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ORIGINAL ARTICLE

Optimizing ANFIS using simulated annealing algorithm for classification of microarray gene expression cancer data

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Abstract
In the medical field, successful classification of microarray gene expression data is of major importance for cancer diagnosis. However, due to the profusion of genes number, the performance of classifying DNA microarray gene expression data using statistical algorithms is often limited. Recently, there has been an important increase in the studies on the utilization of artificial intelligence methods, for the purpose of classifying large-scale data. In this context, a hybrid approach based on the adaptive neuro-fuzzy inference system (ANFIS), the fuzzy c-means clustering (FCM), and the simulated annealing (SA) algorithm is proposed in this study. The proposed method is applied to classify five different cancer datasets (i.e., lung cancer, central nervous system cancer, brain cancer, endometrial cancer, and prostate cancer). The backpropagation algorithm, hybrid algorithm, genetic algorithm, and the other statistical methods such as Bayesian network, support vector machine, and J48 decision tree are used to compare the proposed approach's performance to other algorithms. The results show that the performance of training FCM-based ANFIS using SA algorithm for classifying all the cancer datasets becomes more successful with the average accuracy rate of 96.28% and the results of the other methods are also satisfactory. The proposed method gives more effective results than the others for classifying DNA microarray cancer gene expression data.

Keywords Fuzzy neural networks · Simulated annealing · Machine learning · Optimization · Gene expression

1 Introduction

Due to the developments in medical analyses and imaging technology, there has been a significant increment in the generated data in almost every field and the need for effective methods has also grown in order to develop data mining applications for large-scale data. Laboratory data, which are revealed within the scope of genetic research, are also usually large-scale, and there are considerable difficulties in the applications of classifying these data in practice.

Microarray technology contains hundreds of genes in its structure [1]. With this technology, the diseased and healthy cells activities in the same tissue can be compared with each other. Thus, DNA microarray gene technology is great assistance to researchers to diagnose the genes that cause diseases such as cancer. Additionally, it also supports researchers to diagnose the subtypes of gene-related cancer diseases. Therefore, in order to solve microarray gene expression problems, high-performance classifying methods are of great importance.

The feature selection methods have aroused common interest in the field of microarray gene expression analysis. It determines vital genes related to human cancers. Such data compose of a great number of genes than the number of samples. As the high dimensionality reduces the generalization performance of the classifier, the computational complexity of the problem is significantly increased. The feature selection

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method could be preferred to preserve a few relevant features and separate others, hence, reducing the complexity and searching significant features. Feature selection could commonly be split into two categories as the wrapper and filter in the literature. While the wrapper methods are classifier dependent, the filter methods are classifier independent [2, 3].

In the literature, so as to classify microarray gene expression data, statistical methods like Bayes network (BayesNet), support vector machines (SVM), and the J48 decision tree (J48) are frequently used. For example, a centroid-based gene selection method was suggested by Guo et al. [4] for microarray data classification. The performance of this one was compared to various feature selection methods. The proposed method yielded better performance on all microarray datasets. Dagliyan et al. [5] proposed a method named hyper-box enclosure (HBE) algorithm to classify prostate cancer gene expression data. In this study, they compared the performance of the proposed method with different statistical methods such as BayesNet, SVM, and Random Forest. The HBE achieved better performance on prostate cancer data. In another study, Tan and Gilbert [6] used different machine learning algorithms for cancer classification based on microarray gene expression data where Bagging, C4.5, and AdaBoost algorithms were preferred to classify those data. However, the performances of statistical classifying algorithms may remain limited due to the abundance of genes number. These difficulties have prompted researchers to develop more modern and stronger methods. In this context, the interest of researchers has gradually started to focus on incorporating artificial intelligence methods in their studies.

In the last few decades, various studies based on artificial intelligence methods have proposed for classification problems. Pirooznia et al. [7] conducted a classification study on microarray gene expression data. In that study, artificial intelligence-based methods compared to statistical methods were found be more successful. Sarhan [8] compared the performances of the discrete cosine transform (DCT) and artificial neural network (ANN) methods for classifying microarray cancer dataset. Loganathan and Girija [9] trained the ANFIS parameters using the Runge Kutta learning algorithm. They proposed a model for classification microarray gene expression cancer dataset. AnandaKumar and Punithavalli [10] classified cancer data using ANFIS, and they compared the obtained results with statistical methods. Haznedar et al. [11] trained ANFIS network by using genetic algorithm (GA) to classify microarray gene expression liver cancer data. The performance of proposed model called ANFIS-GA compared with other ANFIS models trained with back propagation and hybrid algorithm (HB). In this study, the proposed ANFIS-GA model was found to be the most successful among all ANFIS models.

The best properties of neural networks and fuzzy systems are combined in the ANFIS structure. Neural networks could find the optimum solutions with back propagation behaviors. Besides, the best characteristic property of fuzzy systems that they reduce the dimension of the search space by distributing input data via the network weights. Thus, these properties ensure important advantages to the ANFIS. The training of the ANFIS structure is an optimization process of finding the optimal values for its premise and consequent parameters. Derivative-based learning algorithms are commonly used such as Levenberg Marquardt (LM), least squares (LS), backpropagation (BP), Kalman filter (KF), and gradient descent (GD) to optimize the ANFIS. But, for derivative-based algorithms, the used chain rule may bring about a local minimum problem and calculating the gradient for each step is also comparatively difficult. Besides, the performance of the algorithms is a vast scale dependent on the initial values, and the convergence of the parameters is quite slow. For these reasons, using derivative-based algorithms to optimize the ANFIS parameters is one of the main problems. So, different approaches are required for optimizing ANFIS successfully. In recent years, multifarious methods have been proposed within this context. Some of these methods are heuristic algorithms such as the GA, differential evolution (DE), artificial bee colony (ABC), and particle swarm optimization (PSO) algorithm [12].

Canayaz [13] trained ANFIS using moth-flame optimization algorithm (MFO) to classify breast cancer dataset. This model was employed for classification problems. The ANFIS was also trained with PSO, GA, and whale optimization algorithm (WOA) where MFO was found to be more successful than the other algorithms. In another study, Jinthanasatian et al. [14] classified seven microarray datasets specifically lung cancer, ovarian cancer, prostate cancer, leukemia (ALL/AML), colon cancer, diffuse large B-cell lymphoma (DLBCL), and breast cancer using ANFIS with firefly Algorithm (FA). The comparison results showed that the proposed model gave better results than other existing ANFIS-GA and ANFIS-PSO models. Thangavel and Kaja Mohidden [15] studied about classification of breast cancer using ANFIS with ant colony optimization (ACO) algorithm. The performance of proposed model was compared with rough set-based ANFIS (RS-ANFIS) and PSO-ANFIS. It was found that ANFIS-ACO achieved better results in comparison with other models. Karaboga and Kaya [16] optimized ANFIS using ABC to estimate number of foreign visitors to Turkey where the ANFIS-ABC was more successful than other optimization methods.

The study of population-based algorithms with a set of candidate solutions usually allows them to quickly access the region of the global optimum. However, since these algorithms have high probability-based search strategies, they often require long computational time to find the optimal solution in the region where they are located. Algorithms such as SA are iterative-based and usually try to find a global

optimum by improving a randomly selected candidate solution. This kind of algorithm can generally obtain the optimal solution in a shorter time interval than population-based algorithms. In this scope, in order to classify microarray gene expression successfully, a hybrid approach is proposed that simulated annealing (SA) algorithm based on artificial intelligence is used to train the ANFIS model that generated by fuzzy c-means clustering (FCM) method. Thereby, proposed hybrid approach that combine ANFIS, FCM, and SA methods together is presented. No study related to the proposed method could be found in the literature. The performance of the proposed method is tested on five different cancer types, and the results from proposed method are compared with those obtained from different algorithms. In the following section, the datasets are introduced and methods are explained. In the third and fourth sections, the results are presented and discussed in detail.

2 Materials and methods

In order to classify microarray gene expression successfully, the consequent and premise parameters of ANFIS model are generated by FCM method and optimized by SA algorithm. Thereby, proposed hybrid approach can be considered as a combination of ANFIS, FCM, and SA methods together. In this section, analyzed cancer datasets are first introduced, and later the ANFIS, FCM, SA, and combined proposed method are presented in details.

2.1 Dataset description

In this study, five different microarray gene expression datasets are used as the data source. These datasets are obtained from the database in the bioinformatics laboratories of Rutgers University. Samples taken from different tissues and cancer types are displayed in Table 1. While the least samples are of brain cancer, the most samples are of lung cancer. Because of the high-leveled cost of microarray data analyses, these analyses cannot be performed on many samples. Therefore, there are very few samples that have the microarray gene expression level.

Lung cancer This dataset, which was provided by Gordon et al. [17], contains the expression levels of 1626 genes. These data consist of two types of lung cancer, 150 of adenocarcinoma of the lung (AD), and 31 of malignant pleural mesothelioma (MPM). The data which contains 1626 genes are taken from lung samples.

Central nervous system cancer This dataset, provided by Pomeroy et al. [18], contains 34 samples in two labels, namely classic medulloblastomas (CMD) and desmoplastic medulloblastomas (DMD), which have 25 and 9 samples, respectively. The data are taken from brain samples. The original dataset contains 857 genes.

Brain cancer This dataset, presented by Nutt et al. [19], comprises the expression levels of 1070 genes. It contains 28 samples and two labels: classic glioblastomas (CG) and non-classic glioblastomas (NG). Among the 28 samples, 14 samples are CG and 14 samples are NG. The data are taken from tumor biopsies collected from brain tumors.

Endometrial cancer This dataset, presented by Risinger et al. [20], consists of 42 samples with 1771 genes taken from tumor biopsies gathered from endometrial tumors, and normal biopsies gathered from the healthy part of the endometrium of the same patient. It comprises four labels: 19 endometrioid cancers (E), 13 serous papillary (SP), 3 clear cell (CC), and 7 age-matched normal endometria (N).

Prostate cancer This dataset, provided by Singh et al. [21], consists of 52 prostate tumor (PR) and 50 normal prostate specimens (N). It comprises 102 samples with the expression levels of 339 genes which are taken from breast tumors.

2.2 Feature selection

Feature selection involves finding a feature subset from the main feature space that will increase the performance of the classifying methods, in other words, reducing the size of the problem by taking a feature subset from the feature set and providing convenience and performance success in solving the problem. If achieving high classifying performances for the microarray datasets is desired, it should be mentioned that feature selection is essential.

Table 1 Detailed information for the used datasets

Dataset	Tissue	Label	Number of genes	Samples
Gordon-2002	Lung	2	1626	181
Pomeroy-2002	Central nervous system	2	857	34
Nutt-2003	Brain	2	1070	28
Risinger-2003	Endometrium	4	1771	42
Singh-2002	Prostate	2	339	102

Feature selection is classified into filter-based and wrapper-based approach. Filter methods measure the efficiency of gene subsets by analyzing only the original data characteristics, in which typically a subset of genes or a single gene is measured toward the label. Generally, the most preferred gene selection methods fall within the filter approach. Even though objects such as division or robustness in multibinary problems are emerging topics, most of the proposed filter approaches are based on knowledge theory [22]. Conventional filter methods are often used for high-dimensional microarray gene expression data, such as fast correlation-based filter (FCBF), correlation feature selection (CFS), or the consistency-based filter [23].

On the other hand, the wrapper approach has not attracted as much notice as the filter approaches do, because of its high computational cost. As the number of features increases, the space of feature subsets increases exponentially. So, the method's computational complexity increases dramatically when tens of thousands of features are considered. Moreover, this brings up the risk of overfitting due to the small sample size of gene expression data. Consequently, the wrapper approach has been majorly avoided in the literature [24].

Some of the studies on feature selection approaches in the literature are the following. Sharma et al. [25] proposed a filter-based method for classification of microarray data. The proposed method yielded a promising accuracy when comparing to other existing methods on several microarray datasets. Lazar et al. [26] presented a study focusing on filter methods by using standardized formula to find out technical details and to accentuate their extensive characteristics. Yu and Liu [27] applied an efficient correlation-based filter algorithm to handle the high-dimensional data. Wanderley et al. [28] presented an evolutionary wrapper method using a Bayesian classifier and a non-parametric estimation method. As a result, the performance of evolutionary wrapper method is better than the others given in literature.

In our study, because of the reasons explained above, correlation-based feature selection algorithm, which is a type of filter approach, is preferred for microarray gene expression data. Thus, useful and the most relevant genes are selected from high-dimensional microarray data.

Correlation-based feature selection Correlation-based feature selection (CFS) evaluates the information of subsets in the feature space. According to this method, high-performance feature subsets consist of features that have a high correlation with the related class and a low correlation with each other [29].

CFS measures the "goodness" of feature subsets and takes into account the usefulness of individual features for predicting the class label along with the level of inter-correlation among them and given by:

$$G_s = \frac{k\bar{r}_{ci}}{\sqrt{k + k(k-1)\bar{r}_{ii}}} \tag{1}$$

where k is the number of features, $\bar{r}_{ci}$ is the average feature correlation, and $\bar{r}_{ii}$ is the average feature inter-correlation parameter. It can be considered that the numerator in (1) represents the estimating skill of a group of features on the class; the denominator represents the redundancy among these features.

2.3 Adaptive neuro-fuzzy inference system

Adaptive neuro-fuzzy inference system (ANFIS), which was developed in 1993 by Jang [30], is a hybrid artificial intelligence method that combines the neural network's parallel computing and learning ability with fuzzy logic's inference property. It uses input and output data pairs with *IF-THEN* rules in its structure. ANFIS is frequently used in prediction problems as it provides decision-making opportunities like experts to neural networks that built-in its structure. The structure of ANFIS consists of two parts. The first part is called initial section, and the second part is called result section. These two sections connect fuzzy rules to each other to form the shape of network. Besides, the parameters found in these sections are used to train ANFIS. These parameters are called premise and consequent parameters. ANFIS consists of five layers. Figure 1 shows a basic ANFIS structure [31].

Training of this network is provided by optimization of the premise and consequent parameters. The learning rule determines how these parameters need to be optimized to minimize a predicted error value. A value of error is a mathematical representation of the difference between the desired output and the actual output of the network. The ANFIS layers are introduced as follows:

Layer 1 The first layer is named as fuzzification layer. Signals received from each node are processed depending on the type of input values and using the membership function. The nodes outputs of this layer are defined in (2) and (3) [33].

$$O_{1i} = \mu A_i(x) \quad i = 1, 2 \tag{2}$$

$$O_{1i} = \mu B_{i-2}(x) \quad i = 3, 4 \tag{3}$$

In this study, the Gaussian membership function given in (4) is used. $\{a_i, c_i\}$ is the parameter set which changes the shapes of the membership function. a_i is the variance of the MFs and c_i the center of the MFs. The parameters in this layer are called the premise parameters.

$$\mu A_i = e^{-\frac{1}{2}\left(\frac{x-c_i}{a_i}\right)^2} \quad i = 1, 2 \tag{4}$$

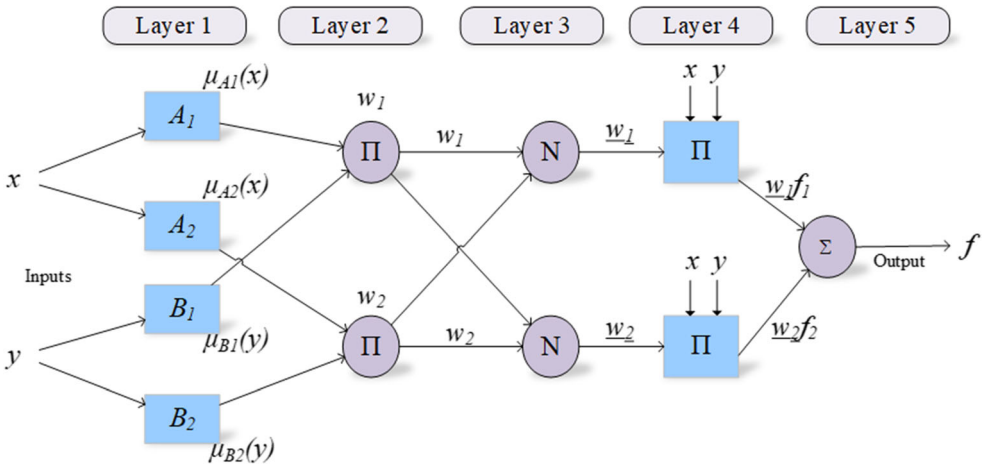

Fig. 1 The basic ANFIS structure [32]

Layer 2 The second layer is known as the rule layer. The firing strength of each rule is calculated using MFs degrees coming from the first layer.

$$O_{2i} = w_i = \mu A_i(x).\mu B_i(y) \quad i = 1, 2 \tag{5}$$

Layer 3 The third layer is the normalization layer of the model. Here, the normalized firing level of each rule is calculated [34] by

$$O_{3i} = \overline{w}_i = \frac{w_i}{w_1 + w_2} \quad i = 1, 2 \tag{6}$$

Layer 4 The fourth layer is called as defuzzification layer. The output values are calculated for each rule in this layer. These are obtained by multiplying the normalized firing strength value coming from the third layer with the first order polynomial [35].

$$O_{4i} = \overline{w_i}.f_i = \overline{w_i}.(p_i x + q_i y + r_i) \tag{7}$$

$\{p_i, q_i, r_i\}$ is the parameter set that called the conclusion parameters.

Layer 5 The final layer is the output layer. The ANFIS's output is obtained by adding the output values of each rule calculated in the defuzzification layer [36, 37] by

$$O_{5i} = f = \sum \overline{w_i}.f_i = \frac{\sum w_i.f_i}{\sum w_i}. \tag{8}$$

The ANFIS consists of two parts: training and construction. In the construction part, the type and number of the membership functions are determined. Also, reflecting the input and output data properly on the rule layers is necessary for the construction. Different methods such as grid partitioning, FCM, and subtractive clustering are used for achieving better ANFIS structure. In this study, in order to obtain a few rules, a fuzzy rule generation technique is used in which ANFIS and FCM clustering are integrated.

In the training part, firstly the training data should be created to optimize the ANFIS. Making changes in the membership function parameters during the training process is possible. Supervised learning is carried out by using the input/output datasets which are given as the training data to the model so as to set these parameters. Various methods can be used for the optimization of the ANFIS parameters, such as BP, LS, KF, or HB learning algorithms, which are formed from merged multiple mathematical optimization [38]. In this study, SA is used for training the ANFIS model that generated by using FCM.

2.4 Fuzzy c-means clustering

Fuzzy c-means clustering (FCM) is a method of data clustering in which each data point belongs to a cluster with a degree specified by a membership. FCM was introduced by Dunn in 1973 [39] and formalized by Bezdek in 1981 [40]. The FCM partitions a collection of n vectors x_i, $i = 1, 2, \ldots, n$ into fuzzy groups and determines a cluster center for each group using the objective function based on minimization.

The steps of the FCM are clarified briefly: Firstly, the centers of each cluster c_i are randomly chosen from the n data patterns $\{x_1, x_2, x_3, \ldots, x_n\}$. Secondly, the membership matrix (μ) is calculated with the following equation:

$$\mu_{ij} = \frac{1}{\sum_{k=1}^{c} \left(\frac{d_{ij}}{d_{kj}}\right)^{\frac{2}{m-1}}} \tag{9}$$

where μ_{ij} is the membership degree of pattern j in cluster i, m is the degree of fuzziness ($m > 1$), and $d_{ij} = \|c_i - x_j\|$ is the Euclidean distance between c_i and x_j. Thirdly, the objective function is computed as follows:

$$J(U, c_1, c_2, \ldots, c_n) = \sum_{i=1}^{c} j_i = \sum_{i=1}^{c} \sum_{j=1}^{n} {\mu_{ij}}^m {d_{ij}}^2 \tag{10}$$

The process works iteratively until the termination criterion is satisfied. Finally, the new c fuzzy cluster centers c_i, $i = 1, 2, \ldots, c$ are computed as follows:

$$c_i = \frac{\sum_{j=1}^{n} {\mu_{ij}}^m x_j}{\sum_{j=1}^{n} {\mu_{ij}}^m} \tag{11}$$

In this study, the FCM is used to partition all data pairs into several subsets. Each membership function of ANFIS is trained by SA algorithm, as proposed by Abdulshahed et al. [41] and Park et al. [42].

2.5 Simulated annealing algorithm

The simulated annealing is a stochastic method that provides optimal solutions for combinatorial optimization problems. This approach has been developed for the solution of combinatorial problems, inspired of the physically annealing of metals. The SA algorithm is based on the logic of gradual cooling of metal crystals containing structural disturbances starting from a high temperature. Thus, metallic crystals are consummated by purified from structural disturbances (transforming into a minimum energy crystal structure). This approach is based on the work of Metropolis et al. (1953) [43–46]. The study was developed in order to find the balanced distribution of atoms at a given temperature level and simulated the energy changes. The idea that this behavior can be used to solve optimization problems was introduced by Kirkpatrick et al. (1983) [44]. The main steps of the SA are given as follows:

Step 1. Construct the initial solution (S)
Step 2. Choose a neighbor solution $S' \in N(S)$, and find the difference between the cost function values of the S and S', $\Delta = C(S) - C(S')$
Step 3. **If**, $(\Delta > 0)$, **or** $\delta \leq e^{\Delta E/T}$
Then, assign S' to $S(S \leftarrow S')$
Else, remain the current solution
Step 4. Update the temperature *(T)*
Step 5. **If** a "stopping criterion" is acquired **then** STOP, **else** GO TO Step 2.

The $T(t+1) = r.\ T(t)$ relation is the cooling function commonly used in literature. In this function, r is a temperature factor. In the literature, the r value is generally between 0.8 and 0.99 [47].

2.6 Training ANFIS using the SA algorithm

In this section, the details of the proposed hybrid approach that combine ANFIS, FCM, and SA methods together are explained. ANFIS has two parameter types to be optimized. These are premise and consequent parameters. The premise parameters pertain to *Gaussian* MFs given as $\{a_i, c_i\}$ in (4). Here, a_i is the variance of the MFs, while the center of the MFs is c_i. Consequent parameters are given as $\{p_i, q_i, r_i\}$ in (7), which is used in the defuzzification layer. The SA algorithm is used to optimize all the parameters of the ANFIS models.

First of all, a solution space is initialized with the FCM clustering method for the initial values of the premise and consequent parameters, which are located in the first and the fourth layers of the ANFIS model shown in Fig. 2. The error values of solutions are determined by the root mean square error (*RMSE*) function that is defined in (12). F and F_d, which are used in this error function, represent the output which is obtained by ANFIS and the actual output of the data.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N} (F(i) - F_d(i))^2}{N}} \tag{12}$$

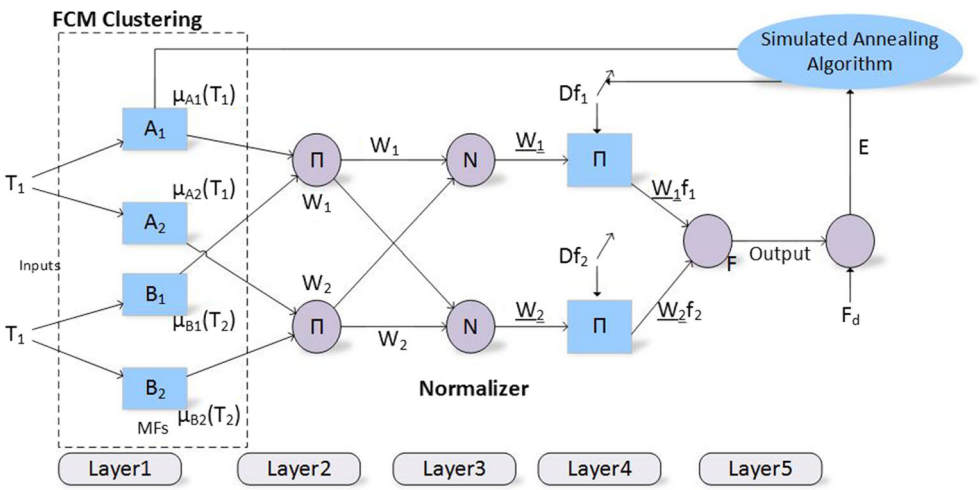

Fig. 2 Basic structure of proposed method

Table 2 The number of genes in the reduced datasets

Dataset	Number of genes
Lung cancer	92
Central nervous system cancer	30
Brain cancer	36
Endometrial cancer	53
Prostate cancer	24

Afterward, the parameters of ANFIS are updated by using the SA algorithm for each iteration. With the purpose of training the ANFIS model for a dataset, the classification architecture shown in Fig. 2 is used in the application of the SA algorithm. The aim is to minimize the active error (RMSE) given in (12) by arranging the premise and consequent parameters of the ANFIS model. In the training stage, firstly, all genes of each sample are applied to the inputs of ANFIS. The efficient error value that is obtained from the actual output and the newly produced neighboring output is compared. If the efficient error value that is obtained with the new output is less, then the new output is assigned as the current output and the search continues. Otherwise, the selection is made according to the Metropolis criteria.

3 Simulation results

In this study, the classification is performed on microarray datasets. Before the simulation process, all the datasets are normalized to [0-1] range, and the feature selection method is applied to the datasets. Feature selection is a process that selects those features in high-dimensional data that are most useful or most relevant for pattern classification problems. For this purpose, in order to create a subset of the datasets, correlation-based feature selection which is a filter approach is preferred. Thus, increasing the performance of the classification methods and getting more successful results become possible with the subsets that express these datasets in a better way rather than with large size datasets. The number of genes for the reduced datasets is given in Table 2.

Table 3 Details of the optimized ANFIS models

Dataset	The number of			The type of MFs
	Inputs	MFs	Rule	
Lung cancer	92	10	10	*gaussmf*
Central nervous system cancer	30	24	24	*gaussmf*
Brain cancer	36	20	20	*gaussmf*
Endometrial cancer	53	29	29	*gaussmf*
Prostate cancer	24	10	10	*gaussmf*

Table 4 Mean test *RMSE* of statistical methods

Dataset	Statistical algorithms		
	BayesNet	SVM	J48
Lung cancer	0	0.1925	0.3333
Central nervous system cancer	0.2287	0.5477	0.6252
Brain cancer	0.2129	0	0.5000
Endometrium cancer	0.3033	0.2774	0.4440
Prostate cancer	0.2536	0.2540	0.3598

Classification with small number of samples is a key issue in statistics and bioinformatics, especially in microarray studies. As for data splitting, usage of validation set requires large number of samples to be able to get estimates with high accuracy. Also, validation with a separate dataset is not much feasible in datasets with small sample sizes similar to the datasets in this study. Because of these reasons, the usage of validation set can be considered as practical and rewarding only for the datasets with large sample size. Likewise, k-fold cross-validation provides unbiased estimation for the datasets with small number of samples. In general, it presents large variability with small samples. In addition, k-fold may not ensure that the data used to validate the classifier is not part of the data used to train it. For these reasons, random sampling is considered as primary methodology instead of cross-validation for data splitting in this study. In addition, k-fold cross-validation method is also used to improve the reliability and significance of the present work.

Simulation results are carried out by using five different microarray cancer datasets to optimize the ANFIS parameters with the SA algorithm. In order to measure the performances of the methods on the datasets, 70% of the data is used for training, and the remaining 30% is used for testing. Due to the abundance number of parameters in the experimental datasets, a fuzzy rule generation method that is integrated with ANFIS and FCM at the first layer is used to create the ANFIS models in which only a few fuzzy rules and membership functions exist. The input number in the ANFIS models which are generated by applying the FCM is equal to the gene number in

Table 5 Mean test *RMSE* of ANFIS models

Dataset	ANFIS			
	BP	GA	HB	SA
Lung cancer	0.3688	0.2807	0.3273	0.1880
Central nervous system cancer	0.3682	0.4436	0.3846	0.2564
Brain cancer	0.3290	0.3312	0.3214	0.1120
Endometrium cancer	0.3536	0.4588	0.6268	0.2548
Prostate cancer	0.3231	0.3056	0.3679	0.3114

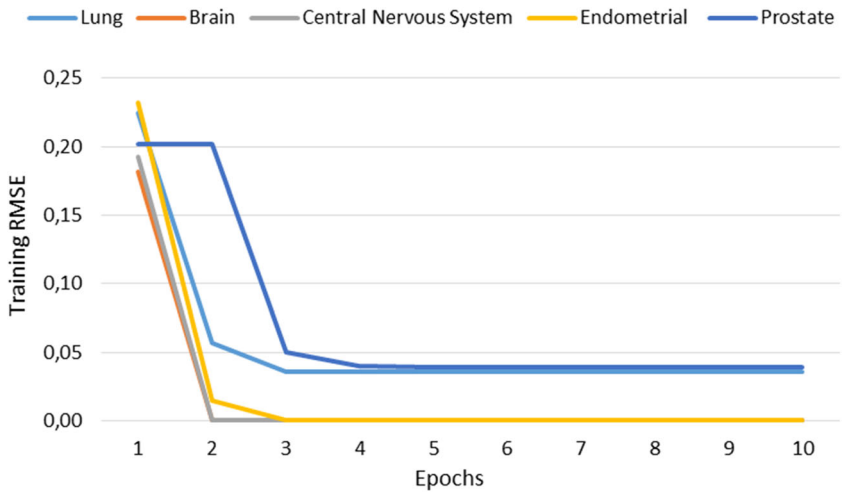

Fig. 3 The *RMSE*-epochs chart

each dataset. For each dataset, the type and number of MFs and the number of fuzzy rules are given in Table 3.

The performance of the artificial intelligence optimization algorithms is largely dependent on the control parameters of the algorithms, and there are no certain methods or rules about which values should be generally used for the control parameters. Within this scope, setting the values which are in the ranges widely recommended by researchers for the parameters, or the approach of determining the optimal parameter values by making many attempts is approved. In the study, many test attempts are applied to decide the SA algorithm's parameter values. As a consequence of the attempts, the number of temperature points is taken as 10, the temperature reduction parameter is chosen as 0.9, and the iteration number which is performed on each temperature point is taken as 2.

The ANFIS network is also trained with GA, BP, and HB algorithms to compare with different methods' performances. In this context for the GA algorithm used, the iteration number, the size of population, the mutation, and crossover rate are taken as 100, 25, 0.8, and 0.01, respectively. The learning rate for the BP algorithm and the momentum coefficient are also chosen as 0.2 and 0.4, respectively. The HB is also used as a method which consists of using least squares estimation and the BP algorithm. In addition, the number of iterations for the BP and HB is defined as 100.

Due to the number of genes being too abundant and usually the non-linear relationship, the performances of statistical classifying algorithms for classifying DNA microarray gene expression data are mostly limited. Therefore, the performance of the proposed method is compared with those of statistical algorithms such as BayesNet, SVM, and the J48. In this context, The C-Style Soft Margin Support Vector Machine (C-SVM) algorithm and radial basis kernel function are used for the SVM method. Also, the cost parameter of the algorithm is defined as 0.5. The K2 search algorithm is preferred for BayesNet. The confidence factor used for pruning is chosen as 0.25, and the minimum number of instances per leaf is taken as 2 for the J48.

Each algorithm is run 15 times to demonstrate the accuracy and reliability of the classification results. Furthermore, the average *RMSE* ($RMSE_{AVG}$) value is obtained by taking the average of the *RMSE* value for each model. The test *RMSE* values of the ANFIS network trained using different optimization algorithms on 5 different microarray gene expression cancer data are given in Tables 4 and 5. As seen from Tables 4 and 5, the smallest test *RMSE* values are obtained by the ANFIS-SA model. Figure 3 shows that the training errors are obtained by using the ANFIS-SA model for five different microarray gene expression cancer data.

The ANFIS models for all the datasets are trained with the SA, GA, BP, and HB algorithms, and their performances are compared. Afterward, the classification results of above-

Table 6 Percentage accuracy (AC), sensitivity (SN), and specificity (SP) of the statistical methods with %70–30 splitting

Dataset	Statistical algorithms					
	BayesNet		SVM		J48	
Lung cancer	AC	100.00	AC	96.30	AC	88.89
	SN	100.00	SN	93.33	SN	79.17
	SP	100.00	SP	100.00	SP	96.67
Central nervous system cancer	AC	90.00	AC	70.00	AC	60.00
	SN	100.00	SN	80.00	SN	50.00
	SP	80.00	SP	60.00	SP	83.33
Brain cancer	AC	87.50	AC	100.00	AC	75.00
	SN	100.00	SN	100.00	SN	75.00
	SP	80.00	SP	100.00	SP	75.00
Endometrium cancer	AC	76.92	AC	84.62	AC	61.54
	SN	50.00	SN	50.00	SN	50.00
	SP	88.89	SP	83.00	SP	75.00
Prostate cancer	AC	93.55	AC	93.55	AC	87.10
	SN	92.86	SN	92.86	SN	100.00
	SP	94.12	SP	94.12	SP	80.00

Table 7 Percentage accuracy (AC), sensitivity (SN), and specificity (SP) of ANFIS models with %70–30 splitting

Dataset	ANFIS							
	BP		GA		HB		SA	
Lung cancer	AC	88.88	AC	90.74	AC	94.44	AC	100.00
	SN	79.17	SN	80.00	SN	86.96	SN	100.00
	SP	96.67	SP	100.00	SP	100.00	SP	100.00
Central nervous system cancer	AC	90.00	AC	70.00	AC	90.00	AC	100.00
	SN	100.00	SN	80.00	SN	100.00	SN	100.00
	SP	80.00	SP	60.00	SP	80.00	SP	100.00
Brain cancer	AC	87.50	AC	75.00	AC	100.00	AC	100.00
	SN	100.00	SN	75.00	SN	100.00	SN	100.00
	SP	80.00	SP	75.00	SP	100.00	SP	100.00
Endometrium cancer	AC	69.23	AC	53.85	AC	76.92	AC	84.62
	SN	50.00	SN	50.00	SN	50.00	SN	66.67
	SP	83.33	SP	75.00	SP	88.89	SP	90.00
Prostate cancer	AC	93.55	AC	93.55	AC	93.55	AC	96.77
	SN	92.86	SN	87.50	SN	92.86	SN	93.33
	SP	94.12	SP	100.00	SP	94.12	SP	100.00

mentioned ANFIS models and the classification results of the statistical algorithms such as BayesNet, SVM, and J48 are compared with each other.

In order to evaluate the performance of the proposed method, three well-known measures are used specifically accuracy, sensitivity, and specificity. Accuracy indicates whether the model classified the instances correctly or not. In addition to accuracy, sensitivity is the percentage of correctly classified actual positives, while specificity shows how well negative examples are predicted by the model. Statistical results for the percentage accuracy, sensitivity, and specificity of classification algorithms obtained by optimal parameter values are presented in Tables 6 and 7. Also, the average accuracy performances of the classification algorithms are shown in Fig. 4.

As depicted in Fig. 4, the ANFIS-SA method maintains the highest performance in classifying all the cancer datasets with the average accuracy rate of 96.28%. The simulation results given in Fig. 4 reveals that the ANFIS-SA method has better performance for classification problems when compared to the other methods.

Different measures are needed to reliably determine the performances of all the methods. The accuracy, sensitivity, and specificity cannot be considered alone for evaluating the methods which classify unbalanced dataset such as microarray. With the scope of the study to evaluate the performance of methods, F-measure, recall, and precision are also used to ensure classification accuracy. According to all the experimental results, the success criterions such as accuracy, precision, recall, and F-measure values for five different cancer data and all classification models are given in Table 8.

In accordance with the average performance measures of the methods, the SA algorithm's performance is more successful than the other algorithms in training the parameters of the ANFIS model. As mentioned in Section 3, k-fold cross-

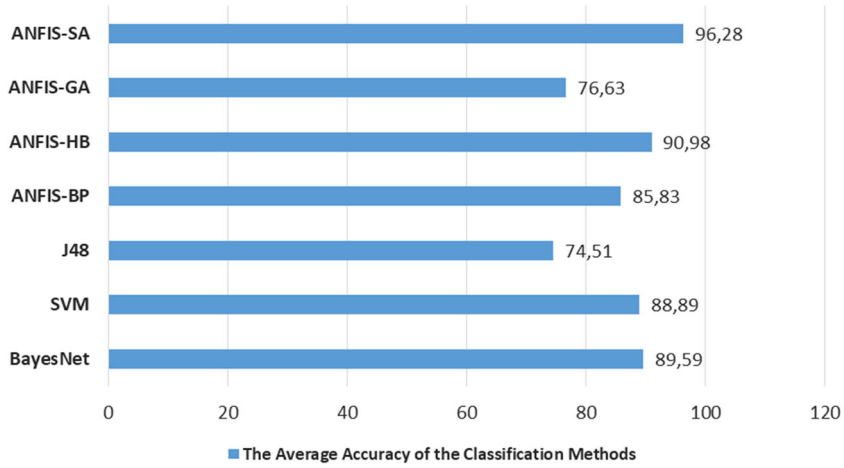

Fig. 4 The average accuracy performances of the classification methods on all microarray gene expression profiles

Table 8 The performance criterions of all methods

Model	Accuracy (%)	Precision	Recall	F-measure
ANFIS-SA	96.28	0.97	0.96	0.96
ANFIS-GA	76.63	0.78	0.77	0.76
ANFIS-BP	85.83	0.88	0.86	0.86
ANFIS-HB	90.98	0.92	0.91	0.91
SVM	88.89	0.86	0.89	0.86
BayesNet	89.59	0.92	0.90	0.89
J48	74.51	0.77	0.75	0.74

validation method is also used to improve the reliability and significance of the present work. Within this scope, the ANFIS models are retrained with the SA, GA, BP, and HB algorithms by using 5-fold cross-validation for data splitting instead of random splitting method. The obtained results by using 5-fold validation are shown in Table 9.

As depicted in Table 9, evaluation measures of the results from the 5-fold validation are acceptable but less than the 70–30% data splitting results presented in Table 8. The average accuracies of the BP, GA, HB, and SA methods with 5-fold cross-validation are 81.36%, 74.20%, 85.60%, and 92.41%, respectively. Again, the highest performance is obtained with ANFIS-SA method.

4 Discussions

The comparison of the obtained results in Table 8 shows that the highest average accuracy rate of 96.28% is achieved by using ANFIS-SA to classify all cancer microarray datasets. In addition, the lowest result belongs to the J48 with the average accuracy rate of 74.51%. Due to the number of genes being too many and usually the non-linear relationship, it is clearly seen that the performances of statistical algorithms for classifying DNA microarray gene expression data become poorer than the ANFIS models.

Calculating the gradient for each step is relatively difficult, and also the used chain rule may cause a local minimum problem in derivative-based algorithms. The obtained results demonstrate that the performance of ANFIS-BP with the average accuracy rate of 85.83% is poorer than that of proposed method.

The study of population-based algorithms with a set of candidate solutions usually allows them to quickly reach to the region of the global optimum. In addition, as these algorithms have high probability-based search strategies, they often require long computational time to find the optimal solution in the region where they are located. On the other hand, iterative-based algorithms such as SA usually try to find a global optimum by improving a randomly selected candidate solution. These kinds of algorithms can generally obtain the optimal solution in a shorter time interval than population-based algorithms. So, the proposed method is more successful than the ANFIS-GA model with the average accuracy rate of 76.63%.

Various statistical methods have proposed for classification of microarray data. For example, Dagliyan et al. [5] applied statistical methods to classify microarray prostate cancer data. This study indicated that the most successful performance is with an accuracy rate of 95.24%. On the same dataset, we achieved better performance via our proposed method with 96.77%. In another study, Tan and Gilbert [6] classified

Table 9 Percentage accuracy (AC), sensitivity (SN), and specificity (SP) of ANFIS models with 5-fold validation

Dataset	ANFIS							
	BP		GA		HB		SA	
Lung cancer	AC	83.33	AC	88.33	AC	90.56	AC	98.33
	SN	75.00	SN	85.00	SN	84.00	SN	100.00
	SP	100.00	SP	89.00	SP	84.00	SP	98.00
Central nervous system cancer	AC	85.71	AC	71.43	AC	88.57	AC	94.29
	SN	81.00	SN	81.00	SN	85.00	SN	92.00
	SP	100.00	SP	40.00	SP	100.00	SP	100.00
Brain cancer	AC	83.33	AC	73.33	AC	90.00	AC	96.67
	SN	62.00	SN	83.00	SN	87.00	SN	90.00
	SP	100.00	SP	60.00	SP	100.00	SP	100.00
Endometrium cancer	AC	64.44	AC	48.89	AC	68.89	AC	77.78
	SN	70.00	SN	43.00	SN	70.00	SN	63.00
	SP	38.00	SP	41.00	SP	41.00	SP	46.00
Prostate cancer	AC	90.00	AC	89.00	AC	90.00	AC	95.00
	SN	90.00	SN	96.00	SN	90.00	SN	98.00
	SP	100.00	SP	81.00	SP	90.00	SP	92.00

microarray cancer datasets by statistical methods. They obtained the accuracy rate of 88.33%, 93.29%, and 73.53% for central nervous system, lung, and prostate cancer datasets, respectively. In our study, we found the accuracy rate of 100%, 100%, and 96.77% on the above-mentioned datasets, respectively.

The number of existing study in the literature is quite limited for classification of microarray cancer datasets using artificial intelligence based methods. Moreover, different datasets are used in the available studies. Therefore, our results are not directly comparable to any of these studies. For example, Haznedar et al. [11] trained ANFIS network by using GA to classify microarray liver cancer data. The performance of their proposed model called ANFIS-GA compared with other ANFIS models trained by BP and HB algorithm. The obtained results showed that ANFIS-GA model with an accuracy of 92.14% was more successful than the other all ANFIS models. Similarly, our present model called ANFIS-SA achieved the average accuracy rate of 96.28% on different microarray datasets. In another study, Loganathan and Girijia [9] trained ANFIS structure to classify lymphoma and leukemia microarray cancer dataset. For this purpose, they used BP and RKLM to train ANFIS model. According to their results, the proposed model called ANFIS-RKLM with the average accuracy rate of 93.22% is more successful than ANFIS-BP with the average accuracy rate of 88%. In our study, the average accuracy rates of 85.83% and 96.28% are obtained on different five microarray cancer datasets by ANFIS-BP and ANFIS-SA models, respectively.

We have analyzed five different microarray gene expression datasets with the proposed method. Due to the high-leveled cost of microarray data analyses, such analyses cannot be performed for datasets with large number of samples. Classification of datasets with very few training samples and more labels is quite a difficult task compared to the others. In this study, the least number of samples are in brain cancer dataset, and the most number of samples is in lung cancer dataset among five datasets. Also, endometrial cancer dataset has the most number of labels. The performance results in Tables 6 and 7 indicate that other algorithms yield very close values to the proposed method for the lung cancer dataset which consists of the most number of samples with 2 labels. However, the performance results obtained by using endometrial cancer dataset which consists of fewer samples with 4 labels show that the proposed method yields much better performance than all other methods. In addition, the highest performance, the average accuracy rate of 96.28%, is obtained by the proposed method in classifying all the cancer datasets. The present study has revealed that the proposed method is especially more successful in classifying datasets with fewer samples and more labels remarkably.

5 Conclusions

In conclusion, a new hybrid approach based on the ANFIS and SA algorithms is suggested for the purpose of classifying microarray data. The performance of the suggested approach is tested on microarray gene expression cancer data that belong to five different cancer types, and the obtained results are compared with the results belonging to the approaches for training ANFIS with the HB, BP, GA, and statistical algorithms such as BayesNet, SVM, and J48.

Statistical performance measures such as precision, recall, and F-measure are important factors in the evaluation of model performance as well as classification measures. In this context, the performances of all the classification models are compared using the above-mentioned measures. By means of statistical measures, the proposed classification model shows a better performance than the other classification approaches. As a result, it is found that ANFIS-SA performance is more successful than the other approaches to classify the microarray cancer gene expression profile. Our results prove the reliability of the proposed method. Because the SA doesn't have limitation as happened for derivative-based algorithms, the proposed model can be applied in studies for different problems.

SA is an iterative-based algorithm and only works on a single solution. Although the algorithm with this series structure yields very successful results for many problems, the time required to reach the global optimum may vary depending on the initial solution. However, since population-based algorithms work with a set of candidate solutions, it is also known that they are generally able to access the global optimum region quickly. Thus, by combining the advantages of iterative and population-based algorithms, the development a new model for the SA algorithm and its implementation for training the ANFIS are planned as a future work.

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