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Fuzzy c-means based support vector machines classifier for perfume recognition

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ABSTRACT

Identification of more than three perfumes is very difficult for the human nose. It is also a problem to recognize patterns of perfume odor with an electronic nose that has multiple sensors. For this reason, a new hybrid classifier has been presented to identify type of perfume from a closely similar data set of 20 different odors of perfumes. The structure of this hybrid technique is the combination of unsupervised fuzzy clustering c-mean (FCM) and supervised support vector machine (SVM). On the other hand this proposed soft computing technique was compared with the other well-known learning algorithms. The results show that the proposed hybrid algorithm's accuracy is 97.5% better than the others.

1. Introduction

Electronic noses are imitated living creatures' olfactory systems to differentiate among odors and volatile compounds by use of different sensor series and pattern recognition techniques. Electronic nose studies have been started at Warwick University at England [1]. In the last few decades, there have been various researches done to improve the hardware and software of electronic noses'. It is possible to access industrial products such as the Aeonose (eNose, Netherlands), Aromascanner (Aromascan plc, UK), Fox (Alpha-MOS, France), and ENOSE 4000 (Neutronics Scientific Ltd., UK). Ryan et al. have developed an electronic nose at the Jet Propulsion Laboratory to monitor spacecraft cabin air for anomalous events such as leaks and spills of solvents, coolants or other fluids with near-real-time analysis [2]. Voss et al. have developed non-invasive method to identify heart failure applying in electronic nose which analyzes sweat volatile gases from the skin surface [3]. Goschnick et al. used an electronic nose called KAMINA to detect levels of water pollution [4] and air quality [5]

There are many different electronic nose applications on cosmetics, food, environmental safety, health, and military. Nakamoto et al. have used an electronic nose to distinguish 5 different perfumes and 5 different fruits [6]. Borah et al. have proposed electronic noses and artificial neural networks to classify tea aromas [7]. Singh has presented an electronic nose to differentiate simple odors for varies coffee, aroma oils and perfumes [8]. Jatmiko et al. has developed an artificial odor discrimination system for recognition both fragrance and the unknown fragrance mixtures. The system has been designed by using quartz resonator sensors and various neural networks [9]. One of the most important components to the electronic nose is the software, which can recognize or classify the information coming from electronic noses.

Electronic noses are used as different machine learning classification algorithms such as artificial neural networks, *k*-nearest neighbor, fuzzy classifier, and support vector machines etc. Recently, some researchers have presented different hybrid methods for electronic nose applications. Karlik and Yuksek have proposed a novel; fuzzy clustering neural network (FCNN) algorithm as pattern classifiers for real time odor recognition system [10]. Temel and Karlik have developed a real-time odor recognition system employing a learning vector quantization as a hybrid classifier [11]. Karlik and Cemel have presented diabetes diagnosing from breathing odor [12].

In this study, 28 samples were obtained from 20 different perfumes using the OMX-GR device. All data was normalized by using min–max normalization method. To classify the perfume data, a novel hybrid method was developed as combination of support vec-

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tor machine and fuzzy c-means clustering which consist of both supervised and unsupervised learning, respectively. Performance results of proposed method are compared with the other well-known machine learning algorithms.

2. Machine learning algorithms

2.1. Artificial neural network

Artificial neural networks (ANN) are also used as a classification algorithm inspired from biological neural networks. ANN has parallel processing elements called nodes which consist of a transfer function and a local memory. Generally, multi layered perceptron (MLP) architecture which has back-propagation (BP) training algorithm is mostly used. Each node receives different input values which are multiplied by the weights. The summation function collects the multiplications and gives the result to the transfer function [13]. Transfer function can be linear or some special functions like sigmoid or tangent hyperbolic functions can be more useful than the others [14].

2.1.1. Gradient descent

Gradient descent is a first-order optimization algorithm which is used to minimize the mean square error (MSE) from the training set. In gradient descent, weights are updated in proportion to the negative of an error derivative with respect to each weight [15].

$$\Delta w_k = -\alpha_k \times g_k \tag{1}$$

Δw_k is a vector of weights changes, α_k is the learning rate, and g_k is a current gradient. If the learning rate gets too large; the weight no longer changes on gradient descent procedure. A method which has been proposed is a momentum term (p) [15]:

$$\Delta w_k = -\alpha_k \times g_k + p \times \Delta w_{k-1} \tag{2}$$

The learning rate is responsively supplied of the complicated local error surface. Gradient descent with adaptive learning rate:

$$\Delta w_k = a\frac{\Delta E_k}{\Delta w_k} \tag{3}$$

Adaptive learning rate and momentum training are combined:

$$\Delta w_k = p \times \Delta w_{k-1} + a \times p \times \frac{\Delta E_k}{\Delta w_k} \tag{4}$$

2.1.2. Resilient back propagation

Rprop algorithm is a short name of resilient back propagation which is generally much faster than gradient descent algorithm. The basic principle of RProp is to eliminate harmful influence of the size of partial derivative on the weight step [16].

$$\Delta w_k = -\text{sign}\left(\frac{\Delta E_k}{\Delta w_k}\right) \times \Delta_k \tag{5}$$

The sign of the partial derivative is considered to indicate the direction of the weight update multiplied by the step size.

2.1.3. Conjugate gradient

Conjugate gradient (CG) is an iterative technique to solve great systems of linear equations. All of the CG algorithms start out by searching in the steepest descent direction (negative of the gradient) on the first iteration [17].

$$p_0 = -g_0 \tag{6}$$

A line search is realized to determine the optimal distance to move along the current search direction.

$$\Delta w_k = \alpha_k \times p_k \tag{7}$$

Next search direction β is defined as conjugate to previous search directions.

$$p_k = -g_k + \beta_k p_{k-1} \tag{8}$$

In the literature there has been proposed several choices for defining the scalar parameter β_k which gives the rise to distinct CG methods as shown below [15].

2.1.3.1. CGF—Fletcher–Reeves. This is the ratio of the norm squared of the current gradient to the norm squared of the previous gradient

$$\beta_k = \frac{g'_k g_k}{g'_{k-1} g_{k-1}} \tag{9}$$

2.1.3.2. CGP—Polak–Ribiere. The product of the previous updating in the gradient is changed by the computing with the current gradient which divided by the square of the previous gradient.

$$\beta_k = \frac{\Delta g'_{k-1} g_k}{g'_{k-1} g_{k-1}} \tag{10}$$

2.1.3.3. CGB—Beale–Powell. The search direction reset the negative of the gradient when this condition is satisfied.

$$|g'_{k-1} g_k| \geq 0.2\|g_k\|^2 \tag{11}$$

CG algorithms considered a line search at iteration. This scaled conjugate gradient algorithm (SCG) has proposed by Moller [18]. SCG kept away from wasting much time on line search. This proposed method is combined with model-trust region of the conjugate gradient approach [18]. Even if this algorithm is established on conjugate directions, it does not perform a line search for iteration.

2.1.4. BFGS quasi-Newton

The Broyden–Fletcher–Goldfarb–Shanno (BFGS) method is defined as $\Delta w_k = -H'_k \times g_k$ where; H is the Hessian matrix of second derivatives. Due to the Hessian matrix, quasi-Newton methods are sometimes more efficient than Newton methods. An approximation of Hessian matrix is updated in every iteration [15,16].

2.1.5. Bayesian regulation

Bayesian regulation (BR) is a network training function that updates the weight and bias values considering the Levenberg–Marquardt optimization. It minimizes a grouping of MSE and weights. Also Bayesian regularization produces a network for generalization [16]. This method is described in MacKay, *Neural Computation* [19].

2.1.6. Levenberg Marquardt

Levenberg Marquardt (LM) method is a hybrid algorithm which is based on both Newton's method and gradient descent. Hybrid method is created by using a damping factor to interpolate between methods. The algorithm obtains the network weight based on the global optimization idea of Newton's method [15,17].

$$\Delta w_k = -H'_k \times g_k \tag{12}$$

$$H' = J'J \tag{13}$$

$$g = J'e \tag{14}$$

"J" is the Jacobian matrix and "e" is a vector of network errors. The Jacobian matrix can be computed through a standard back propagation technique that is much less complex than computing the Hessian matrix [20].

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2.1.7. One step secant

The BFGS algorithm requires more storage and computational time in each learning cycle (or iteration) than the conjugate gradient algorithms. The one step secant (OSS) algorithm is an effort to bridge the gap between CG algorithms and the quasi-Newton (secant) algorithms. Because the OSS does not store the complete Hessian matrix, it requires less storage and calculation per epoch than the BFGS algorithm. The one step secant algorithm is described by Battiti [21].

2.1.8. Random weight/bias rule

For each training cycle, all training vectors are represented in random order, with the neural network, weight and bias values changing in respect of each individual presentation [16].

2.2. Support vector machines

Support vector machines (SVMs) are supervised learning and classifying method to find the best hyper-plane that bisects a space in which both known positive and negative instances [22,23]. For the problems which have two classes and are linearly separable,

$$D = \left\{(x_i, y_i) | x_i \in R^N, y_i \in \left\{-1, 1\right\}\right\}_{i=1}^{n} \quad (15)$$

where, D shows the study set, $x_i \in R^N \quad i = 1, 2, ..N$ and x, an N-dimensional space and $y_i \in \left\{-1, 1\right\}$, the class tags. For n $\{x_i, y_i\}$ belonging to optimum hyperplane are [24]:

$$w \times x_i + b \geq +1 \quad \forall \quad y = +1 \quad (16)$$

$$w \times x_i + b \leq +1 \quad \forall \quad y = -1 \quad (17)$$

If $w \in R^N$veb $\in R$ strangles, the study set can be separated linearly. "w" shows the weighing vectors and "b" shows the bias values. (w, b) couple can define many hyper planes [25]. The purpose is to determine which hyperplane is farther in both of the classes. The vectors that are very close to this plane are called the support vectors. Extensive information can be found in Vapnik's works for hyperplane calculations [22].

$$\min \left[\frac{1}{2}\|w\|^2\right], \quad y_i (w \times x_i + b) - 1 \geq 0 \quad (18)$$

It is known that in real world problems, data is mixed and not linearly separable. Parameter C is used as defined by the user to make the limit in maximum and the false classifications minimum. Then the optimization problem becomes:

$$\min \left[\frac{\|w\|^2}{2} + C \times \sum_{i=1}^{r} \xi_i\right] \quad (19)$$

where $y_i (w \times \varphi(x_i) + b) - 1 \geq 1 - \xi_i$ $(\xi_i \geq 0, i = 1...N)$, and $< C < \infty$.

To solve this optimization problem, the linearly inseparable data is taken to a space with a higher dimension called property space. As seen in Eq. (20), it is possible to separate it linearly in a higher dimension by using a kernel function;

$$K\left(x_i, x_j\right) = \varphi(x_i) \times \varphi\left(x_j\right) \quad (20)$$

$$f(x) = \text{sign}\left(\sum_i \alpha_i y_i \varphi(x) \times \varphi(x_i) + b\right) \quad (21)$$

The most used kernel functions are Gaussian radial basis function, such as "d" degree polynomial etc. SVM's are planned for dual classification. "K" numbers of classifiers are trained in all of the training samples. Researchers have suggested some ways to combine various dual classifiers to make multiple classifications [26].

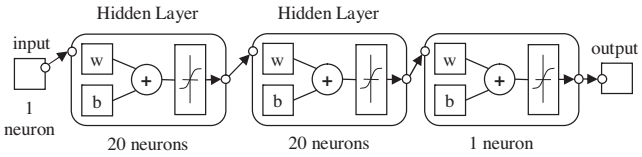

Fig. 1. Structure of the network.

2.3. Fuzzy c-means

Fuzzy c-means (FCM) algorithms are the most well-known and widely used fuzzy separation clustering techniques. FCM algorithms form a basis for clustering techniques which dependent on objective functions. In accordance with fuzzy logic, each data can have a membership value between [0,1], and can belong to two or more clusters. A data which belongs to the clusters is the sum of the degrees of membership is 1. Each cluster is described by its center. The distance between a cluster and a point is measured by a Euclid distance [27].

$$J_m(U, v) = \sum_{k=1}^{N} \sum_{i=1}^{c} (u_{ik})^m \|y_k - v_i\|_A^2 \quad (22)$$

where, $Y = \left\{y1, ..yn\right\} \subset R^n$ shows the data, C *is* the cluster number, v_i center of i'th cluster, $U_{ik}{}^m$ the y_k's value in cluster k, and $J(u,v)$ shows a measure for all the weighted error squares. $J(u,v)$ is minimized for each value of c. Fuzzy c-means algorithm's center vectors is calculated.

$$v_i = \frac{\sum_{k=1}^{N} (u_{ik})^m y_k}{\sum_{k=1}^{N} (u_{ik})^m}; \quad 1 \leq i \leq c \quad (23)$$

After fuzzy c-means algorithm steps are carried out, membership degrees decide which individual belongs to which cluster. Each point joins to each cluster with a certain membership degree, but the cluster which gets the highest membership degree constitutes the actual cluster of that point.

3. Perfume recognition by using different machine learning algorithms

3.1. Perfume recognition by using artificial neural network

As known, it is the general problem to use only one input node of input layer ANN architecture for classification. So it needs the second hidden layer. As it can be seen in Fig. 1, it uses MLP structure is as $1 \times 20 \times 20 \times 1$ which means only one number of neuron for input and output layer and 20 numbers of neurons for both two hidden layers, is trained for BP algorithm by using 14 different training (or activation) functions which are quasi Newton, Bayesian regulation, conjugate gradient with Beale–Powell restarts, conjugate gradient back propagation with Fletcher–Reeves restarts, conjugate gradient with polak–ribiere restarts, gradient descent, gradient descent with momentum, gradient descent with adaptive learning rate, gradient descent with momentum& adaptive LR, Levenberg Marquardt, one step secant, random weight/bias rule, Rprop, and scaled conjugate gradient. Measured data is applied as input of MLP. The output of MLP shows the labels of 20 different perfumes as [type1, type2, type20].

MSE Bayesian regulation and Levenberg Marquardt training functions have shown better performance than the others. Table 1 shows highly successful BP models.

Fig. 2 shows that performance accuracy for each training models. If T is the Target output, O is the output of ANN, all graphs shows that the error (O–T) for training models.

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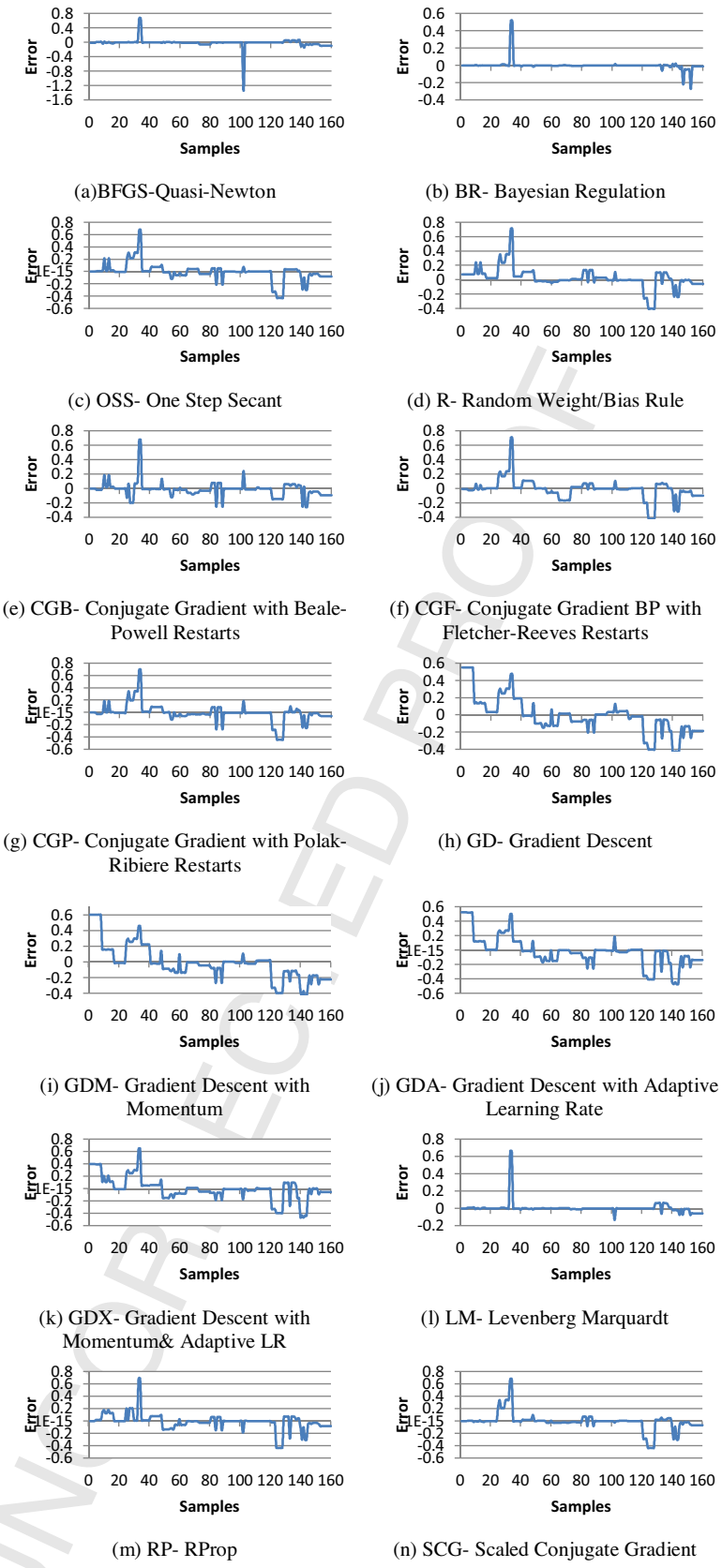

Fig. 2. Error (*O*–*T*) graphs of ANN training functions.

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Table 1
Accuracy results of ANN classifiers.

Data set used (the normalized data for perfumes)	Total number of samples	Number of training sample	Number of test sample	Number of samples classified correctly	ANN classification rate
BR—Bayesian regulation	560	400	160	140	87.5%
LM—Levenberg Marquardt	560	400	160	127	79.375%
BFGS—quasi-Newton	560	400	160	96	60%
CGB—conjugate gradient with Beale–Powell restarts	560	400	160	51	31.875%

Table 2
SVM classification accuracy.

Data set used	Total number of samples	Number of training sample	Number of test sample	Number of samples classified correctly	SVM classification rate	Best *C*
The normalized data for perfumes	560	400	160	133	83.125%	256

Table 3
Classification rates of cascade combination.

Number of cluster centers	Total number of samples	Number of training sample	Number of test sample	Number of samples classified correctly	SVM classification rate	SVM best *C*
14 cluster centers x 20 perfumes	280	200	$4 \times 20 = 80$	57	71.25%	128
10 cluster centers x 20 perfumes	200	140	$3 \times 20 = 60$	39	65%	256
6 cluster centers x 20 perfumes	120	80	$2 \times 20 = 40$	24	60%	256
4 cluster centers x 20 perfumes	80	60	$1 \times 20 = 20$	11	55%	256
2 cluster centers x 20 perfumes	40	20	$1 \times 20 = 20$	11	55%	32

Table 4
Perfume data and cluster centers with their classification rates.

Data Set Used (the normalized data for perfumes + cluster centers obtained from FCM)	Total number of samples	Number of training sample	Number of test sample	Number of samples classified correctly	SVM classification rate	SVM best *C*
Perfume data + 6 set centers	560	400	160	140	87.5%	256
Perfume data + 4 set centers	560	400	160	149	93.125%	256
Perfume data + 2 set centers	560	400	160	156	97.5%	256

3.2. Perfume recognition by using support vector machines

Support vector machines (SVM) is to solve a problem of multi-label and multi-class supervised classification. In this study, the classifications by the support vector machines are done by svmtrain tool in Matlab. 28 measured data is used for 20 different perfumes. Out of the 560 measurement, 400 of them are used for training and 160 are used for test data. Since there are 20 different perfumes, our problem would be 20 different classes. The method we used here is the 1 versus remaining method with kernel type radial basis function. Fig. 3 shows the block diagram of SVM for used perfume recognition system. Table 2 shows accuracy of SVM classification. In this structure, the classification accuracy of test data for 20 different set of perfume was found as 83.125% after given different *C* values from −5 to 8. The best *C* value was found as 256.

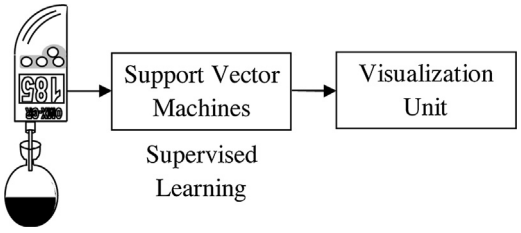

Fig. 3. The block diagram of perfume recognition by SVM.

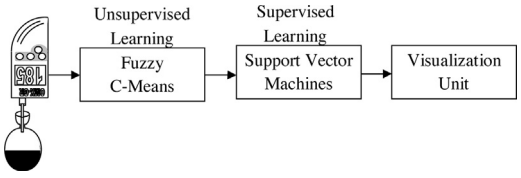

Fig. 4. A block scheme of cluster center based classification.

3.3. Perfume recognition by using cascade combination of fuzzy c-means and support vector machines

A fuzzy clustering based method is proposed for measured data by odor sensors using type-1. Fuzzy c-means (FCM) is an unsupervised learning algorithm to classify different type of perfumes used for input to the SVM classifier (see Fig. 4). This method consists of cascade combination of fuzzy c-mean (FCM) and support vector machines (SVM). Firstly, Matlab's FCM toolset is used for fuzzy clustering to obtain each perfume class as 2, 4, 6, 10 and 14 cluster centers. This way, each cluster center obtained from each class which provides a new attribute for describing the perfume odor. In this proposed method, a new approach is the number of instance in training set which reduced by FCM clustering algorithm and process of reducing was performed on each perfume type separately. As it is seen in Fig. 4, the classification is experimented only on cluster centers, obtained as a result of fuzzy clustering were used in training set of support vector machines. The results can be seen in Table 3.

3.4. Perfume recognition by using FCM based SVM model

In this method, unsupervised fuzzy c-means (FCM) and supervised support vector machines (SVM) has developed as new model that consists parallel combination. Fig. 5 describes block diagram of this hybrid model. Clustering is performed separately for each

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Table 5
Comparison of classification methods.

No.	The methods used	Data set used	Success of the best classification	Error rate
1	Support vector machine	The normalized data for perfumes	83.125%	0.169
2	Cascade binding methods fuzzy c-means and support vector machine	Only cluster centers obtained as a result of fuzzy clustering	71.25%	0.288
3	Hybrid model	The two dimensional data set consisting of normalized data and set centers obtained from FCM	97.5%	0.025
4	The best ANN, Bayesian regulation	The normalized data for perfumes	87.5%	0.125

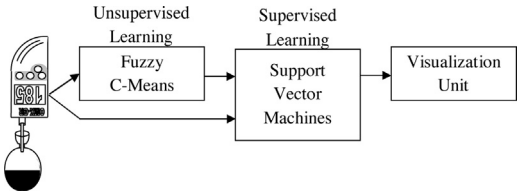

Fig. 5. A block scheme for the hybrid model.

perfume class. For each perfume, 2, 4 and 6 cluster centers are obtained. In this way FCM clustering is used to select instances represented as well features of perfume class for each perfume in original training set. Previous step, original perfume data and the cluster centers obtained from FCM are used for training to support vector machines.

The cluster centers are obtained from a data set which creates a new attribute for data. The two dimensional data set, consisting in perfume odor data and obtained cluster centers drastically increases the SVM's success rates, as seen in Table 4.

4. Results and discussion

In this study, the hybrid system developed using SVM and FCM and proposed to increase the classification success of perfume odor data. The perfume measurement results are formed by single dimensional data. In other words, it is hard to use a single attribute for training by using only the support vector machines. In the proposed model, the clustering results were added as a new attribute of inputs. In this model, first the measurement results are calculated for the cluster centers. Secondly, set centers provide a second attribute for classification. This hybrid system is trained by measurement results and set centers. SVM's success rate was only 83.125%, but with a hybrid structure, the success rate increased to 97.5% as seen in Table 5. This shows that the classification rate is higher than before. According to comparison of all results of used BP with different training functions, proposed hybrid model has shown a better accuracy than the other models.

5. Conclusion

Accuracy of classifier refers to the ability of performance of classifier method. It is estimated the class label correctly and the accuracy of the forecaster refers to how well a given forecaster can estimate the value of predicted attribute for unseen data. For this reason, classifier is requested high accuracy. This paper has presented a novel hybrid classifier model named FCM based on SVM for classification of perfume data. This new model has a positive effect on the accuracy rate of machine learning techniques which is very important for situations in the data mining to reveal accurate information. All used classification algorithms were given acceptable results, but the comparison results of all these algorithms show that proposed hybrid algorithm is better than other algorithms according to the highest accuracy which was found as 97.5%.

For future studies, this proposed hybrid method is useful and can be easily extended for classification of any number of odors. It can be also used to solve various classification problems.

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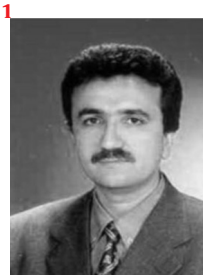

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