



An optimal eighth order derivative free multiple root finding numerical method and applications to chemistry

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Abstract

In this paper, we present an optimal eighth order derivative-free family of methods for multiple roots which is based on the first order divided difference and weight functions. This iterative method is a three step method with the first step as Traub–Steffensen iteration and the next two taken as Traub–Steffensen-like iteration with four functional evaluations per iteration. We compare our proposed method with the recent derivative-free methods using some chemical engineering problems modelled as nonlinear equations with simple and multiple roots. Stability of the presented family of methods is demonstrated by using the graphical tool known as basins of attraction.

Keywords Nonlinear equations · Multiple roots · Derivative free iterative method · Basin of attraction · Order of convergence

Mathematics Subject Classification 65H05

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1 Introduction

Many iterative methods have been developed for the solution of problems modelled as nonlinear equations with simple or multiple roots but it is very difficult to construct an optimal iterative method for finding multiple roots. It is noteworthy that most of the higher order optimal methods that were obtained during the past years require derivative evaluation of the involved function, as in [1], while higher order derivative-free methods exist rarely in literature because it is a difficult task to preserve the order of convergence when we replace derivatives by differences. Kansal et al. [7] and Kumar et al. [8] gave second order iterative schemes to find repeated roots of nonlinear equations. Sharma et al. [17], Kumar et al. [9, 10], Behl et al. [2] and Rani and Kansal [13] proposed a fourth-order root finding methods for multiple roots. Qudsi et al. [11, 12] presented three step sixth order iterative methods for finding the multiple roots. Sharma et al. [15] proposed seventh order convergent iterative scheme for multiple roots. Sharma et al. in [14, 16] presented eight order scheme for computing multiple root of nonlinear equations. nevertheless, other derivative-free methods for multiple roots have been generated by using different approaches, such as [4].

Motivated by the need to find the more efficient iterative method for computing the root of nonlinear equations, we propose an optimal eighth order derivative-free method for computing multiple root of nonlinear equations with multiplicity $\eta \geq 1$ in the next section. This method is derivative-free with four functional evaluations with a univariate and a multivariate weight functions. In Sect. 3, we discuss some particular cases of weight functions and choose four of them for further investigation. We compare our methods with two of the recent derivative-free schemes of seventh [15] and eighth order [14, 16] using physical applications from chemical engineering and dynamical behaviour in Sect. 4. Our proposed method has wider convergence region as compared to recent root-finding iterative method.

2 Proposed optimal eighth order scheme

Let $\tau = w$ be a multiple root with multiplicity $\eta \geq 1$ of the function g . Let $K : \mathbb{C} \rightarrow \mathbb{C}$ and $L : \mathbb{C}^3 \rightarrow \mathbb{C}$ be analytic functions in the neighborhood of 0 and $(0, 0, 0)$ respectively. We propose a family of derivative-free methods of eighth-order involving first-order divided differences for computing multiple roots with multiplicity $\eta > 1$ given by:

$$\begin{aligned} \rho_k &= \tau_k + \gamma g(\tau_k), \quad \text{where } \gamma \in \mathbb{R} \setminus \{0\}, \\ \mu_k &= \tau_k - \eta \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ \nu_k &= \mu_k - \eta p_k K(p_k) \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ \tau_{k+1} &= \nu_k - \eta p_k L(p_k, q_k, r_k) \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \end{aligned} \quad (1)$$

where $p_k = \left(\frac{g(\mu_k)}{g(\tau_k)}\right)^{\frac{1}{\eta}}$, $q_k = \left(\frac{g(\nu_k)}{g(\tau_k)}\right)^{\frac{1}{\eta}}$ and $r_k = \left(\frac{g(\nu_k)}{g(\mu_k)}\right)^{\frac{1}{\eta}}$. Following result can be used to investigate the convergence order of presented method (1) and the conditions to be imposed on weight functions K and L .

Theorem 1 *Let $g : \mathbb{C} \rightarrow \mathbb{C}$ be analytic in a region enclosing multiple root of g with known multiplicity η . Suppose that the initial guess τ_0 be sufficiently close to the multiple zero w . Then, the class of iterative schemes defined by (1) has eighth-order of convergence, when the following conditions are satisfied:*

$$\begin{aligned} K(0) &= 1, \quad K'(0) = 2, \quad K''(0) = -2 \text{ and } K'''(0) = 36, \\ L_{000} &= 0, \quad L_{100} = 0, \quad L_{001} = 1, \quad L_{101} = 2 - L_{010}, \\ L_{110} &= 0, \quad L_{002} = 2, \quad L_{011} = 4, \end{aligned} \tag{2}$$

where

$$L_{ijk} = \frac{\partial^{i+j+k}}{\partial p^i \partial q^j \partial r^k} L(p, q, r) |_{(0,0,0)} \quad i, j, k \geq 0.$$

The error equation for the proposed schemes is:

$$\begin{aligned} e_{k+1} &= -\frac{1}{24\eta^7} (d_1((11 + \eta)d_1^2 - 2\eta d_2)(-12(1 + \eta)^2 d_1^3 + (-665 - 84\eta + 5\eta^2)d_1^4 \\ &\quad - 24\eta(-5 + 2\eta)d_1^2 d_2 - 12\eta^2 d_2^2 + 60\eta^2 d_1 d_3))e_k^8 + O(e_k^9), \end{aligned}$$

being $d_j = \frac{\eta!}{(\eta + j)!} \frac{g^{(\eta+j)}(w)}{g^{(\eta)}(w)}, j \geq 1.$

Proof Let w be a multiple root of g such that $g^{(j)}(w) = 0, j = 0, 1, 2, \dots, \eta - 1$ with $g^{(\eta)}(w) \neq 0$. Let $e_k = \tau_k - w$ be error in the k th iteration. Considering Taylor expansion of $g(\tau_k)$ about w , we have:

$$\begin{aligned} g(\tau_k) &= \frac{g^{(\eta)}(w)}{\eta!} e_k^\eta + \frac{g^{(\eta+1)}(w)}{(\eta + 1)!} e_k^{\eta+1} + \frac{g^{(\eta+2)}(w)}{(\eta + 2)!} e_k^{\eta+2} + \frac{g^{(\eta+3)}(w)}{(\eta + 3)!} e_k^{\eta+3} \\ &\quad + \frac{g^{(\eta+4)}(w)}{(\eta + 4)!} e_k^{\eta+4} + \frac{g^{(\eta+5)}(w)}{(\eta + 5)!} e_k^{\eta+5} + \frac{g^{(\eta+6)}(w)}{(\eta + 6)!} e_k^{\eta+6} + \frac{g^{(\eta+7)}(w)}{(\eta + 7)!} e_k^{\eta+7} \\ &\quad + \frac{g^{(\eta+8)}(w)}{(\eta + 8)!} e_k^{\eta+8} + O(e_k^{\eta+9}), \end{aligned}$$

which can be expressed as:

$$g(\tau_k) = \frac{g^{(\eta)}(w)}{\eta!} e_k^\eta \left(1 + d_1 e_k + d_2 e_k^2 + \dots + d_7 e_k^7 + d_8 e_k^8 + O(e_k^9) \right), \tag{3}$$

where

$$d_j = \frac{\eta!}{(\eta + j)!} \frac{g^{(\eta+j)}(w)}{g^{(\eta)}(w)}, \quad (4)$$

and $j \in \mathbb{N}$. For $\rho_k = \tau_k + \gamma g(\tau_k)$, we obtain:

$$\begin{aligned} \rho_k - w &= \tau_k - w + \gamma g(\tau_k), \\ \rho_k - w &= e_k + \gamma g(\tau_k), \end{aligned} \quad (5)$$

or

$$\rho_k - w = e_k + \frac{\gamma g^{(\eta)}(w)}{\eta!} e_k^\eta \left(1 + d_1 e_k + d_2 e_k^2 + \dots + d_7 e_k^7 + d_8 e_k^8 + O(e_k^9) \right). \quad (6)$$

Using Taylor expansion of $g(\rho_k)$ about w ,

$$\begin{aligned} g(\rho_k) &= \frac{g^{(\eta)}(w)}{\eta!} (\rho_k - w)^\eta \left(1 + d_1(\rho_k - w) + d_2(\rho_k - w)^2 + d_3(\rho_k - w)^3 \right. \\ &\quad + d_4(\rho_k - w)^4 + d_5(\rho_k - w)^5 + d_6(\rho_k - w)^6 + d_7(\rho_k - w)^7 \\ &\quad \left. + d_8(\rho_k - w)^8 + O((\rho_k - w)^9) \right). \end{aligned}$$

By employing (3) and (6) in the first step of (1) and after some algebraic manipulations, we get:

$$\begin{aligned} \mu_k &= \frac{d_1}{\eta} e_k^2 + \frac{2\eta d_2 - (\eta + 1) d_1^2}{\eta^2} e_k^3 + \frac{1}{\eta^3} \left((\eta + 1)^2 d_1^2 + \eta(4 + 3\eta) d_1 d_2 - 3\eta^2 d_3 \right) e_k^4 \\ &\quad + \sum_{i=1}^4 \dot{z}_i e_k^{i+4} + O(e_k^9), \end{aligned} \quad (7)$$

where $\dot{z}_i = \dot{z}_i(\eta, d_1, \dots, d_8)$ for $i = 1, 2, 3, 4$. Now, the Taylor expansion of $g(\mu_k)$ about w is given by;

$$\begin{aligned} g(\mu_k) &= \left(\frac{e_k^2 d_1}{\eta} \right)^\eta \left(\frac{1}{\eta!} + \frac{(2\eta d_2 - (1 + \eta) d_1^2) e_k}{\eta! d_1} + \frac{1}{2\eta \eta! d_1^2} (2(1 + \eta)^2 d_1^3 \right. \\ &\quad + (\eta^3 + \eta^2 - \eta + 1) d_1^4 \\ &\quad \left. + 2\eta(6 + 3\eta - 2\eta^2) d_1^2 d_2 + 4(\eta - 1) \eta^2 d_2^2 - 6\eta^2 d_1 d_3 \right) e_k^2 + \dots + O(e_k^9). \end{aligned} \quad (8)$$

Using (5) and (8) in $p_k = \left(\frac{g(\mu_k)}{g(\tau_k)}\right)^{\frac{1}{\eta}}$,

$$p_k = \frac{d_1 e_k}{\eta} + \frac{(2\eta d_2 - (2 + \eta)d_1^2)e_k^2}{\eta^2} + \frac{1}{2\eta^3} \left(2(1 + \eta)^2 d_1^2 + (5 + 3\eta)d_1^3 + 2\eta(1 + 3\eta)d_1 d_2 - 6\eta^2 d_3\right) e_k^3 + \dots + O(e_k^9). \tag{9}$$

By expanding the weight function $K(p_k)$ in the neighborhood of 0,

$$K(p_k) \approx K(0) + p_k K'(0) + \frac{1}{2} p_k^2 K''(0) + \frac{1}{6} p_k^3 K'''(0) \tag{10}$$

Then, for

$$v_k = \mu_k - p_k \left(K(0) + K'(0) p_k + \frac{K''(0)}{2} p_k^2 + \frac{K'''(0)}{6} p_k^3 \right) (e_k - \mu_k), \tag{11}$$

we get the expansion of v_k around w using (5), (8), (9) and (10):

$$v_k = -\frac{(K(0) - 1)d_1 e_k^2}{\eta} - \frac{(1 + K'(0) + \eta - K(0)(3 + \eta))d_1^2 + 2(K(0) - 1)\eta d_2}{\eta^2} e_k^3 + \frac{1}{2\eta^3} \left(-2(K(0) - 1)(1 + \eta)^2 d_1^2 - (K''(0) - 2K'(0)(5 + 2\eta)) \right. \\ \left. + K(0)(11 + 7\eta)d_1^3 + 2\eta(4 - 4K'(0) - 3K(0)(\eta - 1) + 3\eta)d_1 d_2 + 6(K(0) - 1)\eta^2 d_3 \right) e_k^4 + \dots + O(e_k^9). \tag{12}$$

If we choose the values of $K(0)$, $K'(0)$ and $K''(0)$ in (12), given as:

$$K(0) = 1, \quad K'(0) = 2 \tag{13}$$

we obtain

$$v_k = \frac{(9 - K''(0) + \eta)d_1^3 - 2\eta d_1 d_2}{2\eta^3} e_k^4 - \frac{1}{6\eta^4} (6(1 + \eta)^2 d_1^3 + (119 + K'''(0) + 72\eta + \eta^2) \\ - 3K''(0)(7 + 3\eta))d_1^4 + 12\eta^2 d_2^2 - 24\eta^2 d_1 d_3 + 6\eta(-20 + 3K''(0) + 2\eta)d_1^2 d_2) e_k^5 + \dots + O(e_k^9).$$

Next, from Taylor expansion of $g(v_k)$ about w :

$$\begin{aligned}
g(v_k) = & e_k^{4\eta} \left(\frac{2^{-\eta}}{\eta!} \left(\frac{(11 + \eta) d_1^3 - 2\eta d_1 d_2}{\eta^3} \right)^\eta \right. \\
& - \frac{1}{3(\eta^3 \eta!)} \left(2^{-\eta} \left(\frac{(11 + \eta) d_1^3 - 2\eta d_1 d_2}{\eta^3} \right)^{-1+\eta} \right. \\
& \left. \left(6(1 + \eta)^2 d_1^3 + (161 + K''' + 90\eta + \eta^2) d_1^4 \right. \right. \\
& \left. \left. + 12(\eta - 13)\eta d_1^2 d_2 + 12\eta^2 d_2^2 - 24\eta^2 d_1 d_3 \right) \right) e_k \\
& + \dots + O(e_k^9). \tag{14}
\end{aligned}$$

By using (5) and (14), $q_k = \left(\frac{g(v_k)}{g(\tau_k)} \right)^{\frac{1}{\eta}}$ becomes:

$$\begin{aligned}
q_k = & \frac{((11 + \eta) d_1^3 - 2\eta d_1 d_2) e_k^3}{2\eta^3} - \frac{1}{6\eta^4} (6(1 + \eta)^2 d_1^3 + (194 + K'''(0) + 93\eta + \eta^2) d_1^4 \\
& + 6\eta(-27 + 2\eta) d_1^2 d_2 + 12\eta^2 d_2^2 - 24\eta^2 d_1 d_3) e_k^4 + \dots + O(e_k^9). \tag{15}
\end{aligned}$$

Similarly, from (8) and (14) $r_k = \left(\frac{g(v_k)}{g(\mu_k)} \right)^{\frac{1}{\eta}}$,

$$\begin{aligned}
r_k = & \frac{((11 + \eta) d_1^2 - 2\eta d_2) e_k^2}{2\eta^2} + \frac{1}{6\eta^3} (-6(1 + \eta)^2 d_1^2 - (128 + K'''(0) + 54\eta - 2\eta^2) d_1^3 \\
& + 12(7 - 2\eta)\eta d_1 d_2 + 24\eta^2 d_3) e_k^3 + \dots + O(e_k^9). \tag{16}
\end{aligned}$$

The expansion of the weight function $L(p_k, q_k, r_k)$ in the neighborhood of $(0, 0, 0)$ is given by,

$$\begin{aligned}
L(p_k, q_k, r_k) = & L_{000} + p_k L_{100} + q_k L_{010} + r_k L_{001} + p_k q_k L_{110} + p_k r_k L_{101} \\
& + q_k r_k L_{011} + \frac{r_k^2}{2} L_{002},
\end{aligned}$$

and therefore,

$$\begin{aligned}
e_{k+1} = & v_k - p_k \left(L_{000} + p_k L_{100} + q_k L_{010} + r_k L_{001} + p_k q_k L_{110} + p_k r_k L_{101} \right. \\
& \left. + q_k r_k L_{011} + \frac{r_k^2}{2} L_{002} \right) (e_k - \mu_k).
\end{aligned}$$

After substituting the values of p_k , q_k and r_k from (9), (15) and (16), the error equation becomes:

$$e_{k+1} = -\frac{1}{\eta} (L_{000} d_1 e_k^2) + \frac{1}{\eta^2} ((-L_{100} + L_{000}(3 + \eta)) d_1^2 - 2L_{000} \eta d_2) e_k^3 + \dots + O(e_k^9). \tag{17}$$

As $L_{ijk} = \frac{\partial^{i+j+k}}{\partial p^i \partial q^j \partial r^k} L(p, q, r) |_{(0,0,0)}$, in order to achieve higher order of convergence, we use the values:

$$L_{000} = 0, L_{100} = 0, K''(0) = -2, \tag{18}$$

$$L_{001} = 1, L_{101} = 2 - L_{010}, \tag{19}$$

$$L_{110} = 0, L_{002} = 2. \tag{20}$$

By using (18) in (17),

$$\begin{aligned} e_{k+1} = & -\frac{1}{2\eta^3} \left((-1 + L_{001}) d_1 \left((11 + \eta) d_1^2 - 2\eta d_2 \right) \right) e_k^4 \\ & + \frac{1}{6\eta^4} (6(-1 + L_{001}) (1 + \eta)^2 d_1^3 \\ & + (-161 + K'''(0) (-1 + L_{001}) - 33L_{010} - 33L_{101} \\ & - 90\eta - 3L_{010}\eta - 3L_{101}\eta - \eta^2 \\ & + L_{001} (227 + 96\eta + \eta^2) d_1^4 + 6(26 + L_{010} + L_{101} \\ & + 2L_{001} (-14 + \eta) - 2\eta)\eta d_1^2 d_2 \\ & + 12(-1 + L_{001})\eta^2 d_2^2 - 24(-1 + L_{001})\eta^2 d_1 d_3) e_k^5 + \dots + O(e_k^9). \end{aligned}$$

Furthermore, from (19),

$$e_{k+1} = \frac{1}{24\eta^4} \left(d_1^2 (-2 + L_{010} + L_{101}) \left(2\eta d_2 - (11 + \eta) d_1^2 \right) \right) e_k^6 + \dots + O(e_k^9),$$

and from conditions (20),

$$\begin{aligned} e_{k+1} = & \frac{1}{12\eta^6} (d_1^2 \left((11 + \eta) d_1^2 - 2\eta d_2 \right) ((K'''(0) + 12(8 + \eta) - 3L_{011}(11 + \eta)) d_1^2 \\ & + 6(-4 + L_{011})\eta d_2) e_k^7 + \dots + O(e_k^9). \end{aligned} \tag{21}$$

Now, by using $L_{011} = 4$ in (21), we get

$$e_{k+1} = \frac{1}{12\eta^6} (-36 + K'''(0)) d_1^4 \left((11 + \eta) d_1^2 - 2\eta d_2 \right) e_k^7 + \dots + O(e_k^9).$$

Clearly, for $K'''(0) = 36$ in (21), the error equation indicates eighth order of convergence as an optimal order of convergence:

$$\begin{aligned} e_{k+1} = & -\frac{1}{24\eta^7} (d_1 \left((11 + \eta) d_1^2 - 2\eta d_2 \right) (-12(1 + \eta)^2 d_1^3 + (-665 - 84\eta + 5\eta^2) d_1^4 \\ & - 24\eta(-5 + 2\eta) d_1^2 d_2 - 12\eta^2 d_2^2 + 60\eta^2 d_1 d_3) e_k^8 + O(e_k^9). \end{aligned}$$

□

From Theorem 1, we can get several new root finding methods for multiple roots by using different cases for $K(p_k)$ and $L(p_k, q_k, r_k)$ in the proposed scheme (1). We discuss few particular cases of the proposed class. It is important to note that the choice of specific values of parameter γ can be made under the point of view of an improvement of the stability and a widening of the set of converging initial estimations. However, as in the iterative expression of the new class, $g[\tau_k, \rho_k]$ is an estimation of $g'(\tau_k)$, it is clear that the approximation of the derivative is better when γ is close to zero.

2.1 Some special cases of weight functions

Many special cases of the proposed scheme (1) can be generated by using different forms of weight functions $K(p)$ and $L(p, q, r)$. These weight functions satisfy the conditions given in Theorem 1. We discuss some simple cases as follows:

Case 1 When $K(p)$ is a third-degree polynomial, we can express it as

$$K(p) = a_1 + a_2p + a_3p^2 + a_4p^3.$$

By using the condition set (2), the weight function $K(p)$ becomes:

$$K(p) = 1 + 2p - p^2 + 6p^3.$$

By taking the other weight function $L(p, q, r)$ as a second-degree polynomial,

$$L(p, q, r) = b_1q + b_2qr + b_3r + b_4r^2,$$

and applying the conditions stated in Theorem 1, $L(p, q, r)$ becomes

$$L(p, q, r) = 2q + 4qr + r + r^2.$$

Therefore, the resulting scheme is denoted by FZI and has the iterative expression:

$$\begin{aligned} \rho_k &= \tau_k + \gamma g(\tau_k), \text{ where } \gamma \in \mathbb{R} \setminus \{0\}, \\ \mu_k &= \tau_k - \eta \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ \nu_k &= \mu_k - \eta p_k (1 + 2p_k - p_k^2 + 6p_k^3) \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ \tau_{k+1} &= \nu_k - \eta p_k (2q_k + 4q_k r_k + r_k + r_k^2) \frac{g(\tau_k)}{g[\tau_k, \rho_k]}. \end{aligned}$$

Case 2 By considering the rational form of weight function $K(p)$ as:

$$K(p) = \frac{1 + a_1p + a_2p^2}{1 + a_3p + a_4p^2},$$

and imposing conditions (2), we get $K(p)$ in the form,

$$K(p) = \frac{1 - 9p^2}{1 - 2p - 4p^2}.$$

Let us take $L(p, q, r)$ as the second-degree polynomial

$$L(p, q, r) = b_1pr + b_2qr + b_3r + b_4r^2,$$

which becomes,

$$L(p, q, r) = 2pr + 4qr + r + r^2.$$

Thus, the resulting member of class (1) is denoted by FZ2 and has the following expression:

$$\begin{aligned} \rho_k &= \tau_k + \gamma g(\tau_k), \text{ where } \gamma \in \mathbb{R} \setminus \{0\}, \\ \mu_k &= \tau_k - \eta \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ \nu_k &= \mu_k - \eta p_k \left(\frac{1 - 9p_k^2}{1 - 2p_k - 4p_k^2} \right) \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ \tau_{k+1} &= \nu_k - \eta p_k (2p_k r_k + 4q_k r_k + r_k + r_k^2) \frac{g(\tau_k)}{g[\tau_k, \rho_k]}. \end{aligned}$$

Case 3 Let us consider the weight function $K(p)$ in the form of a proper rational function:

$$K(p) = \frac{1 + a_1p}{a_2 + a_3p + a_4p^2}.$$

By using the conditions of Theorem 1, $K(p)$ becomes;

$$K(p) = \frac{5 + 18p}{5 + 8p - 11p^2},$$

Taking again the second weight function $L(p, q, r)$ as the second-degree polynomial

$$L(p, q, r) = q + pr + 4qr + r + r^2,$$

the obtained element of family (1) is denoted by FZ3 and can be expressed as

$$\begin{aligned} \rho_k &= \tau_k + \gamma g(\tau_k), \text{ where } \gamma \in \mathbb{R} \setminus \{0\}, \\ \mu_k &= \tau_k - \eta \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \end{aligned}$$

$$\nu_k = \mu_k - \eta p_k \left(\frac{5 + 18p_k}{5 + 8p_k - 11p_k^2} \right) \frac{g(\tau_k)}{g[\tau_k, \rho_k]},$$

$$\tau_{k+1} = \nu_k - \eta p_k (q_k + p_k r_k + 4q_k r_k + r_k + r_k^2) \frac{g(\tau_k)}{g[\tau_k, \rho_k]}.$$

Case 4 Let us consider the weight function $K(p)$ in the form:

$$K(p) = \frac{1 + a_1 p + a_2 p^2 + a_3 p^3}{1 + a_4 p}.$$

After applying conditions (2), the weight function $K(p)$ becomes:

$$K(p) = \frac{1 + 3p + p^2 + 5p^3}{1 + p},$$

and $L(p, q, r)$ is the same as in previous cases,

$$L(p, q, r) = 2pr + 4qr + r + r^2.$$

So that, the resulting scheme is denoted by FZ4 and has the iterative expression

$$\rho_k = \tau_k + \gamma g(\tau_k), \text{ where } \gamma \in \mathbb{R} \setminus \{0\},$$

$$\mu_k = \tau_k - \eta \frac{g(\tau_k)}{g[\tau_k, \rho_k]},$$

$$\nu_k = \mu_k - \eta p_k \left(\frac{1 + 3p_k + p_k^2 + 5p_k^3}{1 + p_k} \right) \frac{g(\tau_k)}{g[\tau_k, \rho_k]},$$

$$\tau_{k+1} = \nu_k - \eta p_k (2p_k r_k + 4q_k r_k + r_k + r_k^2) \frac{g(\tau_k)}{g[\tau_k, \rho_k]}.$$

3 Numerical and dynamical analysis

In this section, we check the convergence behavior and performance of Case 1 to Case 4 of our proposed eighth order scheme denoted respectively by FZ1, FZ2, FZ3 and FZ4 by carrying out some nonlinear equations from real life applications of chemical engineering. We compare the methods with the recent derivative free methods of seventh order (see [15], Case I(a), Case II(c)) denoted by SH1, SH2 and eighth order (see [16], M-4 and [14]) denoted as SH3 and SH4. The recent seventh order methods are defined by, in case of SH1

$$\rho_k = \tau_k + \gamma g(\tau_k), \text{ where } \gamma \in \mathbb{R} - \{0\},$$

$$\mu_k = \tau_k - \eta \frac{g(\tau_k)}{g[\tau_k, \rho_k]},$$

$$\begin{aligned}v_k &= \mu_k - \eta p_k \left(1 + 2p_k - p_k^2\right) \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ \tau_{k+1} &= v_k - \eta q_k \left(1 + 2p_k + r_k + r_k^2\right) \frac{g(\tau_k)}{g[\tau_k, \rho_k]},\end{aligned}$$

and SH2 is

$$\begin{aligned}\rho_k &= \tau_k + \gamma g(\tau_k), \text{ where } \gamma \in \mathbb{R} - \{0\}, \\ \mu_k &= \tau_k - \eta \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ v_k &= \mu_k - \eta p_k \left(\frac{2 + 5p_k}{2 + p_k}\right) \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ \tau_{k+1} &= v_k - \eta q_k \left(1 + 2p_k + r_k + r_k^2\right) \frac{g(\tau_k)}{g[\tau_k, \rho_k]},\end{aligned}$$

where

$$p_k = \left(\frac{g(\mu_k)}{g(\tau_k)}\right)^{\frac{1}{\eta}}, \quad q_k = \left(\frac{g(v_k)}{g(\tau_k)}\right)^{\frac{1}{\eta}}, \quad r_k = \left(\frac{g(v_k)}{g(\mu_k)}\right)^{\frac{1}{\eta}}.$$

The above mentioned eight order scheme (see [16]) denoted by SH3 is defined as

$$\begin{aligned}\rho_k &= \tau_k + \gamma g(\tau_k), \text{ where } \gamma \in \mathbb{R} \setminus \{0\}, \\ \mu_k &= \tau_k - \eta \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ v_k &= \mu_k - \eta h_k (1 + 3h_k) \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ \tau_{k+1} &= v_k - \eta p_k q_k \left(\frac{1 + 3h_k + 2q_k + 8h_k q_k - 14h_k^3}{(1 + h_k)(1 + q_k)}\right) \frac{g(\tau_k)}{g[\tau_k, \rho_k]}.\end{aligned}$$

where,

$$p_k = \left(\frac{g(\mu_k)}{g(\tau_k)}\right)^{\frac{1}{\eta}}, \quad q_k = \left(\frac{g(v_k)}{g(\mu_k)}\right)^{\frac{1}{\eta}}, \quad h_k = \frac{p_k}{1 + p_k}.$$

The most recent eighth order method (see [14]), denoted by SH4, is defined as:

$$\begin{aligned}\rho_k &= \tau_k + \gamma g(\tau_k), \text{ where } \gamma \in \mathbb{R} \setminus \{0\}, \\ \mu_k &= \tau_k - \eta \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ v_k &= \mu_k - (3 + 2\eta p_k + (\eta - 3) q_k) p_k \frac{g(\tau_k)}{g[\tau_k, \rho_k]}, \\ \tau_{k+1} &= v_k - s_k ((1 - q_k) (3 + (5r_k - 3p_k - 6) q_k) + \eta (4 + (r_k - 3) q_k) q_k\end{aligned}$$

$$+ 2\eta \left(1 + q_k + (2r_k - 1)q_k^2 \right) p_k - \eta \left(4p_k q_k - \frac{1}{2} (1 + q_k) \right) p_k^2 q_k \frac{g(\tau_k)}{g[\tau_k, \rho_k]},$$

with

$$p_k = \left(\frac{g(\mu_k)}{g(\tau_k)} \right)^{\frac{1}{\eta}}, \quad q_k = \left(\frac{g(\rho_k)}{g(\tau_k)} \right)^{\frac{1}{\eta}}, \quad r_k = \left(\frac{g(v_k)}{g(\mu_k)} \right)^{\frac{1}{\eta}}, \quad s_k = \left(\frac{g(v_k)}{g(\tau_k)} \right)^{\frac{1}{\eta}}.$$

For testing those methods numerically, we have performed all computations in computer algebra software Maple 16 using 300 significant digits of precision. We take the value of $\gamma = 0.001$. Tables show per step numerical errors of approximating real root $|\tau_k - \tau_{k-1}|$ of first three iterations, the absolute residual error of the test function at the third iteration, $|g(\tau_3)|$, and the computational order of convergence (see [6]).

$$COC \approx \frac{\ln |g(\tau_{k+2})/g(\tau_{k+1})|}{\ln |g(\tau_{k+1})/g(\tau_k)|}, \quad k = 1, 2, \dots$$

For dynamical analysis, we use the graphical tool known as basins of attraction. For a polynomial function, basins of attraction is also called a polynomiograph. The dynamical analysis gives us information about the stability and convergence regions of iterative schemes. The choice of initial guess decide the convergence of nonlinear function towards the exact root. Many researchers have used basins of attraction to show the convergence behaviour of their schemes. Consider a function $g_k(\tau)$ where $\tau \in \mathbb{C}$ and w_k be the root of $g_k(\tau)$. We have chosen the parameter $\beta = 0.001$, 10^{-5} as tolerance and we work out the schemes with maximum 15 number of iterations. A grid of 1000×1000 points in the complex plane $[a, b] \times [c, d]$ is taken into consideration where the values of a, b, c and d depends upon the zero of the nonlinear function. We select 'hot' color map and assign black color to the divergence region with few exceptions. Different shades of colors are decided for different number of iterations used by the iterative method to converge to the root with required accuracy. We compare our presented schemes namely $FZ1-FZ4$ with recent methods named as $SH1-SH4$.

3.1 Applications to chemical engineering problems

Chemical Engineering deals with the applications of chemistry for industrial purposes. It effectively analyze the chemical methods to convert materials into more applicable and useful materials. Let us consider some examples from chemical engineering.

Example 1 *Continuous Stirred Tank Reactors (CSTR)* Let us consider an isothermal continuous stirred tank reactor. The components E and M are fed to the reactor at the rates of Q and q-Q respectively. The following reaction scheme develops in the reactor (see [3]):

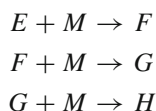


Table 1 Computational comparison of iterative schemes for $g_1(\tau)$

<i>Methods</i>	$ \tau_1 - \tau_0 $	$ \tau_2 - \tau_1 $	$ \tau_3 - \tau_2 $	$ g_1(\tau_3) $	<i>COC</i>
<i>SH1</i>	0.45066	0.22799	0.057457	3.4471×10^{-8}	5.65
<i>SH2</i>	0.45066	0.22800	0.057461	3.4527×10^{-8}	5.65
<i>SH3</i>	0.33512	0.05596	0.000845	1.3030×10^{-27}	5.80
<i>SH4</i>	0.36765	0.09196	0.004311	3.1546×10^{-45}	15.34
<i>FZ1</i>	0.36761	0.09191	0.004304	3.5910×10^{-27}	8.43
<i>FZ2</i>	0.36761	0.09191	0.004305	3.5772×10^{-27}	8.43
<i>FZ3</i>	0.36761	0.09191	0.004304	3.6070×10^{-27}	8.42
<i>FZ4</i>	0.36761	0.09191	0.004304	3.5996×10^{-27}	8.43

$$H + M \rightarrow I$$

For designing simple feedback control system, this problem is analyzed by Douglas (see [5]). Consequently, following equation was obtained for the transfer function of the reactor,

$$K_c \frac{2.98(\tau + 2.25)}{(\tau^4 + 11.50\tau^3 + 47.49\tau^2 + 83.06325\tau + 51.23266875)} = -1,$$

where K_c is the gain of proportional controller. The control system is stable for the values of K_c that yields roots of the transfer function having negative real part. If we consider $K_c = 0$, we get the poles of the open loop transfer function as zero of the nonlinear function

$$g_1(\tau) = (\tau^4 + 11.50\tau^3 + 47.49\tau^2 + 83.06325\tau + 51.23266875),$$

given by $\tau = -1.45, -2.85, -2.85, -4.35$. We take multiple root $w = -2.85$ with multiplicity $\eta = 2$. By taking the initial guess $\tau_0 = -3.13$, the numerical results are given in Table 1.

The basins of attraction obtained for the methods *SH1* – *SH4* and *FZ1* – *FZ4* are shown in Figs. 1, 2. The attraction basins for $g_1(\tau)$ are drawn in the rectangular region $[-5, 0] \times [-2, 2]$. When we observe these basins of attraction, we see that our newly proposed scheme have better convergence as compared to the methods *SH1* – *SH4*. We notice that *SH1* – *SH4* take minimum 2 and maximum 12 iterations, *FZ1* – *FZ4* take minimum 2 and maximum 10 iterations to converge to the root.

3.1.1 Equations of state

An equation of state (EOS) relates the molar volume, temperature and the pressure of a substance. Its simplest form is the ideal gas equation of state:

$$PV = nRT,$$

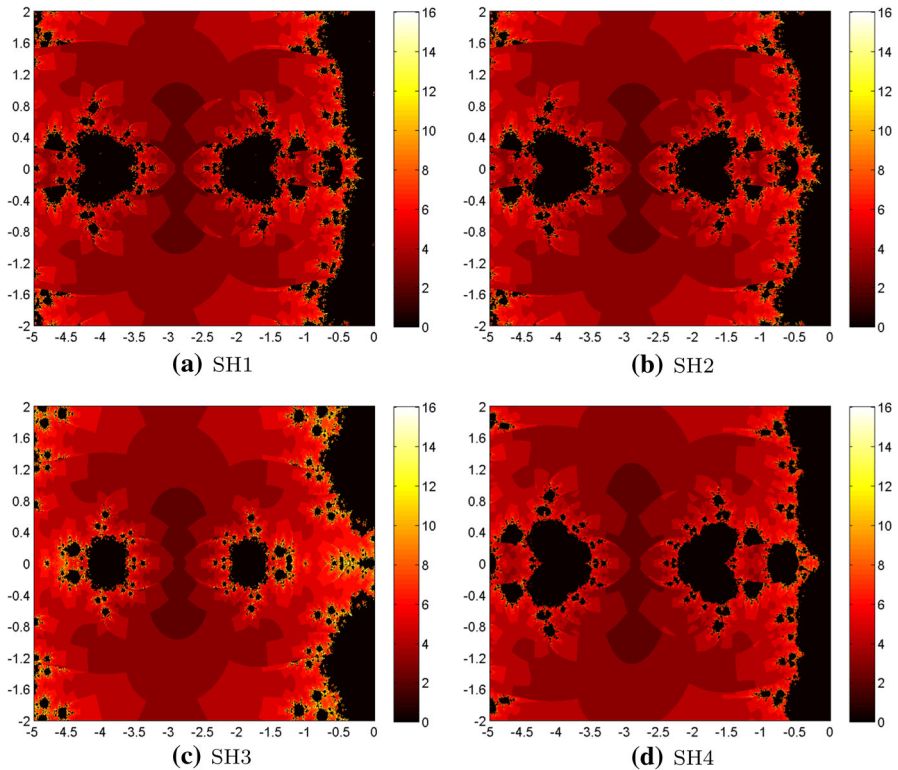


Fig. 1 Attraction basins of SH1–SH4 on $g_1(\theta)$

where P , V and T represents pressure, volume and temperature of a gas respectively. Here n is the number of moles of gas and R is the universal gas constant. There are many improved variants of EOS but we will not discuss all of them. We start with the virial equation of state which is the first improved form of EOS. We also discuss four improved cubic EOS: the Van Der Waals (VW), the Redlich–Kwong (RK), Soave Redlich–Kwong (SRK) and Peng–Robinson (PR) forms. All these equations can be written in the following form (see [18]):

$$V^3 + \left[(c_1 - 1)b - \frac{RT}{P} \right] V^2 + \left[(c_2 - c_1)b^2 - c_1 \frac{RTb}{P} + \frac{a\alpha(T_r)}{P} \right] V - \left(c_2 b^2 + c_2 \frac{RTb}{P} + \frac{a(T_r)}{P} \right) b = 0, \quad (22)$$

with different values of constants c_1 and c_2 . Here a and b are the parameters defined as:

$$a = \lambda_a z \frac{(RT_c)^2}{P_c}, \quad b = \lambda_b z \frac{RT_c}{P_c},$$

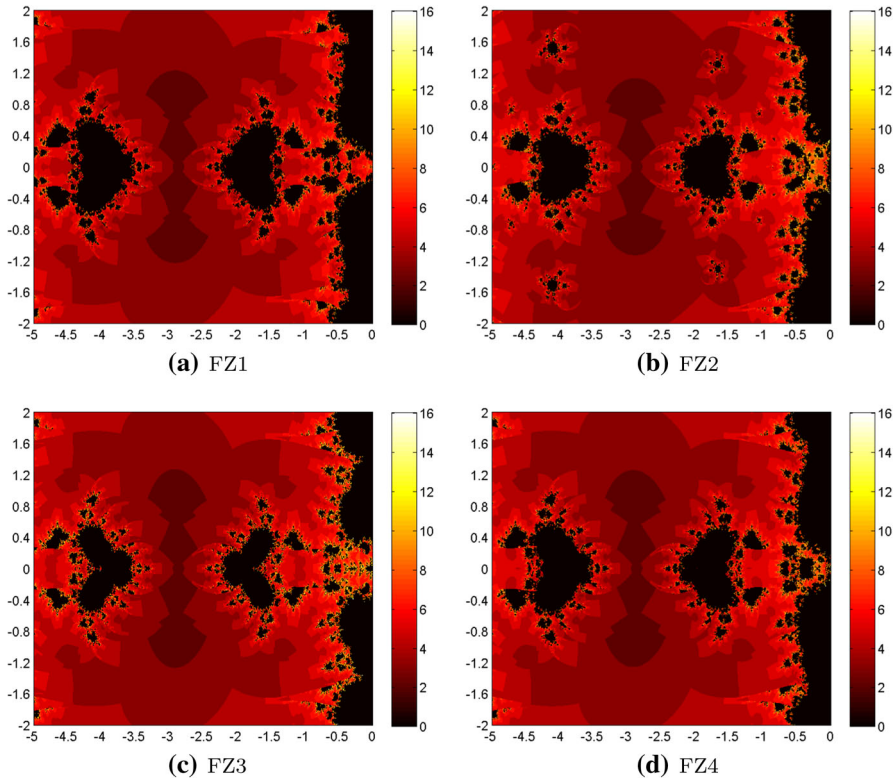


Fig. 2 Attraction basins of FZ1–FZ4 on $g_1(\theta)$

where T_c and P_c represents critical temperature and critical pressure respectively and $T_r = \frac{T}{T_c}$. For Van Der Waals and Redlich–Kwong EOS, $\alpha(T_r) = 1$. Moreover, at the critical isotherm, all equations of state have the value of the function $\alpha(T_r)$ equal to unity.

Example 2 *Virial Equation of State* Let us consider the virial equation of state:

$$V = \frac{RT}{P} \left(1.0 + \frac{b}{V} + \frac{c}{V^2} \right).$$

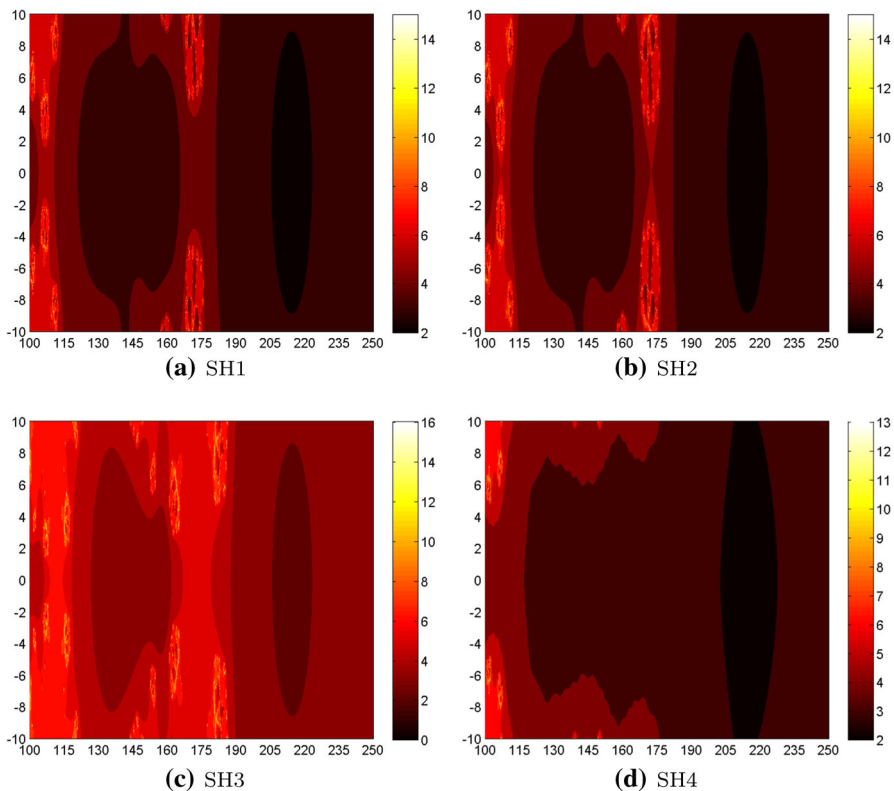
By using the values of parameters of a particular gas $b = -159, c = 9000, P = 75, T = 430.85, R = 82.05$, we obtain the nonlinear function

$$g_2(\tau) = \tau - 471.3499 + \frac{7,49,444.6310}{\tau} - \frac{4.242149100}{\tau^2},$$

where $\tau = V$. Above equation has root $w = 213.0$ with $\eta = 1$. We choose initial guess $\tau_0 = 100$ and numerical results are shown in Table 2.

Table 2 Computational comparison of iterative schemes for $g_2(\tau)$

<i>Methods</i>	$ \tau_1 - \tau_0 $	$ \tau_2 - \tau_1 $	$ \tau_3 - \tau_2 $	$ g_2(\tau_3) $	<i>COC</i>
<i>SH1</i>	57.8615	55.1035	0.03674	3.0740×10^{-22}	6.40
<i>SH2</i>	57.9774	54.9924	0.03196	1.2360×10^{-22}	6.39
<i>SH3</i>	50.2996	65.4799	2.77779	9.3283×10^{-10}	7.34
<i>SH4</i>	61.8919	51.0887	0.02117	2.1628×10^{-13}	3.18
<i>FZ1</i>	63.5901	52.6489	3.23725	5.1981×10^{-10}	8.83
<i>FZ2</i>	61.4648	51.8840	0.34715	2.2013×10^{-17}	7.65
<i>FZ3</i>	63.0133	54.1869	4.19855	3.0668×10^{-9}	9.18
<i>FZ4</i>	63.0860	52.5102	2.59452	8.6714×10^{-11}	8.63

**Fig. 3** Attraction basins of SH1–SH4 of $g_2(\theta)$

It can be observed that the computational estimation of the order of convergence COC is the best at FZ1–FZ4, meanwhile the error at the third iteration is the lowest at SH1–SH2 and FZ2.

In Example 2, the basins of attraction obtained for the methods SH1–SH4 and FZ1–FZ4 are shown in Figs. 3, 4. Observing the region $[100, 250] \times [-10, 10]$, we

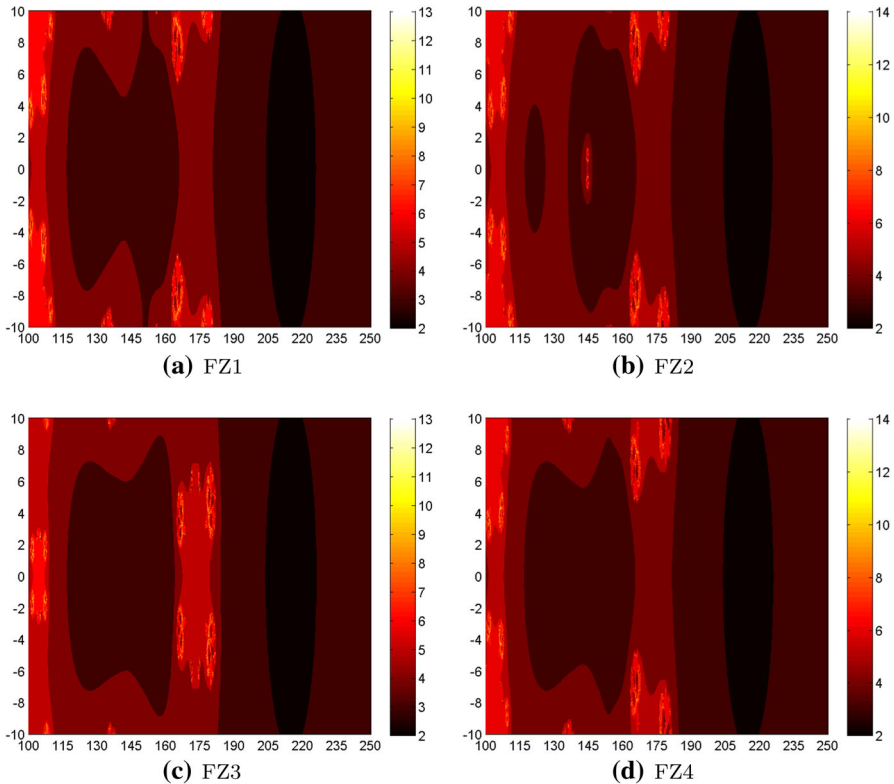


Fig. 4 Attraction Basins of FZ1–FZ4 of $g_2(\theta)$

conclude that SH1–SH4 take minimum two and maximum 10 numbers of iterations to converge to the root. On the other hand, FZ1–FZ4 take minimum two and maximum 8 iterations to converge to the root. In this example, black color shows the divergence region only for SH3 and in all other cases, it indicates the hue of two iterations.

Example 3 *Van Der Waals Equation of State* By using the values $c_1 = c_2 = 0$, $\lambda_b = \frac{1}{3}$, $\lambda_a = \frac{9}{8}$, $z = \frac{3}{8}$ and $\alpha(T_r) = 1$, we get the reduced Eq. (22) in the form:

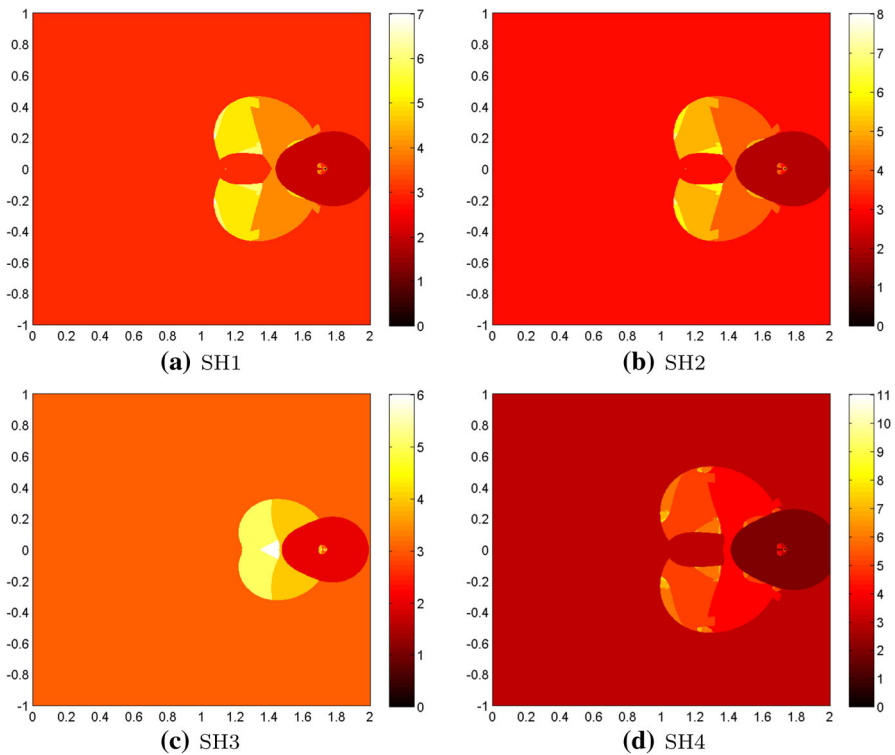
$$V^3 - \left(b + \frac{RT}{P}\right) V^2 + \frac{a}{P} V - \frac{a}{P} b = 0. \tag{23}$$

For finding the volume V of a particular gas, we have to use the values of remaining parameters. For the given parameters a and b of a particular gas, we can get values of n (number of moles), P (pressure) and T (absolute temperature), such that the equation (23) has multiple root with multiplicity 3. By using these values, we get the nonlinear function

$$g_3(\tau) = \tau^3 - 5.22\tau^2 + 9.0825\tau - 5.2675,$$

Table 3 Computational comparison of iterative schemes for $g_3(\tau)$

<i>Methods</i>	$ \tau_1 - \tau_0 $	$ \tau_2 - \tau_1 $	$ \tau_3 - \tau_2 $	$ g_3(\tau_3) $	<i>COC</i>
<i>SH1</i>	0.23667	0.01332	6.2573×10^{-6}	3.2539×10^{-56}	6.39
<i>SH2</i>	0.23667	0.01331	6.2956×10^{-6}	3.7232×10^{-56}	6.38
<i>SH3</i>	0.23399	0.01598	2.0101×10^{-5}	2.1424×10^{-53}	6.97
<i>SH4</i>	0.23825	0.01174	1.3118×10^{-6}	2.7176×10^{-74}	7.49
<i>FZ1</i>	0.23816	0.01182	1.6046×10^{-6}	5.5066×10^{-70}	7.12
<i>FZ2</i>	0.23818	0.01181	1.7411×10^{-6}	1.5188×10^{-69}	7.14
<i>FZ3</i>	0.23817	0.01182	1.5054×10^{-6}	2.4843×10^{-70}	7.11
<i>FZ4</i>	0.23817	0.01182	1.5457×10^{-6}	3.4551×10^{-70}	7.11

**Fig. 5** Attraction basins of SH1–SH4 of $g_3(\theta)$

where $\tau = V$. This equation has the multiple root $w = 1.75$ with multiplicity $\eta = 2$. By taking the initial guess $\tau_0 = 2.00$, the numerical results are presented in Table 3.

Again proposed methods reach better estimations of the theoretical order of convergence in the first three iterations. Moreover, the best error is obtained by SH4, FZ3 and FZ4.

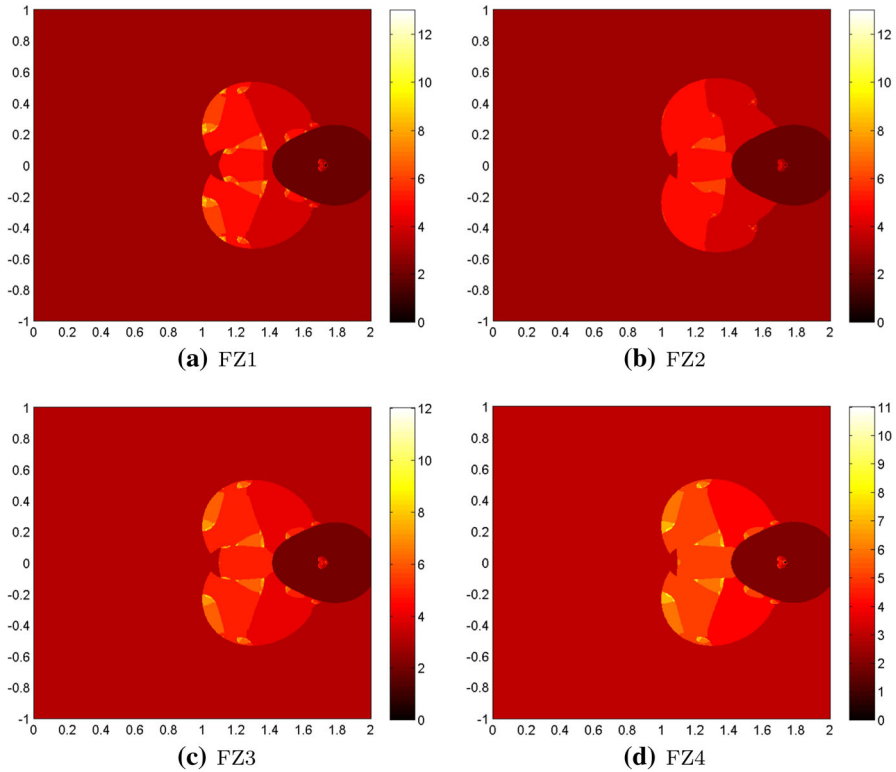


Fig. 6 Attraction basins of FZ1–FZ4 of $g_3(\theta)$

For the Van Der Waals equation of state, the basins of attraction obtained for the methods SH1–SH4 and FZ1–FZ4 are shown in Figs. 5, 6. We use the region $[0, 2] \times [-1, 1]$ to draw the basins of attraction. The dynamical analysis shows that SH1–SH4 take minimum two and maximum eight numbers of iterations to converge to the root and FZ1–FZ4 take minimum two and maximum nine numbers of iterations to converge to the root.

Example 4 Redlich–Kwong Equation of State We consider the RK equation of state for solving V at critical isotherm. For this purpose, we use the values $c_1 = 1$, $c_2 = 0$, $\lambda_b = 0.2599$, $\lambda_a = 1.2824$, $z = 0.333$ and $\alpha(T_r) = 1$ and obtain Eq. (22) in the form of Redlich–Kwong equation of state:

$$V^3 - \frac{RT}{p}V^2 - \left(b^2 + \frac{RTb}{P} - \frac{a}{P}\right)V - \frac{ab}{p} = 0.$$

Let us solve the above equation for Carbon Dioxide (CO_2) at $T = T_c = 304.2$, $P = P_c = 72.85$. By using these values, we get the nonlinear equation:

$$V^3 - 4.175703501V^2R + 5.8123166576VR^2 - 2.696653814R^3 = 0,$$

Table 4 Computational comparison of iterative schemes for $g_4(\tau)$

Methods	$ \tau_1 - \tau_0 $	$ \tau_2 - \tau_1 $	$ \tau_3 - \tau_2 $	$ g_4(\tau_3) $	COC
SH1	0.68578	2.6224×10^{-7}	1.6232×10^{-22}	5.7044×10^{-203}	3.00
SH2	0.68578	2.6224×10^{-7}	1.6232×10^{-22}	5.7044×10^{-203}	3.00
SH3	0.68578	2.6175×10^{-7}	7.0445×10^{-23}	2.7133×10^{-350}	6.06
SH4	0.68578	2.6231×10^{-7}	9.3785×10^{-23}	1.9846×10^{-348}	6.07
FZ1	0.68578	2.6225×10^{-7}	9.3719×10^{-23}	1.9638×10^{-348}	6.07
FZ2	0.68578	2.6225×10^{-7}	9.3719×10^{-23}	1.9638×10^{-348}	6.07
FZ3	0.68578	2.6225×10^{-7}	9.3719×10^{-23}	1.9638×10^{-348}	6.07
FZ4	0.68578	2.6225×10^{-7}	9.3719×10^{-23}	1.9638×10^{-348}	6.07

where $R = 0.082057366080960$, and solving for $\tau = V$,

$$g_4(\tau) = \tau^3 - 4.175703501\tau^2 R + 5.8123166576\tau R^2 - 2.696653814R^3,$$

gives us the multiple root $w = 0.1142157436$ with multiplicity $\eta = 3$. By using the initial guess $\tau_0 = 0.8$, the numerical results are shown in Table 4, with excellent results in the first three iterations.

In Example 4, the basins of attraction obtained for the methods SH1–SH4 and FZ1–FZ4 are shown in Figs. 7, 8. We draw basins of attraction in the region $[-2, 2] \times [-2, 2]$ and conclude that SH1–SH4 and FZ1–FZ4 use minimum two and maximum three numbers of iterations to converge to the root. In this example, black color shows the hue of two iterations for all iterative schemes. FZ1–FZ4 has globally wider black region as compared to SH1–SH4.

Example 5 *Soave Redlich–Kwong Equation of State* Let us take the values $c_1 = 1$, $c_2 = 0$, $\lambda_b = 0.2599$, $\lambda_a = 1.2824$ and $\tau = 0.333$ to get Eq. (22) in the form of Soave Redlich–Kwong equation of state:

$$V^3 - \frac{RT}{P}V^2 - \left(b^2 + \frac{RT}{P} - \frac{a\alpha(T_r)}{P}\right)V - \frac{ab\alpha(T_r)}{P} = 0,$$

where $\alpha(T_r) = [1 + (0.485081 + 1.55171w - 0.15613w^2)(1 - T_r^{0.5})]^2$. w represents the acentric factor of a specific gas. We solve this equation for Ammonia at $T = 302.15$, $P = 229.9 \times 10^3$. We use $T_c = 405.55$, $P_c = 1.128 \times 10^7$, $w = 0.250$ and $R = 8.314$ and get the nonlinear equation:

$$g_5(\tau) = \tau^3 - 0.01092681644\tau^2 + 2.059291793 \times 10^{-6}\tau - 6.067720966 \times 10^{-11},$$

where $\tau = V$. It has a simple root $w = 0.0001547767475$. We choose the initial guess $\tau_0 = 0.0003885$ and the numerical results are presented in Table 5.

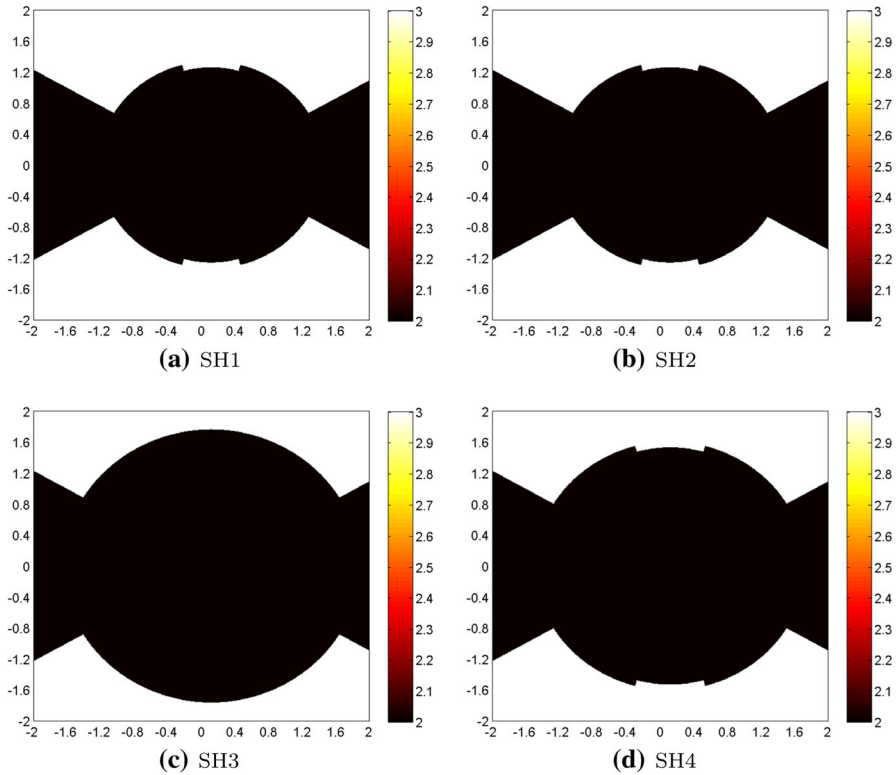


Fig. 7 Attraction basins of SH1–SH4 of $g_4(\theta)$

Table 5 shows the best performance of FZ1–FZ4 schemes, even for simple roots.

For $g_5(\tau)$, the basins of attraction obtained for the methods SH1 – SH4 and FZ1 – FZ4 are shown in Figs. 9, 10. For this example, we consider the region $[-1, 1] \times [-1, 1]$ for dynamical analysis. The basins of attraction of SH1 – SH4 and FZ1 – FZ4 indicate that all iterative schemes take minimum two and maximum six iterations to converge to the root except SH3 which take minimum 2 and maximum 7 numbers of iterations for convergence towards the root. For all iterative schemes, hue of black color shows the divergence region except FZ3 and SH3 in which it indicates two iterations.

Example 6 Peng–Robinson Equation of State We also consider PR equation of state for finding multiple root of V at critical isotherm by using the values $c_1 = 2, c_2 = -1, \lambda_b = 0.2531, \lambda_a = 1.4874, z = 0.3074$ and $\alpha(T_r) = 1$. Equation (22) takes the form:

$$V^3 + \left(b - \frac{RT}{P}\right)V^2 - \left(3b^2 + 2\frac{RTb}{P} - \frac{a}{P}\right)V + \left(b^2 + \frac{RTb}{P} - \frac{a}{P}\right)b = 0.$$

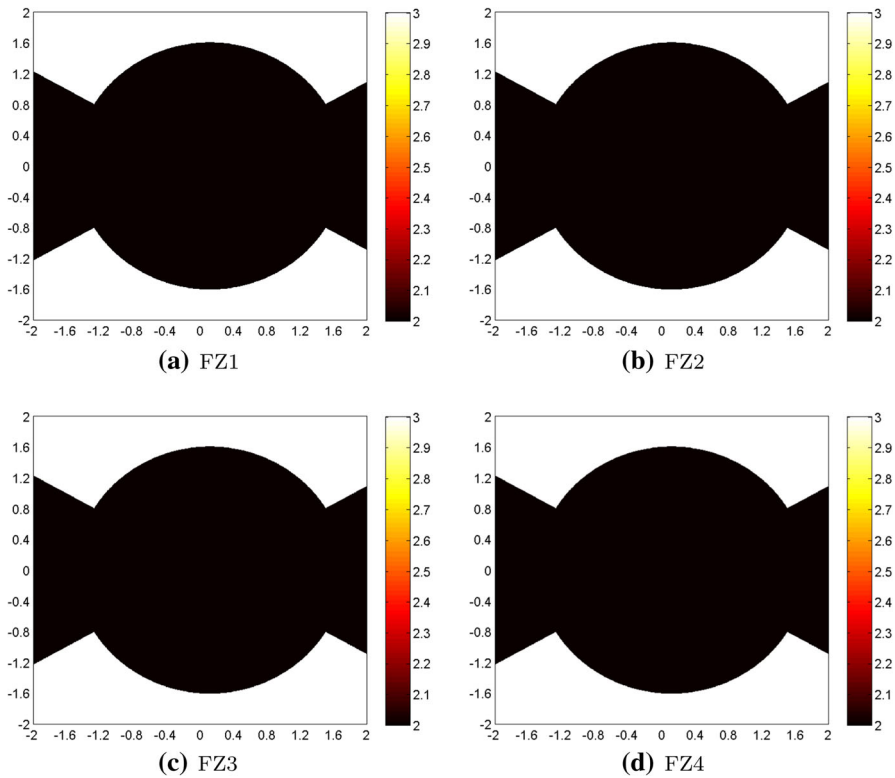


Fig. 8 Attraction basins of FZ1–FZ4 of $g_4(\theta)$

Table 5 Computational comparison of iterative schemes for $g_5(\tau)$

<i>Methods</i>	$ \tau_1 - \tau_0 $	$ \tau_2 - \tau_1 $	$ \tau_3 - \tau_2 $	$ g_5(\tau_3) $	<i>COC</i>
<i>SH1</i>	2.1473×10^{-4}	1.8984×10^{-5}	3.5515×10^{-9}	3.3046×10^{-40}	6.62
<i>SH2</i>	2.1474×10^{-4}	1.8974×10^{-5}	3.5809×10^{-9}	3.5980×10^{-40}	6.62
<i>SH3</i>	2.1016×10^{-4}	2.3538×10^{-5}	1.5977×10^{-8}	3.5683×10^{-38}	7.31
<i>SH4</i>	2.1733×10^{-4}	1.6352×10^{-5}	4.3624×10^{-10}	1.8206×10^{-38}	4.85
<i>FZ1</i>	2.1733×10^{-4}	1.6388×10^{-5}	5.7010×10^{-10}	2.6777×10^{-51}	7.84
<i>FZ2</i>	2.1763×10^{-4}	1.6088×10^{-5}	5.8223×10^{-10}	6.0847×10^{-51}	7.80
<i>FZ3</i>	2.1733×10^{-4}	1.6389×10^{-5}	5.1223×10^{-10}	1.4036×10^{-51}	7.81
<i>FZ4</i>	2.1733×10^{-4}	1.6390×10^{-5}	5.3649×10^{-10}	2.8767×10^{-52}	8.00

Let us solve Peng–Robinson equation of state for Oxygen O_2 at $T = T_c = 153$, $P = P_c = 50$ and using these values we get following nonlinear equation:

$$V^3 - 2.821923704V^2R + 2.654417796VR^2 - 0.8322849442R^3 = 0,$$

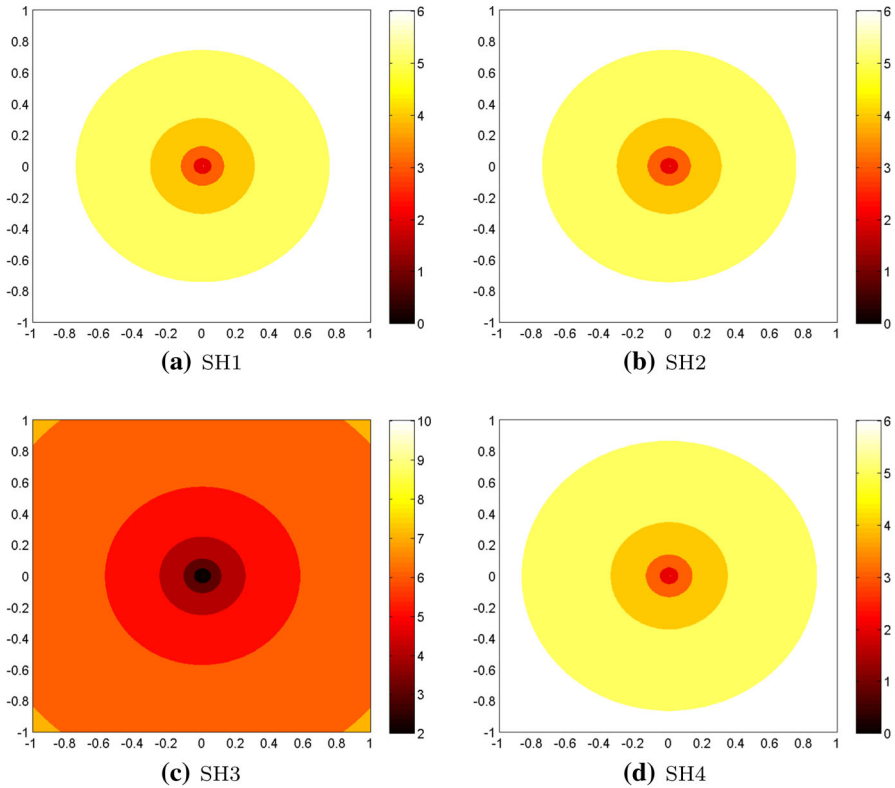


Fig. 9 Attraction basins of SH1–SH4 of $g_5(\theta)$

where $R = 0.0831446261815324$. Solving for $\tau = V$,

$$g_6(\tau) = \tau^3 - 2.821923704\tau^2 R + 2.654417796\tau R^2 - 0.8322849442R^3,$$

gives us the multiple root $w = 0.07820926381$ with multiplicity $\eta = 3$. By using the initial guess $\tau_0 = 0.9$, the numerical results are presented in Table 6.

In this last example, we solve Peng–Robinson equation of state for oxygen O_2 and the basins of attraction obtained for the methods SH1–SH4 and $FZ1 - FZ4$ are shown in Figs. 11, 12 We use the region $[-2, 2] \times [-2, 2]$ to draw the basins of attraction and examine that SH1–SH4 and $FZ1$ – $FZ4$ use minimum two and maximum three numbers of iterations to converge to the root. In this example, the black color indicates the hue of two iterations for all iterative schemes. We observe that newly proposed scheme has globally wider black region as compared to recent methods.

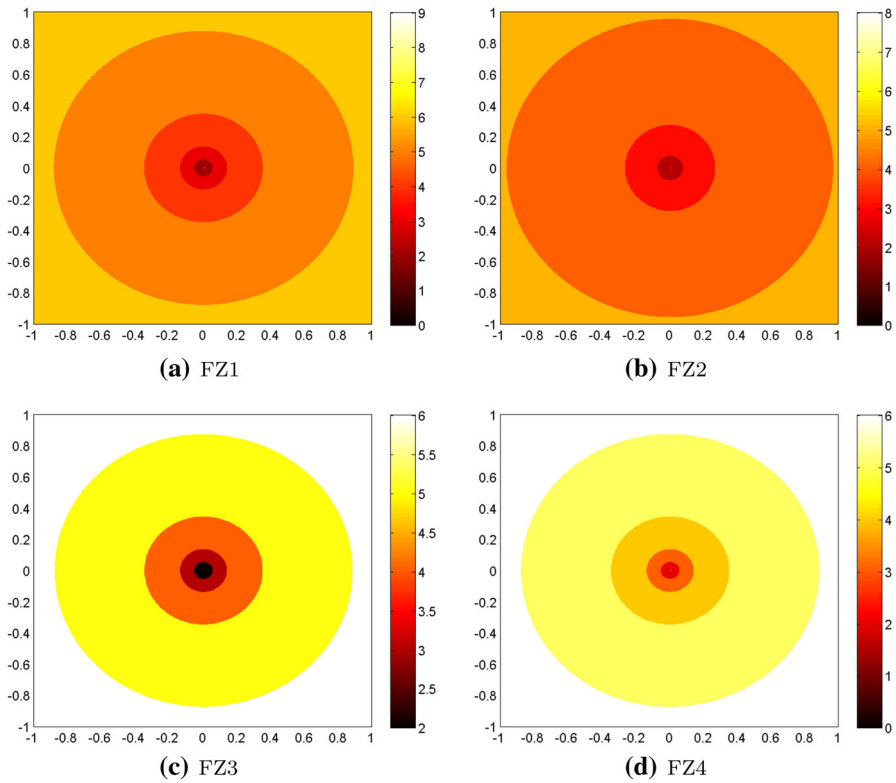


Fig. 10 Attraction basins of FZ1–FZ4 of $g_5(\theta)$

Table 6 Computational comparison of iterative schemes for $g_6(\tau)$

<i>Methods</i>	$ \tau_1 - \tau_0 $	$ \tau_2 - \tau_1 $	$ \tau_3 - \tau_2 $	$ g_6(\tau_3) $	<i>COC</i>
<i>SH1</i>	0.82179	6.4750×10^{-7}	2.4432×10^{-21}	2.2617×10^{-192}	3.00
<i>SH2</i>	0.82179	6.4750×10^{-7}	2.4432×10^{-21}	2.2617×10^{-192}	3.00
<i>SH3</i>	0.82179	6.4575×10^{-7}	1.0577×10^{-21}	1.2054×10^{-332}	6.06
<i>SH4</i>	0.82179	6.4772×10^{-7}	1.4120×10^{-21}	9.1919×10^{-331}	6.08
<i>FZ1</i>	0.82179	6.4750×10^{-7}	1.4106×10^{-21}	9.0543×10^{-331}	6.08
<i>FZ2</i>	0.82179	6.4750×10^{-7}	1.4106×10^{-21}	9.0543×10^{-331}	6.08
<i>FZ3</i>	0.82179	6.4750×10^{-7}	1.4106×10^{-21}	9.0543×10^{-331}	6.08
<i>FZ4</i>	0.82179	6.4750×10^{-7}	1.4106×10^{-21}	9.0543×10^{-331}	6.08

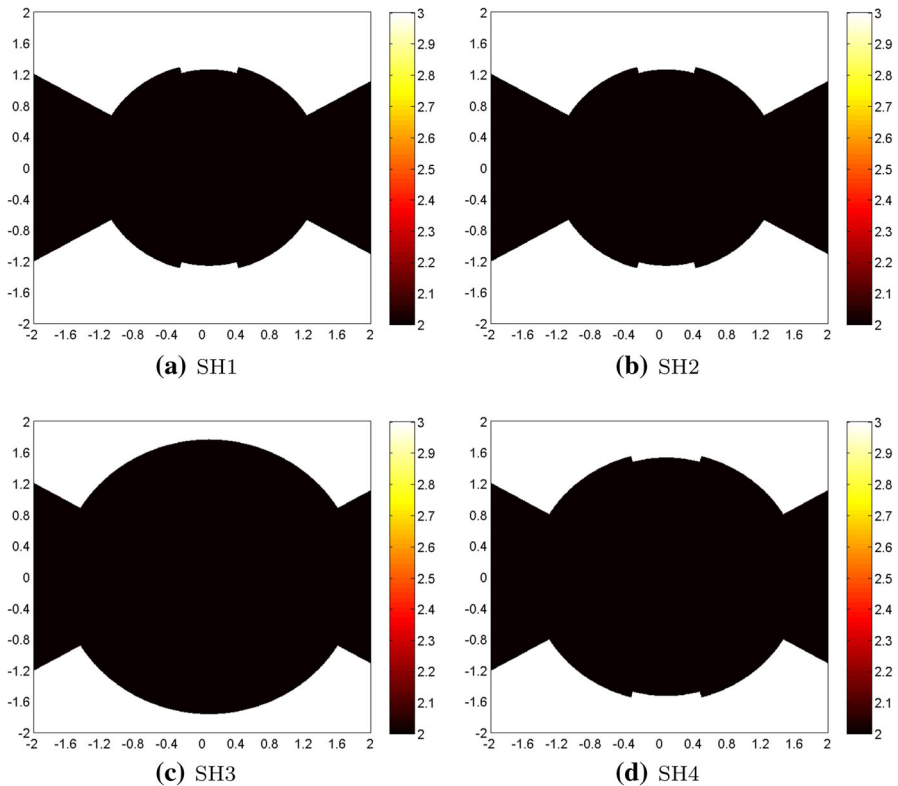


Fig. 11 Attraction basins of SH1–SH4 of $g_6(\theta)$

4 Conclusion

There exist many numerical root-solvers with high order of convergence that require derivative evaluations for finding the multiple root of a function. The derivative free higher-order techniques for computing multiple root are rare and yet to be explored. It is not an easy task to attain an optimal derivative-free root-finder family of methods. We have presented a derivative-free optimal eighth order iterative scheme for finding the zeros of a nonlinear equations with known multiplicity of zeros with a univariate and a multivariate weight functions. The number of functional evaluations required for our presented scheme is four. We have compared the numerical results of our presented scheme with the most recent methods in the literature. We conclude that our method gives eight order of convergence also for the case when function has root of multiplicity one. The dynamical comparison of our presented method with recent seventh and eighth order methods shows that newly proposed method has, in general, wider convergence region. It is apparent from the numerical results and construction that our presented family of method is optimal and efficient in terms of small residual errors.

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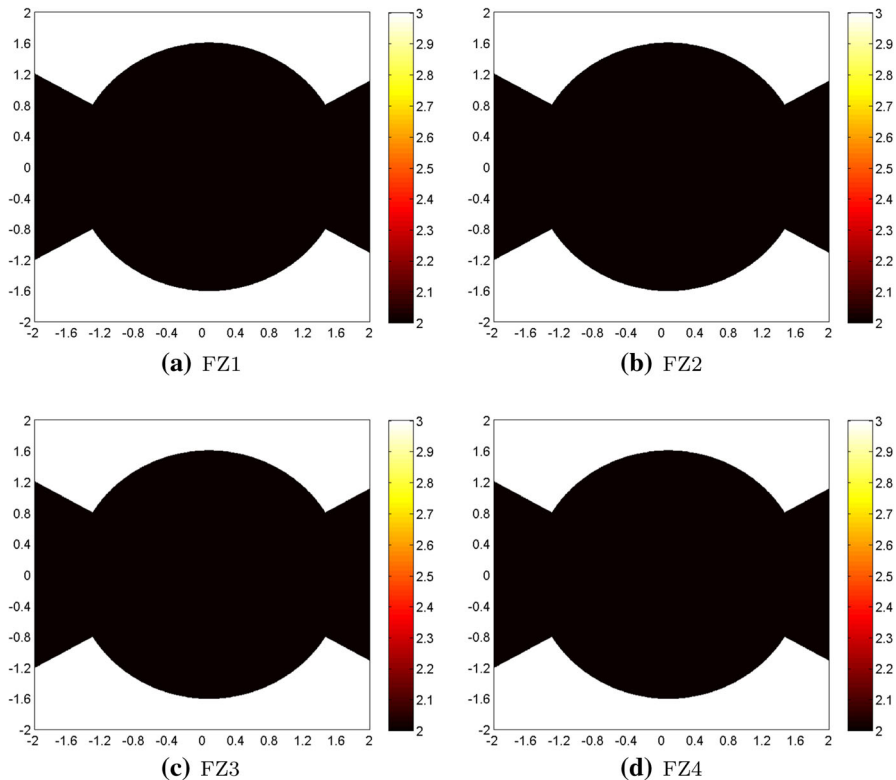


Fig. 12 Attraction basins of FZ1–FZ4 of $g_6(\theta)$

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