than once. The main objective of this work is to enhance the applicability of Interval Newton method in cases where no efficient alternative are available. Thus, in this paper, the Interval Newton method is studied and an adjusted perturbation technique is proposed to address the cases where multiple zeros exist. In particular, the given function is vertically shifted. Then, the Interval Newton operator is applied once to this shifted function. The resulting enclosures are then used to efficiently partition the search interval. The successful application of the Interval Newton method is expected to improve overall performance and reduce reliance on bisection schemes. Experimental results on a set of problems demonstrate the effectiveness of the proposed technique.

Key-Words: nonlinear equations, interval bisection, perturbation technique, pathological cases, bisection schemes

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1 Introduction

This paper addresses the problem of solving reliably and with certainty the equation

$$f(x) = 0, \tag{1}$$

within a closed interval $[a, b] \subset \mathbb{R}$, where $f : \mathbb{R} \to \mathbb{R}$ is a differentiable nonlinear function over the real numbers.

The importance of (1), [1] arises in various numerical analysis problems, including solving systems of nonlinear equations and optimization problems, [2], [3], as well as real-world applications in fields such as chemical engineering (process design and flowsheeting), computer graphics (render implicit surfaces), robotics (determine the efficiency of the used motors), and control theory (stability assessment of a linear time-invariant system, robust mobile robot path planning), [4], [5], [6], [7], [8].

Several methods have been proposed to solve (1), such as Newton-Raphson method, bisection method, secant method etc., each having distinct characteristics and advantages, [9]. Although certain techniques, such as the Newton-Raphson method, demonstrate favorable characteristics like quadratic convergence when locating single or multiple zeros, their drawback resides in their capacity to approximate only a single zero during each iteration. In addition, for the efficient discovery of zeros with multiplicities greater than one, a series of modifications has been proposed, under the assumption that the multiplicity of the zero being sought is already known, [10].

An alternative and efficient approach involves using Interval Arithmetic, initially introduced by Moore in 1966, [11]. These methods reliably enclose all zeros of (1) within a given search interval with arbitrary precision. Interval Newton is a typical and well-known method from the class of interval methods.

The Interval Newton method exhibits appealing properties, such as quadratic convergence and zero uniqueness (Theorems 2 and 3) and, recently, some improvements in the performance of the method have been proposed, [12], [13]. Nevertheless, there exist certain cases in which the method fails to provide sharp zero enclosures. One such case is the existence of multiple zeros. To address such pathological cases, a bisection scheme is employed on the current search interval. This approach successfully reduces the search interval, which is the primary objective of interval algorithms (Algorithm 1). However, it is important to note that the bisection scheme may, at times, generate multiple sequences of intervals that enclose the same zero. This can lead to an increase in the number of final zero enclosures and, consequently, a rise in the computational cost of the method.

It is worth noting that Interval methods generally efficiently handle the problem of enclosing zeros with multiplicity greater than one, [14]. Although the computational cost increases, the method will eventually provide enclosures for these zeros with arbitrary precision.

The aforementioned pathological cases have been acknowledged within the scholarly discourse. In some instances, no proposals for solutions are given. In others, directions for a possible search strategy are provided, depending on the zero multiplicity, [13]. Alternatively, more precise interval arithmetics may be adopted to obtain sharp enclosures, but these approaches do not clearly avoid bisection schemes in these cases, [12].

In this work, the behavior of the Interval Newton method is studied for cases where a bisection scheme is required in the execution flow of the algorithm, due to the existence of multiple zero. Such pathological cases occur when there exists a possible multiple zero located in the middle point of the search interval. The inability of Interval Newton to derive better enclosures leads to the adoption of a bisection scheme. This increases the computational cost of the method, especially given the lack of an efficient alternative.

Targeting this weakness of the method, a technique is proposed to directly enclose a multiple zero. In particular, a temporary perturbation of the initial function is considered, and then the Interval Newton operator is applied once to it to enclose its zeros. These zeros, referred to as pseudo-zeros, are not the actual zeros of $f(x) = 0$. The resulting 'pseudo-enclosures' are employed to deliver an efficient partition of the search interval. The proposed technique enables the inclusion of a multiple zero within a single sequence of intervals, significantly enhancing the overall performance of the method. The given numerical results support the efficiency of the proposed technique.

The paper's structure is as follows: The next section briefly introduces the interval methods framework. Subsequently, the motivation behind this work is discussed, and the proposed idea, along with an algorithm, is presented. Following that, numerical results are provided, and finally, the paper concludes with a brief discussion of future research directions.

2 Interval Methods

Following are some definitions regarding the concept of intervals and their corresponding arithmetic that are used in this work. An extensive study of Interval arithmetic and interval methods can be found in [11], [15], [16], [17], [18], [19].

2.1 Notation and basic concepts

A closed, compact interval, denoted as $[x]$, is the set of all points

$$[x] = [\underline{x}, \overline{x}] = \{x \in \mathbb{R} \mid |\underline{x} \leq x \leq \overline{x}\}$$

where $\underline{x}$, $\overline{x}$ denotes the lower and upper bound of interval $[x]$, respectively, and the set of all closed an compact intervals is denoted as $\mathbb{IR}$. The intersection of two intervals $[x] \cap [y]$, is defined as the common points between the two intervals, while the empty intersection, the lack of common points is defined as $[/]$. The width of an interval $[x]$ is defined by

$$w([x]) = \overline{x} - \underline{x},$$

while the midpoint of an interval $[x]$ is defined as

$$m([x]) = \frac{\overline{x} + \underline{x}}{2}.$$

For operations between two intervals $[a]$, $[b] \in \mathbb{IR}$, a corresponding interval arithmetic was defined, which, in general, is described as a set extension of real arithmetic, using the elementary operations $\circ \in \{+, -, \cdot, \div\}$

$$[a] \circ [b] = \{a \circ b \mid \forall a \in [a], \forall b \in [b]\}.$$

The above definition is equivalent to the following simpler rules, [20],

$$[a] + [b] = [\underline{a} + \underline{b}, \overline{a} + \overline{b}]$$
$$[a] - [b] = [\underline{a} - \overline{b}, \overline{a} - \underline{b}]$$
$$[a] \cdot [b] = \left[\min\left\{\underline{ab}, \underline{a}\overline{b}, \overline{a}\underline{b}, \overline{ab}\right\}, \max\left\{\underline{ab}, \underline{a}\overline{b}, \overline{a}\underline{b}, \overline{ab}\right\}\right],$$
$$\frac{[a]}{[b]} = \left[\min\left\{\frac{\underline{a}}{\underline{b}}, \frac{\underline{a}}{\overline{b}}, \frac{\overline{a}}{\underline{b}}, \frac{\overline{a}}{\overline{b}}\right\}, \max\left\{\frac{\underline{a}}{\underline{b}}, \frac{\underline{a}}{\overline{b}}, \frac{\overline{a}}{\underline{b}}, \frac{\overline{a}}{\overline{b}}\right\}\right]$$

where $0 \notin [b]$ for the case of interval division. For the case where $0 \in [b]$ an extended interval arithmetic have been proposed, [21].

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a real function. An interval extension of f is an interval function $F : \mathbb{IR}^n \to \mathbb{IR}$ such that for each $[\boldsymbol{x}] \in \mathbb{IR}^n$ and for each $\boldsymbol{x} \in [\boldsymbol{x}]$ $f(\boldsymbol{x}) \in F([\boldsymbol{x}])$. F is inclusion isotonic if $[\boldsymbol{y}] \subset [\boldsymbol{x}]$ implies $F([\boldsymbol{y}]) \subset F([\boldsymbol{x}])$, where $[\boldsymbol{x}], [\boldsymbol{y}] \in \mathbb{IR}^n$.

The following theorem, known as the Fundamental Theorem of Interval Analysis, [11], [15], can be used to bound the exact range of a given expression.

Theorem 1 *If F is an inclusion isotonic interval extension of f, then*

$$f([x]) \subseteq F[([x])].$$

The resulting enclosure of the range f is, in general, overestimated due to the phenomenon of dependency, as described in [15]. Specifically, the more occurrences a variable has in an expression, the higher the overestimation will be.

2.2 The form of Interval algorithms

The fundamental principle behind interval algorithms employed to solve (1) is centered on generating sequences of nested intervals, [11]. The primary goal is to iteratively produce narrower intervals in each iteration, converging eventually to a zero enclosure. The conceptual framework of these methods is illustrated in Algorithm 1. The basic implementations of this approach occurs when a simple bisection scheme is adopted (Algorithm 1 without Lines 7-11 and 14-15). This method, known as Interval Bisection, remains a reliable and widely used technique for determining all solutions of a non-differentiable equation to this day.

1 **Function** ***genIZF*** *(f,$[x]$,ε)*
2   **if** $0 \in F([x])$ **then**
3   **if** $w([x]) \leq \varepsilon$ **then**
4   Accept $[x]$ as a zero-enclosure
5   **end**
6   **else**
7   Reduce the search interval - find a new $[x']$
8   **if** $[x'] \subset [x]$ **then**
9   Initiate the method on $[x']$
10   **end**
11   **else**
12   Bisect the search interval $[x]$
13   Initiate the method on both of them
14   **end**
15   **end**
16   **end**
17   **else**
18   Discard search interval - $[x]$ contains no zeros
19   **end**
20 **end**

Algorithm 1: General Zero-Finding Interval Algorithm

If the reduction of the search interval is done using the following Interval Newton operator

$$\begin{aligned} m_k &= m([x]_k) \\ N([x]_k) &= m_k - \frac{f(m_k)}{F'([x_k])}\ , \\ [x]_{k+1} &= [x]_k \cap N(x[x]_k) \end{aligned} \tag{2}$$

then the Interval Newton method will be obtained. The basic properties of this method are described by the following Theorems.

Theorem 2 (Proof can be found in [11] and [18]) *Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a continuously differentiable function and let $[x] \in \mathbb{IR}$ be a given search interval. Then Interval Newton operator given by* (2) *has the following properties.*

1. *If $x^* \in [x]$ is a zero of $f(x) = 0$ then $x^* \in N([x])$.*
2. *If $N([x]) \cap [x] = [/]$ then there exist no zero of f in $[x]$.*
3. *If $N([x]) \subset [x]$ then there exist a unique zero of f in $[x]$ and therefore in $N([x])$.*

Theorem 3 (Proof can be found in [14] and [22]) *Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a continuously differentiable function and let $[x] \in \mathbb{IR}$ be a given search interval.*

1. *If $0 \notin f'([x]_i)$ for some $i \geq N$ then $w([x]_{i+1}) \leq \frac{1}{2} w([x]_i)$ for all $i \geq N$.*
2. *If $0 \notin f'([x]_i)$ there exists a constant C such that $w([x]_{i+1}) = [w([x]_i)]^2$.*

The above theorems tell us that, on the one hand, if there is no zero of the equation, the algorithm will yield this result. On the other hand, if the function is monotonic within a search interval, the algorithm can computationally prove both the monotonicity of the function and the uniqueness of the enclosing zero. Additionally, it will converge to the zero enclosure very fast, even if the search interval is very wide. The following Algorithm 2 describes the Interval Newton method employing extended interval arithmetic.

2.3 Pathological cases

In certain instances, the Interval Newton method fails to return a narrower interval. This occurs when both the numerator and denominator of the operator are zero or contain zero:

$$\begin{aligned} m_k &= m([x]_k) \\ N([x]_k) &= m_k - \frac{0}{[a, 0] \cup [0, b])} = [-\infty, +\infty]. \\ [x]_{k+1} &= [x]_k \cap [-\infty, +\infty] = [x]_k \end{aligned}$$

```
Function inewton (f, f', [x], ε)
    if 0 ∈ F([x]) then
        if w([x]) ≤ ε then
            Accept [x] as a zero-enclosure
        end
        else
            [x'] = [x] ∩
              (m([x]) − f(m([x]))/F'([x]))
            if [x'] = [/] then
                Discard search interval
            end
            else
                if [x'] ⊂ [x] then
                    Initiate the method on [x']
                end
                else
                    Bisect the search interval [x]
                    Initiate the method on both
                      of them
                end
            end
        end
    end
    else
        Discard search interval - [x] contains
          no zeros
    end
end
```

Algorithm 2: Interval Newton Algorithm

This pathological case may occur when the method attempts to enclose a possible multiple zero and the midpoint of search interval coincides with a zero of f, i.e. $f(m([x])) = 0$ (Figure 1). At this point, a bisection scheme is applied to the current search interval:

$$[x] = [\underline{x}, \overline{x}] = [x]_1 \cup [x]_2 = [\underline{x}, m([x])] \cup [m([x]), \overline{x}].$$

It is clear that both of the generated interval sequences containing $[x]_1$ and $[x]_2$, respectively, will converge to at least an enclosure containing $m([x])$, a zero of $f(x) = 0$. For example, consider the equation $x^2 = 0$ defined over the interval $[-1, 1]$ with $F([-1, 1]) = [0, 1]$ and $F'([-1, 1]) = [-2, 2]$. The application of Interval Newton on this problem, given a solution tolerance of $\varepsilon = 10^{-8}$, will perform as it is shown in Table 1. The application of the method in the third example results in two enclosures of a single zero, due to the aforementioned pathological case.

Again, a bisection scheme will be needed when there is an overestimation in the enclosure of the derivative of f, but f is actually monotone on the current search interval, as shown in Figure 2. For example, consider, now, the equation $x^3 = 0$ defined over the interval $[-1, 1]$ with $F([-1, 1]) = [-1, 1]$

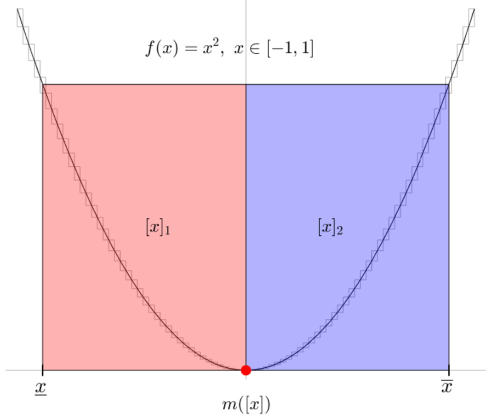

Figure 1: An example of pathological case with even multiplicity.

Table 1: Application of Interval Newton [$f(x) = x^2$, $\varepsilon = 10^{-8}$]

SI	NZ	ENCL	ITS	FE	DE	BS
$[-1, 0]$	1	**1**	20	**39**	19	0
$[0, 1]$	1	**1**	20	**39**	19	0
$[-1, 1]$	1	**2**	41	**80**	19	1

SI: Search Interval, NZ: Number of zeros, ENCL: Enclosures found, ITS: Iterations, FE/DE: Function and Derivative evaluations, BS: Needed bisections.

and $F'([-1, 1]) = [0, 3]$. The application of Interval Newton on this equation, given a solution tolerance of $\varepsilon = 10^{-8}$, will perform as it is shown in Table 2. The application of the method in the third example results in two enclosures of a single zero, due to the aforementioned pathological case.

Table 2: Application of Interval Newton [$f(x) = x^3$, $\varepsilon = 10^{-8}$]

SI	NZ	ENCL	ITS	FE	DE	BS
$[-1, 0]$	1	**1**	25	**49**	24	0
$[0, 1]$	1	**1**	25	**49**	24	0
$[-1, 1]$	1	**2**	51	**100**	49	1

SI: Search Interval, NZ: Number of zeros, ENCL: Enclosures found, ITS: Iterations, FE/DE: Function and Derivative evaluations, BS: Needed bisections.

Finally, due to the nature of certain functions, there is often a significant overestimation of their range, and Interval Newton method cannot provide sharp bounds for the zero enclosures, returning $[x] \subseteq N([x])$. These cases arise when the search interval is of short width, and as in the earlier cases, the method proceeds using a bisection scheme.

The issue of overestimation is addressed by choos-

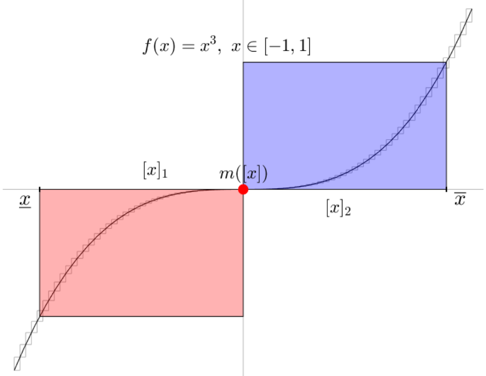

Figure 2: An example of pathological case with odd multiplicity.

ing appropriate interval extensions, [11], [16], which is beyond the scope of this paper.

2.4 Function perturbation

In this paper, a new technique is introduced to address pathological cases that may arise during the application of the Interval Newton method. The proposed technique is described as follows: If function f perturbed by a small amount, denoted as p, a new function f_p is derived. Consequently, the midpoint of $[x]$ will no longer be a zero of $f_p(x) = 0$, resulting in $f_p(m([x])) \neq 0$. Additionally, the equation $f_p(x) = 0$ will exhibit either two zeros or a single one, all different from those of $f(x) = 0$, for the cases of even or odd multiplicity respectively. These zeros will be referred to as pseudo-zeros (Figure 3 and Figure 4).

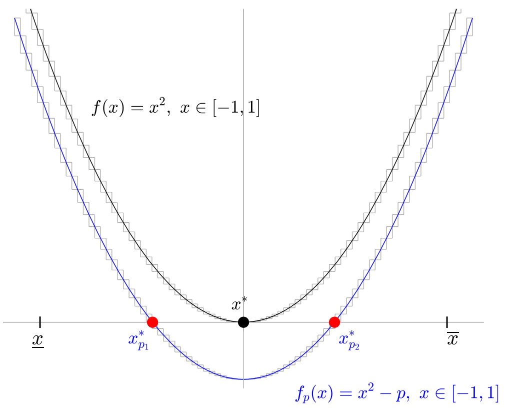

Figure 3: Function perturbation - Case with even multiplicity.

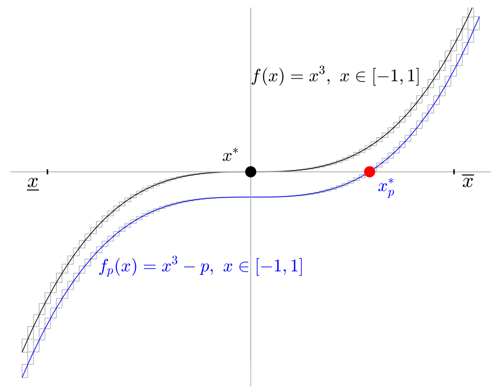

Figure 4: Function perturbation - Case with odd multiplicity.

By employing the Interval Newton method on the function $f_p(x)$, we can obtain enclosures for these pseudo-zeros. It is essential to emphasize that our primary objective is to provide zero-enclosures for the function $f(x) = 0$, rather than for $f_p(x) = 0$. These resulting enclosures serve as an efficient way to partition the search interval. For the case of even multiplicity the search interval will be partitioned as follows:

$$[x] = [\underline{x}, \overline{x}^*_{p_1}] \cup [x_{p_m}] \cup [\underline{x}^*_{p_2}, \overline{x}],$$

where $[x^*_{p_1}]$, $[x^*_{p_2}]$ denotes the zero enclosures of $f_p(x) = 0$ and $[x_{p_m}]$ the mid-interval. For the case of odd multiplicity the partition of the search interval is given as follows:

$$[x] = [\underline{x}, \overline{x}^*_p] \cup [x_{p_c}] \text{ or } [x] = [x_{p_c}] \cup [\underline{x}^*_p, \overline{x}],$$

where $[x^*_p]$ denotes the zero enclosure of $f_p(x) = 0$ and $[x_{p_c}]$ the complementary interval. Subsequently, the next step for the method is to search for zeros within these intervals.

Remark 1 *It is clear that in the case of a multiple zero of even multiplicity, the proposed technique can yield its existence, given that it can be proved that the pseudo-zeros enclosures contain simple zeros. This can be achieved, for instance, utilizing the method's property* $N([x]) \subset [x]$. *This holds since, as the perturbed function tends to the original one, the pseudo-zeros gradually shift towards the endpoints of the mid-interval. Consequently, the mid-interval will contain at least one zero of* $f(x) = 0$.

Remark 2 *For the case of a multiple zero of odd multiplicity the same result can be obtained by simply* *choosing an alternative to the midpoint. Assuming that* $0 \in F'(x)$ *and* $f(m(x)) = 0$ *it is not possible to determine the type of multiplicity. Thus, choosing a different point for Interval Newton method is not effective in all cases.*

2.5 The Special Interval Newton step

The implementation of the proposed technique modifies the Lines 16-17 of Algorithm 2 and it is described by the following Algorithm 3.

1 **Function** ***sinewton*** *(f,f′,* $[x]$*,p)*
2   **if** $0 \in f(m[x])$ **then**
3   Define $f_p(x) = f(x) - p$
4     $[x]_p = [x] \cap \big(m([x]) - f_p(m([x]))/F'([x])\big)$
5   Partition $[x]$ based on $[x]_p$
6   Initiate inewton method on each non-empty interval
7   **if** *pathology exists* **then**
8   Bisect the search interval $[x]$
9   Initiate inewton method on both of them
10   **end**
11   **end**
12 **end**

Algorithm 3: Special Interval Newton Step

The amount of perturbation p is chosen heuristically such that it satisfies the condition $d \leq \varepsilon$, where ε is the given tolerance for the problem (1). In Line 7, the statement "if the pathology exists", indicates that, due to overestimation issues, both enclosures $[x^*_{p_1}]$ and $[x^*_{p_2}]$ may result in an empty intersection with $[x]$, leading to the mid-interval $[x_{p_m}]$ being equal to the current search interval. In this case, the use of a bisection scheme becomes unavoidable.

3 Numerical Results

This section presents the application of the proposed step in different instances. To evaluate the performance of the method using the proposed step a set of eight test-functions was considered containing simple and multiple zeros (Table 3). The experiments were performed using MATLAB and intlab toolbox, [23], requiring an accuracy of $\varepsilon = 10^{-12}$ and a perturbation size of $p \in \{10^{-6}, 10^{-8}, 10^{-12}\}$. The results of the experiments in this work are summarized in the following Table 4. Based on the numerical findings, it is clear that when the equation has a unique zero, a significant improvement can be achieved by choosing an appropriate amount of perturbation. Even in the cases where multiple zeros exists and there is a substantial overestimation, employing an appropriate amount of perturbation appears to reduce the reliance on bisection schemes, making the Interval Newton method more efficient and reliable.

Table 3: Test Functions

PR	f	SI	NZ	ML
1	$x^2 - 4$	$[-4, 4]$	2	1
2	$x^2 - 4$	$[0, 4]$	1	1
3	x^2	$[-2, 2]$	1	2
4	$x^4 - x^2$	$[-2, 2]$	2	2
5	$x^6 - 2x^4 + x^2$	$[-2, 2]$	3	2
6	x^3	$[-2, 2]$	1	3
7	$(x^3 - 1)^2$	$[0, 2]$	1	6
8	$x^4 - 2x^3 - 3x^2$	$[-4, 4]$	3	1&2

PR: Problem, **f**: Test function, SI: Search Interval, NZ: Number of zeros, ML: Multiplicity.

Remark 3 *The numerical results show that the smaller the perturbation, the smaller the required bisections.*

4 Conclusions - Further Work

In this paper, we have considered the problem of finding all zeros of a differentiable function within a closed search interval. Specifically, we have studied the pathological cases that arise from the existence of multiple zeros within a given search interval. In these cases, the efficiency of the Interval Newton method decreases due to the employment of bisection schemes. This is because the Interval Newton operator is unable to reduce the search interval, and therefore cannot improve the bounds of zero enclosures.

The proposed Special Newton Step, temporarily transforms a function with a multiple zero x^* into a function where x^* is not a zero. This transformation is achieved by vertically shifting the original function by an appropriate amount, effectively reducing the limitations of the Interval Newton operator. The application of this step creates more favorable conditions for the method, significantly enhancing its efficiency. Our numerical results show that it is feasible to avoid the use of bisection schemes in cases where the application point of the method coincides with a multiple zero. Moreover, we demonstrate that a multiple zero is not only enclosed faster but, also, large intervals surrounding the zero can also be discarded. Additionally, it is evident from the results that the efficiency and effectiveness of the method depend significantly on the amount of the perturbation applied to the function.

The rapid inclusion of a multiple zero raises questions about existence and uniqueness, which, along with the problem of finding the optimal perturbation, should be topics for a future research.

Table 4: Numerical Results [$\varepsilon = 10^{-12}$]

$p = 10^{-6}$						
PR	**Interval Newton**			**Interval Newton+**		
	ENCL	FE+DE	BS	ENCL	FE+DE	BS
1	2	35	0	2	35	0
2	2	32	1	1	17	0
3	2	179	1	2	88	1
4	6	265	3	4	208	1
5	170	2177	169	148	2046	161
6	2	227	1	1	119	0
7	2	179	1	1	59	0
8	4	256	1	3	203	0
$p = 10^{-8}$						
PR	**Interval Newton**			**Interval Newton+**		
	ENCL	FE+DE	BS	ENCL	FE+DE	BS
1	2	35	0	2	35	0
2	2	32	1	1	17	0
3	2	179	1	2	58	1
4	6	265	3	4	196	1
5	170	2177	169	148	1956	143
6	2	227	1	1	119	0
7	2	179	1	1	36	0
8	4	256	1	3	197	0
$p = 10^{-12}$						
PR	**Interval Newton**			**Interval Newton+**		
	ENCL	FE+DE	BS	ENCL	FE+DE	BS
1	2	35	0	2	35	0
2	2	32	1	1	17	0
3	2	179	1	1	6	0
4	6	265	3	3	192	0
5	170	2177	169	135	1880	130
6	2	227	1	1	116	0
7	2	179	1	1	6	0
8	4	256	1	3	203	0

Interval Newton: Interval Newton Method,
Interval Newton+: Interval Newton method using Special Interval Newton Step, SI: Search Interval, NZ: Number of zeros, ENCL: Enclosures found, ITS: Iterations, FE/DE: Function and Derivative evaluations, BS: Needed bisections.

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