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Chaotic Binary Manta-Ray Foraging Optimization Algorithm Based Descriptor Selection for Amphetamine-Type Stimulants Drug Classification

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ABSTRACT

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This study proposes a novel approach to optimize descriptor selection for classifying Amphetamine-Type Stimulants (ATS) and non-ATS drugs. The approach applies a Manta Ray Foraging Optimization (MRFO) framework enhanced with time-varying transfer function and a chaotic map. These enhancements aim to achieve a balance between exploration (finding new possibilities) and exploitation (refining promising solutions) within the improved version of binary MRFO (BMRFO) algorithm to solve descriptor selection problem. Two types of time-varying transfer functions recommended by earlier research are used to convert continuous MRFO to binary MRFO (BMRFO) for binary optimization problem. In addition, the pseudorandom number of the MRFO's probability operator is replaced with eleven different chaotic maps to prevent convergence problem. To evaluate the effectiveness of the suggested approach, a particular high-dimensional chemical dataset containing molecular descriptors of ATS and non-ATS drugs was utilized. The experimental results and statistical analysis show that the proposed BMRFO_{TV2}-C9 employing the non-linear time-varying Sigmoid transfer function and Sinusoidal chaotic map is superior with lowest average fitness indicating its ability to convergence to optimal solution by selecting relevant descriptor subset and achieved better classification accuracy. Additionally, this study evaluated the performance of BMRFO_{TV2}-C9 to other known BMRFO variations from the literature and the findings show that it is more efficient than others.

Keywords:

Binary manta ray foraging optimization; descriptor selection; chaotic map; drug classification

1. Introduction

Domestically and globally, the drug situation is unprecedented, with a massive increase in the sorts of drugs accessible on the market, including new synthetic pharmaceuticals. According to research published in World Drug 2023, there was a significant increase in drug seizures between

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2018 and 2019, particularly for the ATS drug group [1]. ATS, which includes amphetamine (AMP), methamphetamine (MET) and 3,4-methylenedioxymethamphetamine (MDMA), are exemplary synthetic drugs that are experiencing rapid growth in Europe. The EU retail market for AMP and MET is estimated to be worth 1 billion EUR, while the market for MDMA is around 0.5 billion EUR. With increasing rivalry among suppliers, the creation of synthetic drugs is getting increasingly complex, varied and aggressive, especially in the ecstasy market. In order to curb drug misuse, seizures and trafficking in the market, there is a great need for a rapid and efficient analytical technique for ATS drug classification [2].

The challenges in drug development are now the excessive cost and low efficacy of traditional approaches. Cheminformatics plays an important part in drug discovery and gives a computational strategy for shortening this timescale [3]. Within cheminformatics, the chemical or molecular descriptors are quantitative representations of chemical compounds' structural, physicochemical and biological attributes [4]. Consequently, the dimensional curse that results from repetitive and irrelevant data as well as the small sample size may affect molecular descriptors [5]. A feature selection process is carried out that can improve the accuracy of the data mining activity and lower its computing cost to identify the most relevant features and diminish the curse of dimensionality issue. It decreases the dimensionality of the data by removing irrelevant, redundant or noisy data [6].

The process of selecting the most relevant characteristics from the enormous feature space of the data is referred to as feature selection. Feature selection has proven to be a major difficulty in machine learning. Because finding the most essential features within a huge dataset takes an increasing amount of time, it is referred to as an NP-hard task [7]. One class of metaheuristic algorithms that have shown potential in resolving feature selection issues in a variety of applications is swarm intelligence (SI) [8]. In cheminformatics, various SI algorithms have been effectively used as strategies for selecting molecular descriptors. These encompass the Harris Hawk Optimization (HHO) by Houssein *et al.*, [5], Firefly Algorithm (FA) by Fouad *et al.*, [9] and Grasshopper Optimization Algorithm (GOA) [10].

There are two main types of feature selection methods: filter and wrapper [6]. The filter model does not employ any learning algorithm to assess the importance of characteristics. As a result, the filter approach's procedures are usually quick [6]. This technique surpasses the wrapper in computational efficiency. Conversely, wrapper approaches use classifiers and are related to the features in the data. Wrapper methods, on the other hand, are known to be computationally costly while outperforming filter approaches in terms of output quality. For this reason, wrapper approaches, often called metaheuristic procedures, are frequently employed to assess the efficacy of features [11]. Since achieving high classification accuracy is crucial for identifying ATS drugs, this research focuses on using wrapper feature selection for selecting the appropriate molecular descriptors.

This research is driven to employ a native MRFO by Zhao *et al.*, [12] as a wrapper feature selection method in ATS drug categorization, inspired by the No Free Lunch theorem by Wolpert *et al.*, [13], which acknowledges that no single algorithm can address all optimization challenges. This theorem emphasizes that a single, universal optimization algorithm is unlikely to excel across all problem domains. MRFO is particularly well-suited for this task due to its ability to effectively balance exploration and exploitation during the search process. Exploration allows the algorithm to identify promising new regions within the solution space, while exploitation focuses on refining solutions within these identified areas. This balanced approach enables MRFO to achieve near-optimal solutions, making it a compelling choice for tackling diverse optimization problems in various fields [14].



Zhao *et al.*, [12] introduced the first MRFO algorithm to deal with continuous optimization. Because attributes in an attribute selection space are binary in nature, two situations occur: selection and non-selection, resulting in the establishment of BMRFO, that best represents the attribute space [15]. One fundamental feature of an FS problem is a discrete binary search space. To describe solutions to the feature selection problem, a vector of 0 and 1 is required, where 0 signifies the feature not selected and 1 denotes the selected one. The feature dimension of the dataset under consideration correlates to the length of the vector. Thus, a binary vector is used to represent a Manta Ray. Binary issues can be created by converting the variables in continuous search space problems to binary variables. Everyone's position in the continuous search space is indicated by a position vector. Positions in a discrete search space can be updated by flipping between 0 and 1. In order to convert the actual manta ray position into binary data, a transfer function is applied [16].

Feature selection is a type of combinatorial problem that is classified as NP-hard since it requires a longer period to choose the most pertinent descriptors. For this reason, binary meta-heuristic methods have been used to tackle them throughout the previous several decades. Most metaheuristic algorithms were developed for the continuous search space and should be transferred to binary form to solve these challenges. The simplest technique to handle FS difficulties is to use a transfer function to transform the continuous search space to binary [17].

Like most metaheuristic algorithms in the literature reviews, MRFO has several inherent algorithmic inefficiencies, such as delayed and premature convergence and unexpected entrapment to the local optimal locations in the search domain. Lately, the metaheuristic algorithms for solving these problems have been extended to include random numbers produced by chaos theory [18,19]. The chaotic approach is distinguished by three characteristics: ergodicity, quasi-stochastic property and sensitive initial conditions. Chaos sequences are integrated with metaheuristic algorithms to boost algorithm performance. Random variables or parameters are replaced with chaos variables [20].

Furthermore, previous researchers have been interested in utilizing a set of chaotic variables on the MRFO algorithm to improve the solution's effectiveness and accuracy. Based on the existing literature research by Turgut [18], Xu et al., [21], Ćalasan et al., [22] and Qiufeng et al., [23], we have become interested in applying chaotic theory to the domain of feature selection in MRFO algorithm. This study investigates the possibilities of several chaotic maps, including Chebyshev, Circle, Gauss/Mouse, Iterative, Logistic, Piecewise, Sine, Singer, Sinusoidal, Logistic-Tent and Logistic-Sine maps in MRFO.

2. Research Background

2.1 Binary Method

This approach has been successful in producing binary versions of numerous SI algorithms, including Binary Particle Swarm Optimization, Binary Bat algorithm and Binary Artificial Bee Colony [24]. Recent years have seen a rise in the use of binary MRFO in many applications; some of the works are included in Table 1.

Table 1Some works on binary MRFO

References	Algorithms	Application	Transfer function used
Ghosh et al., [25]	BMRFO	Feature Selection	S-shaped and V-shaped
Tayal <i>et al.,</i> [16]	MRFO	Feature Selection	S-shaped and V-shaped
Hassan et al., [15]	BMRF	Feature Selection	Adaptive S-shaped
Ansari Shiri et al., [26]	CBBMRF	Feature Selection	S-shaped



Yıldızdan [27]	Bin_MRFOA	Binary Optimization	S-shaped and V-shaped
Zhang et al., [28]	IMRFO	Engineering	S-shaped

2.2 Chaotic in Metaheuristics Algorithm

The incorporation of chaotic maps in metaheuristic algorithms has grown widespread in various applications and some of the works are given in Table 2.

Table 2Some of chaotic map works in metaheuristics algorithms

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References	Algorithms	Application
Mohmmadzadeh et al., [29]	Chaotic Symbiotic Search	Feature Selection
Zhang <i>et al.,</i> [28]	Gaussian Mutational Chaotic Fruit Fly-Built	Feature Selection
Too <i>et al.,</i> [30]	Chaotic Atom Search	Feature Selection
Singh <i>et al.,</i> [31]	Chaotic Flower Pollination Algorithm	Optimization Problem

2.3 Chaotic in MRFO Algorithm

The employment of chaotic in MRFO algorithm are shown in Table 3 below.

Table 3Some of the implementation of chaotic map in MRFO algorithm

References	Algorithms	Application
Xu et al., [21]	Chaotic	Function Optimization
	MRFO	
Turgut [18]	Chaotic	Function Optimization and maintaining thermos-economic scheme optimization
	MRFO	of an air-fin cooler
Ćalasan et al.,	CMRFO	Finding parameters of a single phase and two new transformers
[22]		
Qiufeng et al.,	IMFRO	Energy fibre Bragg grating demodulation
[23]		

Section 2 introduces the methodologies employed in the research. It provides a comprehensive overview of the concepts, algorithms or techniques used in the case of study. Section 3 presents the findings and outcomes obtained from the conducted experiments or analyses. Lastly, is Section 4. This section interprets the results within the context of the existing literature, highlights the key contributions of the study and offers suggestions for potential future research directions. It concludes by summarizing the main findings and their significance.

3. Methodology

3.1 Chaotic Binary Manta-Ray Foraging Algorithm

The selection of an appropriate time-varying update strategy for the transfer function (TF) is crucial in MRFO to prevent convergence to local optima. This strategy facilitates exploration of diverse regions within the search space, thereby enhancing the algorithm's ability to locate the global optimum. This study employs a modified Sigmoid transfer function within the MRFO algorithm. This function originally proposed by Mohd Yusof *et al.*, [32], effectively transforms real-valued position data of search agents into probability values ranging from 0 to 1. The author has shown significant improvement in terms of selecting informative descriptors and obtaining high classification accuracy compared to standard Sigmoid transfer function. The transfer function is depicted in Eq. (1),



Sigmoid
$$\left(x_i^d(t+1)\right) = \frac{1}{1+0^{-10}\left(\frac{x_i^d(t+1)}{Tv}0.5\right)}$$
 (1)

Where, agent represents the position of a manta ray or search agent, t denotes the current iteration number, i signifies the order of the search agent within the population and d represents the dimensionality of the search space. Tv is a control parameter that systematically decreases over time. Following the transformation using the transfer function, Eq. (2) from Kennedy *et al.*, [33] is utilized to update the position vector based on the obtained probability values. The equation is presented below:

$$x_i^{d}(t+1) = \begin{cases} 1, & \text{if rand } < \text{Sigmoid} \left(x_i^{d}(t+1)\right) \\ 0, & \text{Otherwise} \end{cases}$$
 (2)

with rand signifying a random number drawn from the uniform distribution [0,1]. This study investigates the efficacy of two time-varying updating schemes for the control parameter (Tv) within the Manta Ray Foraging Optimization (MRFO) algorithm.

The first scheme, designated as TV1, adopts a linear time-varying approach. This strategy aligns with the findings of several prior works by Algamal *et al.*, [34], Kahya *et al.*, [35], Chantar *et al.*, [36], Beheshti [17] and is mathematically represented by Eq. (3),

$$t = t_{\text{max}} + (t_{\text{min}} - t_{\text{max}})(\frac{itr_{t+1}}{itr_{\text{max}}})$$
(3)

Conversely, the second scheme, denoted as TV2, utilizes a non-linear time-varying approach. This strategy finds support in references by Hussien *et al.*, [37] and is depicted in Eq. (4),

$$t = t_{\text{max}} + (t_{\text{min}} - t_{\text{max}}) \left(\frac{itr_{t+1}}{itr_{\text{max}}}\right)^{\alpha}$$
(4)

Within this equation, itr_{t+1} signifies the current iteration number, while itr_{max} is the maximum number of iterations represents the maximum number of iterations permitted for the optimization process. Additionally, t_{min} and t_{max} denote the minimum and maximum allowable values, respectively, for the control parameter Tv. For these purposes of this research, the specific values chosen for t_{min} , t_{max} and α are set at 4, 0.01 originally introduced by Chantar *et al.*, [36] and 0.5 respectively, based on findings reported by Kahya *et al.*, [35].

In the original MRFO, the pseudorandom numbers are assigned to random values, rand() to help in controlling the exploration and exploitation. Nature-inspired optimization algorithms allow for changes to avoid premature convergence and achieve more accurate solutions. Chaos maps' dynamic properties have been frequently employed to address inadequacies, improve intensification and diversification and evaluate stochastic algorithm performance [19]. In this study, the chaotic mapping mechanism is combined with the traditional MRFO in both search strategies and speed parameters to obtain the global optimum for the challenging high-dimensional problem. The chaotic time-varying manta ray foraging optimization was generated by substituting random values in the basic MRFO with a chaotic variable, $chaos_idx(index)$ explained in Figure 1.



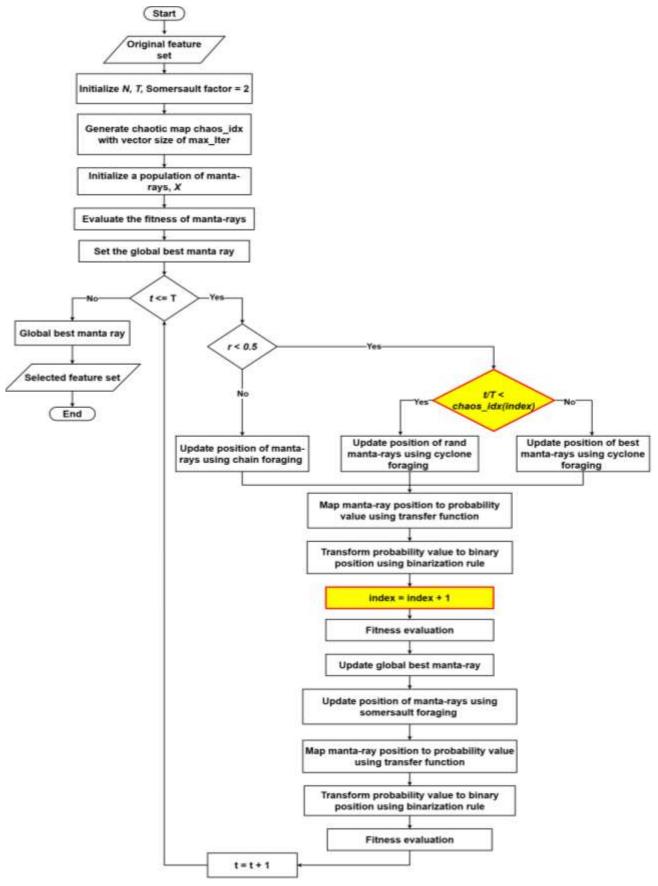


Fig. 1. Flowchart of the proposed chaotic BMRFO algorithm (yellow boxes indicate the change of chaotic map implementation)



3.2 Chaotic Binary Manta-Ray Foraging Wrapper Feature Selection Algorithm

This study employs a Chaotic BMRFO-based wrapper feature selection algorithm to intelligently select the relevant descriptor subset from a large chemical dataset to accurately classify between ATS or non-ATS drug. The methodology involves initializing the process with the inclusion of all descriptors from a specific data partition into the designated algorithm for feature selection, as illustrated in Figure 2.

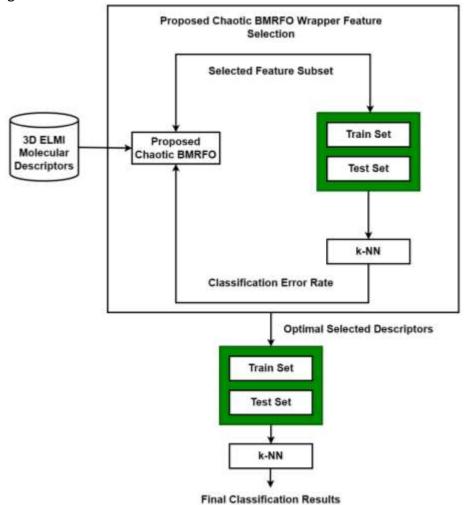


Fig. 2. Framework of the proposed Chaotic BMRFO-based wrapper feature selection model

Upon reaching the predetermined number of iterations, the descriptor search and selection procedures are performed. Since a wrapper approach is employed, a K-Nearest Neighbors (K-NN) classifier is utilized to evaluate the quality of the selected feature subsets. K-NN is a well-established classification method known for its simplicity, speed and ease of implementation [38-40]. Eq. (5) defines a fitness function that incorporates the K-NN classifier's classification error rate. This error rate is then used by the proposed BMRFO algorithm to assess the fitness of the selected feature subsets.

$$\downarrow \text{Fitness} = \alpha \cdot E + \beta \frac{|SF|}{|F|} \tag{5}$$



The fitness function incorporates two constant parameters, α and β , are constant parameters that regulating the trade-off between classification performance and descriptor subset length, where $\alpha \in (1,0)$ and $\beta \in (1-\alpha)$. E represents the rate of classification error. The original feature size in the dataset is denoted by |F|, while the selected feature size is represented by |SF|. Given that classification performance is the primary objective, a high weight of 0.99 is assigned to this metric within the fitness function.

A lower fitness value obtained by the proposed Chaotic BMRFO algorithm indicates the selection of a more informative feature subset. This selected subset is then evaluated using the same K-NN classifier to determine the final classification accuracy for ATS and non-ATS drug classification. Subsequently, the obtained classification performance is compared against the results achieved by other benchmark algorithms.

3.3 Dataset

The dataset incorporated in this study is the 3D Exact Legendre Moment Invariant (ELMI) molecular descriptors [41]. It contains 1187 descriptors of 7109 drug instances (3,595 ATS drugs and 3,595 non-ATS drugs). The attributes of the descriptors include a molecular identifier, 1,185 moment invariant values and a binary classification label (0 for non-ATS, 1 for ATS). It is important to note that the molecule ID descriptor was excluded from the experiments.

3.4 Parameter Setting

In the experiment, every algorithm was run ten times via a diverse set of random seeds. Random seeds are used to ensure reproducibility, as all algorithms begin with the same number and data partition. Additionally, each random seed was subjected to 150 iterations. A stratified hold-out validation technique was employed [39,42]. This method divides the data into training (80%) and testing (20%) sets. During optimization, the classifier is trained on the training data, while the testing data is used to assess the chosen features' performance. To account for potential variations, the results are presented as average metrics calculated from the ten independent runs. The algorithm was developed and executed using MATLAB R2023b on a PC with an Intel Xeon CPU E5-1603 (2.80 GHz), running Windows 10 Pro and equipped with 8 GB of RAM.

3.5 Performance Measurement

This research examines how well the proposed Chaotic BMRFO algorithm performs by looking at several performance metrics. These metrics include an average fitness (Avg. Fitness) and its standard deviation (Std.) that helps to observe the convergence ability in finding the optimal features and their consistency and robustness from run-to-run. Besides, an average classification accuracy (Avg. Accuracy) shows how accurate the classifier to classify ATS and non-ATS drug using descriptors selected by algorithm. Moreover, another performance measurement used in this study is an average number of selected descriptor (Avg. No. of Descriptors) that shows how many relevant features subset selected by the algorithm. The algorithm convergence speed is measure based on the average computational time (Avg. CT), where it is the time taken by the algorithm to complete the searching and selection process. A qualitative analysis is conducted by generating a convergence graph in Figure 5 visualize the convergence ability of each algorithm. The non-parametric statistical analysis, Wilcoxon signed-rank test with significant level of 0.05 is performed to discover if there is a significant performance differences by the proposed algorithm from existing algorithms. The null hypothesis



states that no significant difference between the two algorithms is accepted when the p-value is greater or equal to 0.05. Otherwise, the null hypothesis is rejected when the p-value is lower than 0.05.

4. Results

To comprehensively evaluate the proposed Chaotic BMRFO algorithm, several experiments were designed. The first experiment conducted is to identify which chaotic maps is suitable for the BMRFO implementing linear (BMRFO_{TV1}) and non-linear (BMRFO_{TV1}) time-varying Sigmoid transfer functions. The experiment turns out having different result of BMRFO_{TV1} for each different chaotic map. For BMRFO_{TV1} the best performance emerged for BMRFO_{TV1}-C10 employing hybrid Logistic-Tent map with the highest average accuracy as seen in Figure 3.

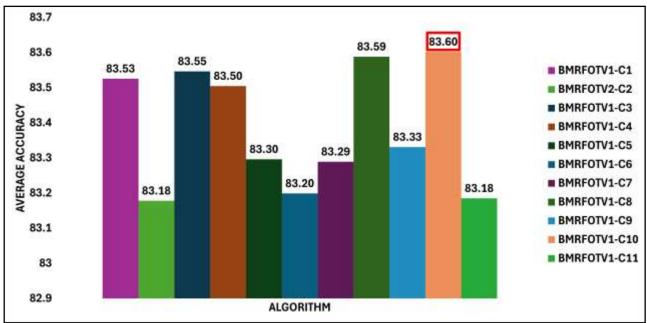


Fig. 3. Result of average accuracies of enhanced BMRFO $_{TV1}$ with different chaotic maps other comparative algorithms

Figure 4 depicted the best chaotic map for BMRFO $_{TV2}$ is Sinusoidal map in BMRFO $_{TV2}$ -C9 which obtained the highest average accuracy. These results indicate that both Logistic-Tent and Sinusoidal map have produced the improvement in the exploration and exploitation processes in BMRFO which led to better quality solutions especially in feature selection domain.



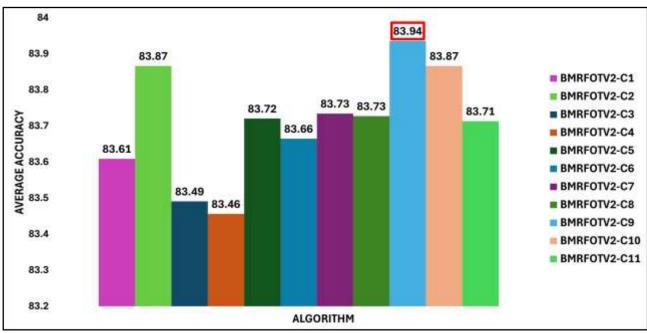


Fig. 4. Results of average accuracies of proposed BMRFO_{TV2} algorithm with different chaotic maps

The next experiment is to measure the effectiveness of the proposed algorithm with the existing BMRFO variants in the literature: MRFOv3, BMRFO_{TV1}, BMRFO_{TV2}, BMRFO_{TV2}-C10 and BMRFO_{TV2}-C9. The outcomes of the experiment presented in Table 4.

Table 4
Results of the average fitness, fitness of standard deviation and average computational time (CT) (seconds) of MRFOv3, BMRFO_{TV1}, BMRFO_{TV2}, CBMRFO_{TV1} and CBMRFO_{TV2}

Algorithm	Avg. Fitness	Std.	Avg. CT (seconds)	Avg. Accuracy	Avg. No. of Descriptors
MRFOs3 [44]	0.18099	0.00667	4629.19	82.03	366
MRFOv3 [25]	0.18878	0.18878	426.22	82.03	33
BMRFO _{TV1} [43]	0.16341	0.01308	1270.51	83.57	94
BMRFO _{TV2} [43]	0.16145	0.01297	1488.79	83.79	116
BMRFO _{TV1} -C10	0.16302	0.01374	3230.21	83.60	80
BMRFO _{TV2} -C9	0.15989	0.01358	2419.64	83.94	101

The algorithm demonstrating the most promising performance is highlighted for clarity. The implementation of chaotic map in each of the existing algorithms, BMRFO $_{\text{TV1}}$ and BMRFO $_{\text{TV2}}$ proposed by Yusof et~al., [43] have shown an improvement in convergence performance after obtaining lower average fitness by BMRFO $_{\text{TV1}}$ -C10 using Logistic-Tent map and BMRFO $_{\text{TV1}}$ -C9 using Sinusoidal map. Moreover, it is observed that BMRFO $_{\text{TV2}}$ -C9 has scored the lowest average fitness among other algorithms proving its ability to escape from local minima and converge near to the optimal solution. It is evidenced by the convergence graph illustrated in Figure 5.



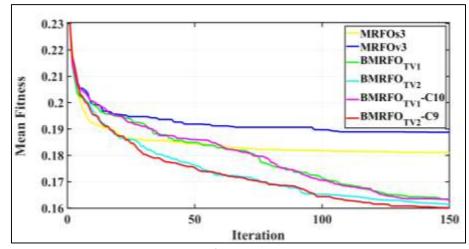


Fig. 5. Convergence curves of proposed BMRFO $_{TV2}$ -C9 and another comparative BMRFO

Moreover, by referring to Table 4, BMRFO_{TV2}-C9 algorithm also seen to exhibits the highest average accuracy. This implies that BMRFO_{TV2}-C9 possesses a better performance, enabling it to produce solutions that are demonstrably close to optimal. MRFOv3 proposed by Ghosh *et al.*, [25] shows the lowest average number of selected descriptors during the optimization process, however not able to find and select the relevant descriptors and obtain lowest average classification accuracy. This highlights that the algorithm is not suitable to be employed with the 3D-ELMI dataset for drug classification although it has shown an outstanding performance in several benchmark datasets. On the other hand, the existing algorithm of BMRFO_{TV2} introduced by Yusof *et al.*, [43] has the lowest standard deviation advocating it robustness and converge consistently in each run. In terms of convergence speed, the MRFOv3 algorithm is seen to converge rapidly with the shortest average computational time and it justifies that MRFOv3 has faced with premature converge issue and failed to find the optimal solution. The employment of chaotic maps in the existing BMRFOTV1 and BMRFOTV2 have increased the average computational time (Avg CT) since the generated chaotic map numbers have assisted the algorithm to traverse to wider search space to find for relevant descriptors.

To statistically assess potential performance differences among the proposed and existing binary algorithms, a Wilcoxon signed-rank test was employed based on the average classification accuracy in Table 4. By observing on the data presented in Table 5, there are significant improvements shown between BMRFO $_{TV2}$ -C9 with MRFOs3 and MRFOv3. Both algorithms achieved p-values of 0.004 and 0.002 which is less than 0.05. Therefore, the null hypothesis is rejected. Conversely, BMRFO $_{TV1}$, BMRFO $_{TV2}$ and BMRFO $_{TV1}$ -C10 display less significant improvements performance compared to BMRFO $_{TV2}$ -C9 with the calculated p-values larger than 0.05 indicating the null hypothesis is accepted. However, their performance is still comparable.

Table 5Results of p-values of Wilcoxon signed-rank test based on the average classification accuracy between BMRFO_{TV2}-C9 with other algorithms

	 5
Algorithms	p-values
MRFOs3	0.004
MRFOv3	0.002
BMRFO _{TV1}	0.161
BMRFO _{TV2}	0.444
BMRFO _{TV1} -C10	0.153



Table 6 shows the average classification accuracies of three classifiers: k-NN (k = 5) with Euclidian distance metric, support vector machine (SVM) with radial basis function (RBF) and random forest (RF) using the original dataset. The results show that RF is the best classifier, with 83.11% classification accuracy. The employment of proposed BMRFO_{TV2}-C9 algorithm has demonstrated excellent performance in finding 101 important descriptors and successfully increased the classification accuracy to 83.94%. It shows that feature selection is essential in refining the efficiency of classifier to learn and predict better result from large dataset.

Table 6Difference of classification performance with different classifier using original datasets and our proposed technique

	Original (1185 descriptors)	BMRFO _{TV2} -C9 (101 descriptors)
Classifier	Avg. accuracy (%)	Avg. accuracy (%)
k-NN	62.89	83.94
SVM (RBF)	68.41	
RF	83.11	

5. Conclusions

This study introduces an enhanced version of BMRFO algorithm that employ the time-varying transfer function and chaotic map. Experimental works have embedded 2 version of time-varying Sigmoid transfer functions with 11 chaotic maps on standard MRFO on a descriptor selection problem of a high-dimensional chemical dataset for improving ATS drugs classification. The results show that among several variations of the BMRFO algorithm, BMRFOTV2-C9 performed best. This version was particularly effective at selecting relevant and informative features, leading to high classification accuracy. This research opens doors for future studies to employ different transfer function parameters value in other optimization algorithms, both existing and newly developed. To further validate the effectiveness of the proposed algorithm, future work could involve testing it on a wider range of problems and datasets from the University of California Irvine (UCI) Machine Learning repository. Additionally, exploring different initial parameter settings of chaotic map and incorporating other types of chaotic theory novels could potentially improve the performance of BMRFO in classifying ATS drugs.

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