# A NEW SECOND DERIVATIVE FREE ITERATIVE METHOD OF FIFTH ORDER OF CONVERGENCE AND ITS APPLICATIONS 

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#### Abstract

The primary objective of this article is to derive a new free-from-second derivative iterative method for solving nonlinear equations. The proposed method is proven to have fifth order of convergence. Comparisons with other iterative methods represent the advantage of the modified method. Observation of applications of the method in problems of chemical equilibrium, binary azeotropic problem, volume from van der Waals equations, and eccentric anomaly in Kepler's law exhibit that our method is applicable and preferable. Keywords: Nonlinear equations, iterative method, Halley's method


## 1. Introduction

Finding solution of non-linear equation, $f(x)=0$, has been a challenging as well as progressing subject. Numerous equations of this kind are typical in real life problems. Many researchers have developed methods on root-finding problems in order to update the methods or to overcome some drawbacks that come with the modification of the methods. Generally, subjects of improvement are how to reduce the number of iterations needed to obtain the root and how to increase efficiency index or the order convergence order of the method.

Halley's method, which is defined by

$$
\begin{equation*}
x_{k+1}=x_{k}-\frac{2 f\left(x_{k}\right) f^{\prime}\left(x_{k}\right)}{2 f^{\prime}\left(x_{k}\right)^{2}-f\left(x_{k}\right) f^{\prime \prime}\left(x_{k}\right)}, \tag{1.1}
\end{equation*}
$$

has third order of convergence and requires calculation of second derivative, see ([1],[2]). It has been modified by many researchers in pursuit of finding better methods. One of the ways is by combining the method with other methods in order to attain better results and higher order of convergence; for instance see ([3], [4], [5], [6], [7]).

There is a problem in an iterative method if second derivative appears. Due to the cost of calculating it or the problematic practicality in applying the method, free derivative method is preferable. Many researchers have employed several techniques in order to avoid these problems. There is a vast literature on how to avoid the calculation of second derivative in an iterative methods as one can find in ([5], [8], [9], [10], [11], [12], [13]).

This paper studies about adopting a technique to modify method in [14] to give a new second derivative free iterative method. This paper is organized as follows: The derivation of our proposed method as well as the convergence analysis of the proposed method is carried out in Section 2. In Section 3, we test the proposed method and other iterative methods on several transcendental functions. Finally in Section 4, we draw the conclusion.

## 2. A New Free Second Derivative Iteration Method

In [8], Noor presented the method based on the method in [14] as follows:

$$
\begin{align*}
y_{k} & =x_{k}-\frac{2 f\left(x_{k}\right) f^{\prime}\left(x_{k}\right)}{2 f^{\prime}\left(x_{k}\right)-f\left(x_{k}\right) f^{\prime \prime}\left(x_{k}\right)}  \tag{2.1}\\
x_{k+1} & =x_{k}-\frac{2\left[f\left(x_{k}\right)+f\left(y_{k}\right)\right] f^{\prime}\left(x_{k}\right)}{2 f^{\prime 2}\left(x_{k}\right)-\left[f\left(x_{k}\right)+f\left(y_{k}\right)\right] f^{\prime \prime}\left(x_{k}\right)}, \quad n=0,1,2, \cdots \tag{2.2}
\end{align*}
$$

This method has fifth order of convergence and takes evaluation of two functions, one first derivative and one second derivative. The efficiency index of the method is $5^{1 / 4} \approx 1.4953$.

In order to avoid calculating second derivative, we utilize a technique by [5] where the approximation of $f^{\prime \prime}(x)$ is done by making use of parabola of the form

$$
\begin{equation*}
a y^{2}+y+b x+c=0 . \tag{2.3}
\end{equation*}
$$

Upon imposing tangency conditions $y\left(x_{k}\right)=f\left(x_{k}\right), y^{\prime}\left(x_{k}\right)=f^{\prime}\left(x_{k}\right)$ and $y\left(w_{k}\right)=$ $f\left(w_{k}\right)$ on (2.3) where $w_{k}$ is defined as

$$
\begin{equation*}
w_{k}=x_{k}-\frac{f\left(x_{k}\right)}{f^{\prime}\left(x_{k}\right)} \tag{2.4}
\end{equation*}
$$

then the approximation of $f^{\prime \prime}(x)$ is presented as follows,

$$
\begin{equation*}
f^{\prime \prime}\left(x_{k}\right) \approx y^{\prime \prime}\left(x_{k}\right)=\frac{2 f\left(w_{k}\right) f^{\prime}\left(x_{k}\right)^{2}}{\left(\left(x_{k}\right)-f\left(w_{k}\right)\right)^{2}} \tag{2.5}
\end{equation*}
$$

Substituting (2.5) to (2.1) and (2.2), we obtain a new method free of second derivative

$$
\begin{align*}
w_{k} & =x_{k}-\frac{f\left(x_{k}\right)}{f^{\prime}\left(x_{k}\right)}  \tag{2.6}\\
y_{k} & =x_{k}-\frac{f\left(x_{k}\right)\left(f\left(w_{k}\right)-f\left(x_{k}\right)\right)^{2}}{f^{\prime}\left(x_{k}\right)\left(f\left(w_{k}\right)^{2}-3 f\left(x_{k}\right) f\left(w_{k}\right)+f\left(x_{k}\right)^{2}\right)}  \tag{2.7}\\
x_{k+1} & =x_{k}-\frac{\left(f\left(x_{k}\right)+f\left(y_{k}\right)\right)\left(f\left(w_{k}\right)-f\left(x_{k}\right)\right)^{2}}{f^{\prime}\left(x_{k}\right)\left(f\left(w_{k}\right)^{2}+f\left(x_{k}\right)^{2}-f\left(w_{k}\right)\left(3 f\left(x_{k}\right)+f\left(y_{k}\right)\right)\right)} \tag{2.8}
\end{align*}
$$

The method describes in (2.6) - (2.8) is a three-step method that requires evaluations of three functions and one first derivative. We call the method as new method free of second derivative and for simplicity will be referred to as NMFSD. The convergence of the method is given by the following theorem.

Theorem 2.1. Let $\alpha \in \mathcal{D}$ be a simple root of the function $f: \mathcal{D} \subset \mathbb{R} \longrightarrow \mathbb{R}$, where $f(x)$ is sufficiently differentiable in an open interval $\mathcal{D}$. If $x_{0}$ be an initial guess that properly close to $\alpha$, then NMFSD has fifth order of convergence.

Proof. Let $\alpha$ be a simple root of $f(x)$. Expanding $f(x)$ around $x=\alpha$ using Taylor series, one obtains

$$
\begin{align*}
f(x)=f(\alpha) & +f^{\prime}(\alpha)(x-\alpha)+\frac{1}{2!} f^{\prime \prime}(\alpha)(x-\alpha)^{2}+\frac{1}{3!} f^{\prime \prime \prime}(x)(x-\alpha)^{3}  \tag{2.9}\\
& +\frac{1}{4!} f^{(4)}(x)(x-\alpha)^{4}+\frac{1}{5!} f^{(5)}(x)(x-\alpha)^{5}+\frac{1}{6!} f^{(6)}(x)(x-\alpha)^{6} \\
& +O(x-\alpha)^{7}
\end{align*}
$$

Evaluating $f(x)$ at $x_{k}$ and $e_{k}=x_{k}-\alpha$ be the error at the $k$ th-iteration, one attains

$$
\begin{equation*}
f\left(x_{k}\right)=f^{\prime}(\alpha)\left(e_{k}+C_{2} e_{k}^{2}+C_{3} e_{k}^{3}+C_{4} e_{k}^{4}+C_{5} e_{k}^{5}+C_{6} e_{k}^{6}+O\left(e_{k}^{7}\right)\right) \tag{2.10}
\end{equation*}
$$

where $C_{n}=(1 / n!)\left(f^{(n)}(\alpha) / f^{\prime}(\alpha)\right), n=1,2,3, \cdots$.
Differentiating (2.9) and evaluating the derivative at $x_{k}$, resulting in

$$
\begin{equation*}
f^{\prime}\left(x_{k}\right)=f^{\prime}(\alpha)\left(1+2 C_{2} e_{k}^{2}+3 C_{3} e_{k}^{2}+4 C_{4} e_{k}^{3}+5 C_{5} e_{k}^{4}+6 C_{6} e_{k}^{5}+O\left(e_{k}^{6}\right)\right) \tag{2.11}
\end{equation*}
$$

From (2.10) and (2.11) we have

$$
\begin{align*}
\frac{f\left(x_{k}\right)}{f^{\prime}\left(x_{k}\right)}=e_{k} & -C_{2} e_{k}^{2}+\left(2 C_{2}^{2}-2 C_{3}\right) e_{k}^{3}+\left(4 C_{2}^{3}+7 C_{2} C_{3}-3 C_{4}\right) e_{k}^{4} \\
& +\left(16 C_{2}^{2} C_{3}+10 C_{2} C_{4}+6 C_{3}^{2}\right) e_{k}^{5}+O\left(e_{k}^{6}\right) \tag{2.12}
\end{align*}
$$

Using (2.4), $w_{k}$ is obtained as

$$
\begin{align*}
w_{k}=e_{k} & -C_{2} e_{k}^{2}+\left(2 C_{2}^{2}-2 C_{3}\right) e_{k}^{3}+\left(4 C_{2}^{3}+7 C_{2} C_{3}-3 C_{4}\right) e_{k}^{4}+\left(16 C_{2}^{2} C_{3}\right. \\
& \left.+10 C_{2} C_{4}+6 C_{3}^{2}\right) e_{k}^{5}+\left(20 C_{2}^{2} C_{4}+21 C_{2} C_{3}^{3}+17 C_{3} C_{4}\right) e_{k}^{6}+O\left(e_{k}^{7}\right) \tag{2.13}
\end{align*}
$$

Substituting $w_{k}$ to $f(x)$ we have,

$$
\begin{align*}
f\left(w_{k}\right)=f^{\prime}(\alpha) & \left(C_{2} e_{k}^{2}-\left(2 C_{2}^{2}-2 C_{3}\right) e_{k}^{3}-\left(4 C_{2}^{3}+7 C_{2} C_{3}-3 C_{4}\right) e_{k}^{4}\right. \\
& \left.-\left(16 C_{2}^{2} C_{3}+10 C_{2} C_{4}+6 C_{3}^{2}\right) e_{k}^{5} 10 C_{2} C_{4}+6 C_{3}^{2}\right) e_{k}^{5} \\
& \left.+\left(20 C_{2}^{2} C_{4}+21 C_{2} C_{3}^{3}+17 C_{3} C_{4}\right) e_{k}^{6}+O\left(e_{k}^{7}\right)\right) \tag{2.14}
\end{align*}
$$

Using (2.10) and (2.14) and some simplification, we have

$$
\begin{align*}
f\left(x_{k}\right)\left(f\left(w_{k}\right)-f\left(x_{k}\right)\right)^{2}=f^{\prime} & \left(x_{k}\right)^{3}\left(e_{k}^{3}+C_{2} e_{k}^{4}+\left(4 C_{2}^{2}-C_{3}\right) e_{k}^{5}\right. \\
& \left.+\left(12 C_{2}^{3}+12 C_{2} C_{3}-3 C_{4}\right) e_{k}^{6}+O\left(e_{k}^{7}\right)\right) \tag{2.15}
\end{align*}
$$

Next, utilizing (2.10), (2.11), and (2.14) yields

$$
\begin{align*}
& f^{\prime}\left(x_{k}\right)\left(f\left(w_{k}\right)^{2}-3 f\left(x_{k}\right) f\left(w_{k}\right)+f\left(x_{k}\right)^{2}\right) \\
& =f^{\prime}(\alpha)^{3}\left(e_{k}^{2}+C_{2} e_{k}^{3}\left(2 C_{2}^{2}-C_{3}\right) e_{k}^{4}+\left(24 C_{2}^{3}+7 C_{2} C_{3}-3 C_{4}\right) e_{k}^{5}\right. \\
& \left.\quad+\left(36 C_{2}^{4}+104 C_{2}^{2} C_{3}+8 C_{2} C_{4}+5 C_{3}^{2}-5 C_{5}\right) e_{k}^{6}+O\left(e_{k}^{7}\right)\right) . \tag{2.16}
\end{align*}
$$

Substituting (2.15) and (2.16) to (2.7) and simplifying, we have

$$
\begin{align*}
y_{k}=\alpha & -C_{2}^{2} e_{k}^{3}-\left(-12 C_{2}^{3}+5 C_{2} C_{3}\right) e_{k}^{4}-\left(-12 C_{2}^{4}-111 C_{2}^{2} C_{3}\right. \\
& \left.-8 C_{2} C_{4}-5 C_{3}^{2}+5 C-5\right) e_{k}^{5}+O\left(e_{k}^{6}\right) \tag{2.17}
\end{align*}
$$

Employing the same technique to get $f\left(w_{k}\right)$, we obtain

$$
\begin{align*}
f\left(y_{k}\right)=f^{\prime}(\alpha)( & -C_{2}^{2} e_{k}^{3}-\left(-12 C_{2}^{3}+5 C_{2} C_{3}\right) e_{k}^{4}-\left(-12 C_{2}^{4}-111 C_{2}^{2} C_{3}\right. \\
& \left.\left.-8 C_{2} C_{4}-5 C_{3}^{2}+5 C-5\right) e_{k}^{5}+O\left(e_{k}^{6}\right)\right) \tag{2.18}
\end{align*}
$$

Following on, from (2.10), (2.14), and (2.17) we have

$$
\begin{align*}
\left(f\left(x_{k}\right)\right. & +f\left(y_{k}\right)\left(f\left(w_{k}\right)-f\left(x_{k}\right)\right)^{2} \\
& =f^{\prime}(\alpha)^{3}\left(e_{k}^{3}+C_{2} e_{k}^{4}+\left(3 C_{2}^{2}-C_{3}\right) e_{k}^{5}+\left(24 C_{2}^{3}+7 C_{2} C_{3}-3 C_{4}\right) e_{k}^{6}+O\left(e_{k}^{7}\right)\right) \tag{2.19}
\end{align*}
$$

and also,

$$
\begin{align*}
& f^{\prime}\left(x_{k}\right)\left(f\left(w_{k}\right)^{2}+f\left(x_{k}\right)^{2}-f\left(w_{k}\right)\left(3 f\left(x_{k}\right)+f\left(y_{k}\right)\right)\right) \\
& \quad=f^{\prime}(\alpha)^{3}\left(\left(e_{k}^{2}+C_{2} e_{k}^{3}+(3 C) 2^{2}-C_{3}\right) e_{k}^{4}+\left(25 C_{2}^{3}+7 C_{2} C_{3}-3 C_{4}\right) e_{k}^{5}\right. \\
& \left.\quad+\left(24 C_{2}^{4}+111 C_{2}^{2} C_{3}+8 C_{2} C_{4}+5 C_{3}^{2}-5 C_{5}\right) e_{k}^{6}+O\left(e_{k}^{7}\right)\right) \tag{2.20}
\end{align*}
$$

Substituting (2.19) and (2.20) into (2.8) and after some simplification we obtain

$$
\begin{aligned}
x_{k+1}=\alpha- & -\left(-14 C_{2}^{4}-114 C_{2}^{2} C_{3}-8 C_{2} C_{4}-5 C_{3}^{2}+5 C_{5}\right) e_{k}^{5}-\left(128 C_{2}^{5}\right. \\
& \left.+113 C_{2}^{3} C_{3}-C_{2}^{2} C_{4}+8 C_{2} C_{3}^{2}-5 C_{2} C_{5}\right) e_{k}^{6}+O\left(e_{k}^{7}\right), \\
e_{k+1}= & \left(14 C_{2}^{4}+114 C_{2}^{2} C_{3}+8 C_{2} C_{4}+5 C_{3}^{2}-5 C_{5}\right) e_{k}^{5}-\left(128 C_{2}^{5}\right. \\
& \left.+113 C_{2}^{3} C_{3}-C_{2}^{2} C_{4}+8 C_{2} C_{3}^{2}-5 C_{2} C_{5}\right) e_{k}^{6}+O\left(e_{k}^{7}\right) .
\end{aligned}
$$

## 3. Numerical Results

In this section we present some numerical results of our iterative method and its contrasts to several other methods. The software we use for the simulations is Maple v.2018. We additionally apply our method on some real life problems. The methods used in the comparison are Newton's method (NM), Halley's method (HM), fifthorder method composed of Newton and third-order Halley's method (NHM) [6], improvement of Super-Halley Method (ISHM) [9] and two step Halley's method (TSHM) [14]. The functions being tested are

- $f_{1}(x)=x^{3}-4 x^{2}-10$ with root $\alpha=1.3652300134140968457608068$,
- $f_{2}(x)=x^{2}-e^{x}-3 x+2$ with root $\alpha=0.2575302854398607604553673$,
- $f_{3}(x)=x^{3}-10$ with root $\alpha=2.1544346900318837217592936$,
- $f_{4}(x)=\cos (x)-x$ with root $\alpha=0.7390851332151606416553145$,
- $f_{5}(x)=\sin (x)^{2}-x^{2}+1$ with root $\alpha=1.4044916482153412260350868$,
- $f_{6}(x)=x^{2}+\sin (x / 5)-1 / 4$ with root $\alpha=1.2634012757103932674282872$,
- $f_{7}(x)=e^{x}-4 x^{2}$ with root $\alpha=0.7148059123627778061376222$,
- $f_{8}(x)=e^{-x}+\cos (x)$ with root $\alpha=1.7461395304080124176507031$.

The stopping criteria in the program are $\left|x_{k+1}-x_{k}\right| \leq 10^{-15}$ or $\left|f\left(x_{k+1}\right)\right| \leq 10^{-15}$.
Table 1 displays the comparisons between the proposed method and other iterative methods for functions $f_{1}(x)$ through $f_{8}(x)$. We observe number of iterations, absolute value of function at $k$-th iteration and distance of each iteration for every discussed method. It can be seen that NMFSD needs fewer or equal number of iterations compared to the competitor methods. In addition, the discussed method gives a more precise solution. For instance, in the case where the number of iterations are the same, our proposed method gives a better precision than other methods where it can be seen from the values of $|f(x)|$ of NMFSD that are relatively smaller for all cases except in $f_{1}(x)$. In this case, NMFSD produces the smallest number of iterations among others. Furthermore, although ISHM and TSHM are of the same order of convergence with NMFSD, the numerical results are not overall accurate as NMFSD and same goes with the rest of the compared methods with lower order of convergence.

Table 1. Comparison of discussed iterative methods for functions $f_{1}(x)$ through $f_{8}(x)$

| function | Methods | $k$ | $x_{k}$ | $\left\|f\left(x_{k}\right)\right\|$ | $\left\|x_{k+1}-x_{k}\right\|$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | NM | 54 | 1.3652300134140968457608068 | $8.1 e-30$ | $1.0 e-15$ |
|  | HM | 58 | 1.3652300134140968457608069 | $6.8 e-25$ | $6.1 e-09$ |
| $f_{1}(x)$ | NHM | 56 | 1.3652300134140968457608068 | $5.3 e-26$ | $1.0 e-07$ |
| $x_{0}=-0.3$ | ISHM | 27 | 1.3652300134140968457608068 | $8.4 e-48$ | $6.6 e-16$ |
|  | TSHM | 19 | 1.3652300134140968457607650 | $6.9 e-22$ | $5.3 e-05$ |
|  | NMFSD | 4 | 1.3652300134140968457591418 | $2.8 e-20$ | $1.2 e-04$ |
|  | NM | 4 | 0.2575302854398607604553673 | $1.1 e-26$ | $1.8 e-13$ |
|  | HM | 3 | 0.2575302854398607604553673 | $1.4 e-32$ | $4.2 e-11$ |
| $f_{2}(x)$ | NHM | 2 | 0.2575302854398608296848409 | $2.6 e-16$ | $1.9 e-04$ |
| $x_{0}=0.5$ | ISHM | 2 | 0.2575302854398609247347169 | $6.2 e-16$ | $4.9 e-05$ |
|  | TSHM | 2 | 0.2575302854398607604553673 | $4.5 e-27$ | $1.1 e-05$ |
|  | NMFSD | 2 | 0.2575302854398607604553673 | $4.7 e-37$ | $1.9 e-07$ |
|  | NM | 5 | 2.1544346900318837218052378 | $6.4 e-19$ | $3.2 e-10$ |
|  | HM | 3 | 2.1544346900318837216602636 | $1.4 e-18$ | $8.8 e-07$ |
| $f_{3}(x)$ | NHM | 3 | 2.1544346900318837217592937 | $2.4 e-24$ | $3.1 e-07$ |
| $x_{0}=1.7$ | ISHM | 3 | 2.1544346900318837217592936 | $4.1 e-28$ | $2.3 e-09$ |
|  | TSHM | 3 | 2.1544346900318837216602636 | $1.4 e-18$ | $8.8 e-07$ |
|  | NMFSD | 3 | 2.1544346900318837217592936 | $5.1 e-64$ | $2.3 e-13$ |


| function | Methods | $k$ | $x_{k}$ | $\left\|f\left(x_{k}\right)\right\|$ | $\left\|x_{k+1}-x_{k}\right\|$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | NM | 4 | 0.7390851332151606416617026 | $1.1 e-20$ | $1.7 e-10$ |
|  | HM | 3 | 0.7390851332151606416553121 | $5.6 e-29$ | $6.6 e-10$ |
| $f_{4}(x)$ | NHM | 3 | 0.7390851332151606416553121 | $3.6 e-57$ | $1.0 e-14$ |
| $x_{0}=1.0$ | ISHM | 3 | 0.7390851332151606416553121 | $1.9 e-41$ | $1.1 e-13$ |
|  | TSHM | 2 | 0.7390851332151606416553145 | $4.1 e-24$ | $3.6 e-05$ |
|  | NMFSD | 2 | 0.7390851332151606416553121 | $2.4 e-32$ | $1.7 e-06$ |
|  | NM | 6 | 1.4044916482153412260354817 | $9.8 e-22$ | $2.5 e-11$ |
|  | HM | 4 | 1.4044916482153412260351022 | $3.8 e-23$ | $3.1 e-08$ |
| $f_{5}(x)$ | NHM | 4 | 1.4044916482153412260350868 | $4.8 e-35$ | $1.4 e-09$ |
| $x_{0}=3.5$ | ISHM | 3 | 1.4044916482153412261236135 | $2.2 e-19$ | $1.5 e-06$ |
|  | TSHM | 3 | 1.4044916482153412260350868 | $2.1 e-26$ | $6.3 e-06$ |
|  | NMFSD | 3 | 1.4044916482153412260350868 | $1.8 e-36$ | $7.0 e-08$ |
|  | NM | 3 | 1.2634012757103931737831137 | $1.8 e-17$ | $6.0 e-08$ |
|  | HM | 3 | 1.2634012757103932674282872 | $6.1 e-45$ | $1.6 e-14$ |
| $f_{6}(x)$ | NHM | 2 | 1.2634012757103932674282872 | $8.3 e-28$ | $1.8 e-06$ |
| $x_{0}=1.0$ | ISHM | 2 | 1.2634012757103932649724849 | $4.8 e-19$ | $1.4 e-05$ |
|  | TSHM | 2 | 1.2634012757103932674282872 | $8.4 e-39$ | $1.9 e-07$ |
|  | NMFSD | 2 | 1.2634012757103932674282872 | $4.5 e-49$ | $3.6 e-09$ |
|  | NM | 5 | 0.7148059123627778061382883 | $2.5 e-21$ | $2.9 e-11$ |
|  | HM | 3 | 0.7148059123627777997252275 | $2.4 e-17$ | $2.0 e-06$ |
|  | NHM | 4 | 0.7148059123627778061376222 | $1.5 e-47$ | $7.5 e-13$ |
|  | NHM | 3 | 0.7148059123627778061376222 | $3.9 e-35$ | $8.0 e-12$ |
| $f_{7}(x)$ | ISHM |  |  |  |  |
| $x_{0}=0.5$ | TSHM | 3 | 0.7148059123627778061376222 | $6.3 e-63$ | $2.5 e-13$ |
|  | NMFSD | 3 | 0.7148059123627778061376222 | $3.3 e-70$ | $1.2 e-14$ |
| $x_{0}=2.4$ | NMFSD | 3 | 1.7461395304080124176507031 | $2.4 e-74$ | $6.2 e-15$ |
|  | NM | 5 | 1.7461395304080124176507030 | $6.7 e-26$ | $6.2 e-13$ |
|  | NHM | 4 | 1.7461395304080124176507031 | $4.8 e-42$ | $3.2 e-14$ |
|  | NHM | 3 | 1.7461395304080121277471630 | $3.4 e-16$ | $2.2 e-04$ |
|  | TSHM | 3 | 1.7461395304080124176506969 | $7.2 e-24$ | $7.4 e-08$ |
|  | 3 | 1.7461395304080124176507031 | $1.7 e-48$ | $4.8 e-10$ |  |
|  |  |  |  |  |  |

Next, we investigate the proposed method by applying it to chemical engineering problems and physics and do some comparison with methods used in the preceding numerical simulations. The stopping criteria and tolerance used are the same with the previous simulation done above.

Example 3.1. Consider a chemical equilibrium problem showed in [16],

$$
\begin{equation*}
g_{1}(x)=x^{4}-7.79075 x^{3}+14.7445 x^{2}+2.511 x-1.674 \tag{3.1}
\end{equation*}
$$

which represents a conversion of ammonia from the fraction of nitrogen-hydrogen feed (also known as fractional conversion) at 250 atm pressure and temperature of $500^{\circ} \mathrm{C}$. The roots of (3.1) are $x_{1}=0.278, x_{2}=-0.384, x_{4}=3.949+0.316 i$ and $x_{4}=3.949-0.316 i$. Fractional conversion is a number between 0 and 1 . Hence, the only solution that is physically meaningful is $x_{1}$. For the numerical simulation, we use initial guess $x_{0}=0.5$.

Example 3.2. Consider the problem from [17] to find the azeotropic point of a binary solution:

$$
\begin{equation*}
g_{2}(x)=\frac{A B\left(B\left(1-x^{2}\right)-A x^{2}\right)}{\left(x(A-B)+B^{2}\right)}+0.14845 \tag{3.2}
\end{equation*}
$$

where $A$ and $B$ are coefficients in the van Laar equation that describe phase equlibria of liquid solutions, see [18] and the reference therein. Let $A=0.38969$ and $B=$ 0.55954 , then the root of (3.2) is $x=0.6914737357$. We apply initial guess $x_{0}=1.0$ in the simulation.

Example 3.3. Kepler's law of planetary motion states that a planet revolves around the sun in an elliptic orbit. Position of a planet, $(\alpha, \beta)$, at time $t$ can be determined by solving

$$
\begin{aligned}
& \alpha=a \cos (E-e) \\
& \beta=a \sqrt{1-e^{2}} \sin (E)
\end{aligned}
$$

where $E$ and $e$ are the eccentric anomaly and the eccentricity of the ellipse respectively and $0<e<1$, see [19] and the reference therein. In order to find $(\alpha, \beta)$, one must solve the following formula:

$$
g_{3}(E)=e \sin (E)-E+M
$$

where $M$ is the mean anomaly. The arising problem is to find the root of

$$
\begin{equation*}
g_{3}(x)=M-x+e \sin (x)=0 \tag{3.3}
\end{equation*}
$$

The root of (3.3) is 0.5236038 . Consider $M=\frac{\pi}{6}$ and use initial guess $x_{0}=M$.
Example 3.4. Van der Waals' equation for $n$ moles of gas is given by:

$$
\begin{equation*}
\left(P+\frac{n^{2} a}{V^{2}}\right)(V-n b)=n R T \tag{3.4}
\end{equation*}
$$

where $R=0.0820578$ is gas constant and $n$ is number of moles of gas, $P$ is pressure, $V$ is volume and $T$ is temperature, see [20]. In addition, $a$ and $b$ are constants which are obtained experimentally for each gas.

Formula (3.4) is reduced in order to find the volume of a certain gas:

$$
g_{4}(V)=p V^{3}-n(R T+b p) V^{2}+n^{2} a V-n^{3} a b
$$

Volume of 1.00 moles of neon at temperature of 355 K under pressure of 500 atm , given that van der Waals constants for neon are $a=0.2135$ and $b=0.01709$, can be found by finding the roots of following equation

$$
\begin{equation*}
g_{4}(x)=500 x^{3}-37.4905190 x^{2}+0.208 x-0.00347776 \tag{3.5}
\end{equation*}
$$

The roots of (3.5) are $x_{1}=0.0022882-0.0098929 i, x_{2}=0.0022882+0.0098929 i$ and $x_{3}=0.070776$. Since the goal is to find volume, we only consider the third root $x_{3}$. The test is done by considering $x_{0}=2.0$.

Table 2 illustrates the comparisons between the studied iterative methods with other methods to solve Example 3.1 through Example 3.4, where $k$ denotes the

Table 2. Comparison of discussed iterative methods for functions $g_{1}(x)$ through $g_{4}(x)$

|  | Methods | $k$ | $x_{k}$ | $\left\|g\left(x_{k}\right)\right\|$ | $\left\|x_{k+1}-x_{k}\right\|$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{array}{r} g_{1}(x) \\ x_{0}=0.5 \end{array}$ | NM | 5 | 0.2777594235836338613571836 | $4.7 e-26$ | $7.4 e-14$ |
|  | HM | 3 | 0.2777594235836338626272471 | $1.1 e-17$ | $9.1 e-07$ |
|  | NHM | 4 | 0.2777594235836338613571836 | $1.3 e-57$ | $1.4 e-15$ |
|  | ISHM | 3 | 0.2777594235836338613571836 | $1.1 e-29$ | $2.5 e-10$ |
|  | TSHM | 3 | 0.2777594235836338613571836 | $1.8 e-70$ | $4.7 e-15$ |
|  | NMFSD | 2 | 0.2777594235836338613570451 | $1.2 e-21$ | $5.9 e-05$ |
| $\begin{array}{r} g_{2}(x) \\ x_{0}=1.0 \end{array}$ | NM | 5 | 0.6914737357471414206321227 | $9.4 e-25$ | $1.2 e-12$ |
|  | HM | 3 | 0.6914737357471414206321218 | $2.2 e-32$ | $8.1 e-11$ |
|  | NHM | 2 | 0.6914737357471411393975076 | $3.1 e-16$ | $1.9 e-04$ |
|  | ISHM | 3 | 0.6914737357471414206321013 | $2.3 e-23$ | $5.1 e-08$ |
|  | TSHM | 2 | 0.6914737357471414206321218 | $2.6 e-27$ | $1.4 e-05$ |
|  | NMFSD | 2 | 0.6914737357471414351059217 | $1.6 e-17$ | $5.9 e-04$ |
| $\begin{array}{r} g_{3}(x) \\ x_{0}=\frac{\pi}{6} \end{array}$ | NM | 1 | 0.5236037756416005182695768 | $6.3 e-17$ | $5.0 e-06$ |
|  | HM | 1 | 0.5236037756416004557679530 | $1.8 e-22$ | $5.0 e-06$ |
|  | NHM | 1 | 0.5236037756416004557677725 | $1.3 e-32$ | $5.0 e-06$ |
|  | ISHM | 1 | 0.5236037756416004557677725 | $4.5 e-28$ | $5.0 e-06$ |
|  | TSHM | 1 | 0.5236037756416004557677725 | $2.0 e-38$ | $5.0 e-06$ |
|  | NMFSD | 1 | 0.5236037756416004557677725 | $2.8 e-44$ | $5.0 e-06$ |
| $\begin{gathered} g_{4}(x) \\ x_{0}=2.0 \end{gathered}$ | NM | 14 | 0.0704788277033310934161193 | $3.6 e-17$ | $7.3 e-10$ |
|  | HM | 9 | 0.0704788277033310780934677 | $1.7 e-33$ | $1.1 e-12$ |
|  | NHM | 10 | 0.0704788277033310780934677 | $2.0 e-34$ | $1.9 e-10$ |
|  | ISHM | 6 | 0.0704788277033310780934677 | $1.8 e-35$ | $1.4 e-13$ |
|  | TSHM | 7 | 0.0704788277033310780934677 | $9.1 e-59$ | $1.3 e-13$ |
|  | NMFSD | 4 | 0.0704788277033310780958190 | $5.4 e-21$ | $4.9 e-06$ |

number of iterations needed to satisfy the stopping criteria, $x_{k}$ is the approximate root at iteration $k,\left|g\left(x_{k}\right)\right|$ is the value of approximate root at iteration $k$, and $\left|x_{k+1}-x_{k}\right|$ is the distance between two successive iterations. From the simulation, it can be concluded that NMFSD has better approximation to the solution of each example. It is shown in the table that NMFSD needs fewer or equal number of iterations for $g_{1}(x), g_{2}(x)$ and $g_{4}(x)$. Finally, In the case of $g_{3}(x)$, although all of discussed methods need one iteration to approximate the solution, NMFSD does better in approximating by providing a more accurate solution where its $\left|g\left(x_{k}\right)\right|$ being the smallest among all.

## 4. Conclusion

In this study, we have derived a new iterative method free from second derivative. We have approximated the second derivative by applying a parabola equation and imposing the tangency conditions, obtaining a new iterative method of fifth order of convergence. Order of convergence of the method has been proven. Numerical simulations and comparisons have been carried out for five other iterative methods, two of which are of the same order with the discussed method. Four real life problems from chemical engineering and physics have been borrowed to test the method
and its competitors. Overall, the proposed method shows more accurate solutions compare to the other methods.

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