CHEMICAL RING HANDWRITTEN RECOGNITION BASED ON NEURAL NETWORKS

Nabil Hewahi*, Mohamed N. Nounou, Mohamed S. Nassar, Mohamed I. Abu-Hamad, Husam I. Abu-Hamad
Computer Science Department,
Islamic University of Gaza (IUG), Palestine
nhewahi@iugaza.edu *

ABSTRACT
This paper is focused on pattern recognition for Heterocyclic chemical handwritten recognition using Neural Networks. The idea is to develop a software to make the recognition simple with a very high accuracy. The development stage is based on two phases. In the first phase, a neural network is used as a classifier to classify to which class the chemical rings can be classified, where four classes are defined (S, N, O and others). In the second phase, a neural network to recognize the type and name of the chemical rings within the classified class in the first phase is performed. A comparative study has been done to distinguish the results of various used approaches.

Keywords: neural networks, chemical rings, pattern recognition **.**

1 INTRODUCTION

Pattern is an object, process or event that can be given a name. Watanabe [13] defines a pattern as opposite of a chaos; it is an entity, vaguely defined, that could be given a name. Pattern could be a fingerprint image, a handwritten cursive word, chemical rings, DNA sequence, UPC Bar Code, a human face, or a speech signal.

Etymologically, the act of thinking again involves “identifying” or “acknowledging”, so we can say that Pattern Recognition is “the study of how machines can observe the environment, learn to distinguish and identify patterns of interest, and make a reasonable decision about the categories of the patterns”. Where, the patterns which is sharing common attributes and usually originating from the same source, categorized to specific category defined by the system designer (in supervised classification) or are learned based on the similarity of patterns (in unsupervised classification).

Pattern recognition has been an active subject of research since the early days of computers. It has been developed significantly in the 1960s as a field of science and it kept developing through the rapid growth of the computation power and techniques. In 1970s nevertheless, in it is early development, pattern recognition had a lot of works [11].

The four best known approaches for pattern recognition are 1- Template Matching 2-Syntactic (Structural) Approach. 3- Statistical Approach. 4- Neural Networks. These models are not necessarily independent and sometimes the same pattern recognition method exists with different interpretations [1-5][9-11][13]. In many of the emerging applications, it is clear that no single approach for classification is the optimal and that multiple methods and approaches have to be used. By merging several models together in one system, the system called hybrid system.

1.1 PATTERN RECOGNITION SYSTEMS

The design of a pattern recognition system essentially involves the following three aspects:

1) Data acquisition and preprocessing.
2) Data representation.
3) Decision making.

These three aspects contain a complex processes as shown in Fig. 1. The real challenging facing the designer of any Pattern Recognition system is to the choice the correct sensors, preprocessing techniques, well extraction of features and representation schema and decision making model.

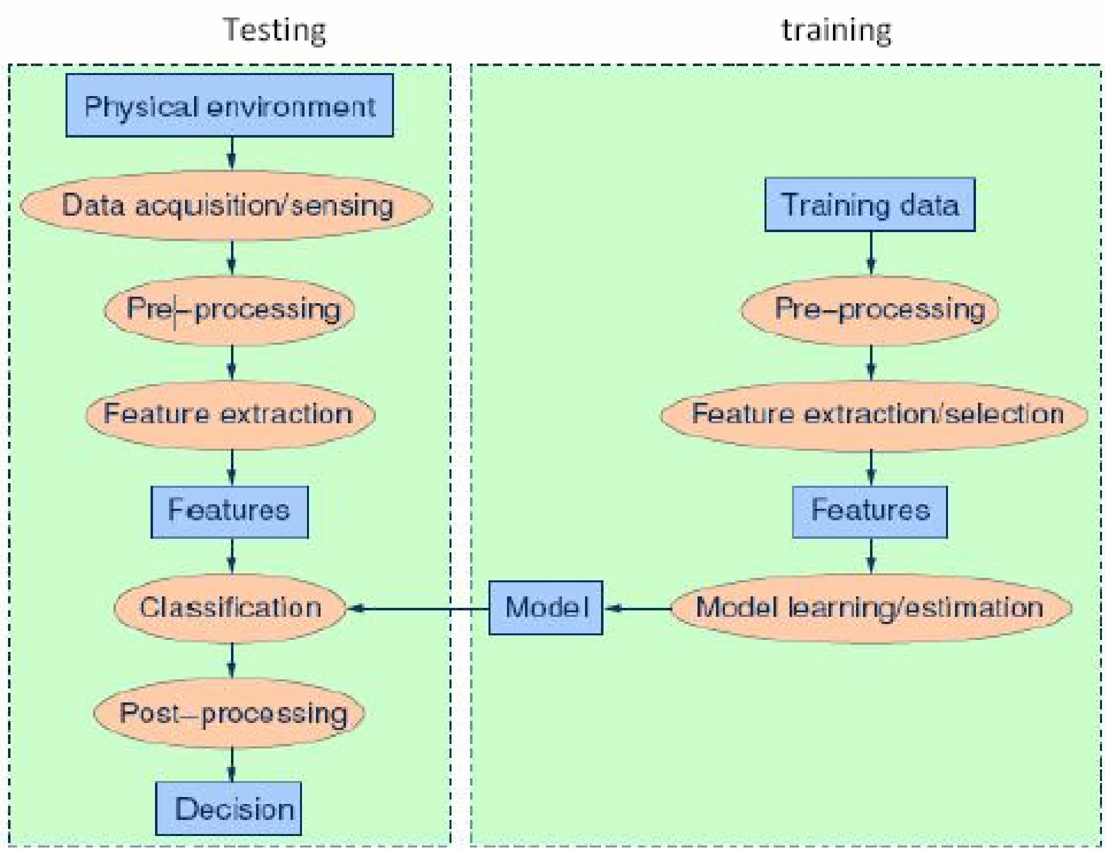

Figure 1: Pattern Recognition System General Components

1.2 THE RESEARCH GOAL & THE USED METHODOLOGY

The goal of our project is to develop a software that can recognize the chemical rings with high performance and accuracy. The chemical rings included in our study is called heterocyclic rings which is considered one of the chemical ring groups. It consists of 23 rings as shown in Fig. 2. As far as we know and based on our survey, chemical rings recognition weren't performed before. Other chemical recognition applications are already exist [6] [7] [8] [12].Most chemical rings papers talk about the 3D rotating, drawing rings or combination rings together when putting the equation. In [8], Johann Gasteiger talks about how long it took of him with his staff to build a database of chemical rings figures and names, and to translate the chemical reactions to electronic to generate the structure of the reactions, and they proposed a plan in the application as a Data Flow Diagram (DFD) to follow it. In [6] an analysis to the properties of the rings and creation of a virtual library of Aromatic rings by calculations to put it in N.N. to identify very well the areas of property space typical for active or inactive rings have been presented.

The difficulty of recognition here is due to the close similarity of the shapes (rings). In our recognition process, we shall use neural networks approach as we shall see in the next sections. There are five main reasons why we choose chemical rings for our study:

a) Chemical rings handwriting recognition has not been done before (or few research has been done on that) and it is very useful for the chemical departments in the universities.
b) Most of the projects concerned with chemistry are not in the pattern recognition or handwriting recognition, but in other applications.
c) The project helps the chemists and the students to know the patterns easily.
d) Web engine search -which almost the search engines recognize letters, words, and statements, but if you want to search by images you have to enter a name of that image to see it, and the engines, search only in the name of those pictures or images, not on the contents of the images, But if you have an image that you don't know any information about it, you can't search. But by this project you can put your image and you can find any information about it.(backward process).
e) The common use of these projects, in new versions of mobile (I-mate) that you write by your pen on the screen and the software will recognize your writing.

In this paper, neural network has been chosen to be the recognition approach. Based on the previous studies on various applications, neural network showed very high performance in recognition of characters in general, moreover, conceiving the features by the neural network is an easier task compared to other methods. The main characteristics of neural networks are that they have the ability to learn complex nonlinear input-output relationships, use sequential training procedures, and adapt themselves to the data.

One use of a neural network is classification. For this purpose each input pattern is forced, adaptively, to output the pattern indicators that are part of the training data; the training set consists of the input covariate x and the corresponding class labels.

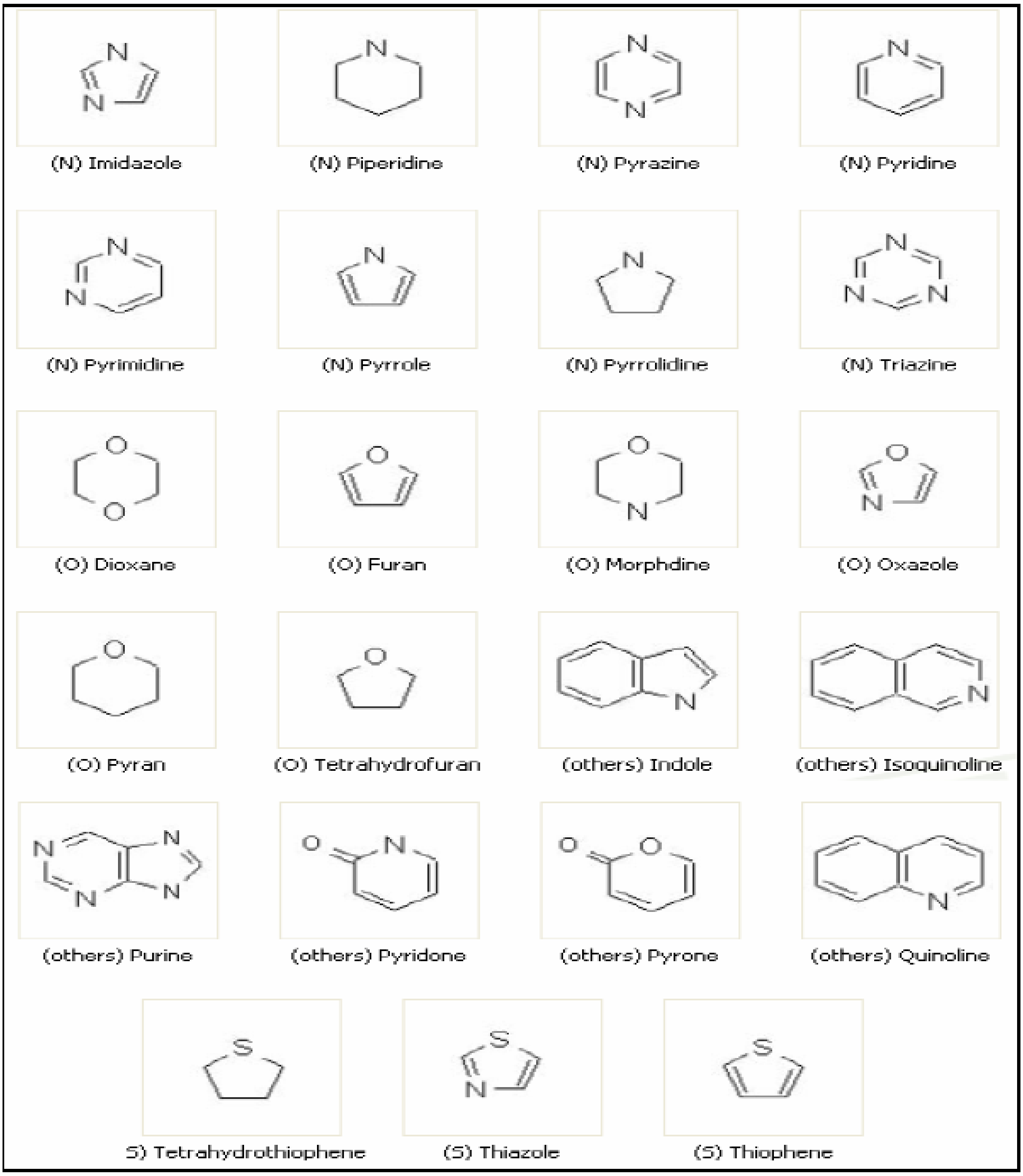

Figure 2: The heterocyclic chemical rings that are included in our handwritten recognition process (along with their categorized class as we shall explain later).

2. THE PROPOSED APROACHED

Before going straight forward to the technique used to solve our problem, we tried the ordinary method of recognition using the neural network. The inputs is 1600 units (pixel values 0 or 1 and the grid used 40X40) , hidden layer 1600 (many other numbers less or more have been tried) and 23 outputs represent the 23 chemical rings to be recognized. This method is usually used for recognitions of English Alphabetic and Arabic numerals and shows very high performance reaches about 95%. The network structure that represent the case is shown in Fig. 3. The results were very poor in terms of training and recognition. The system performance was only 7%.

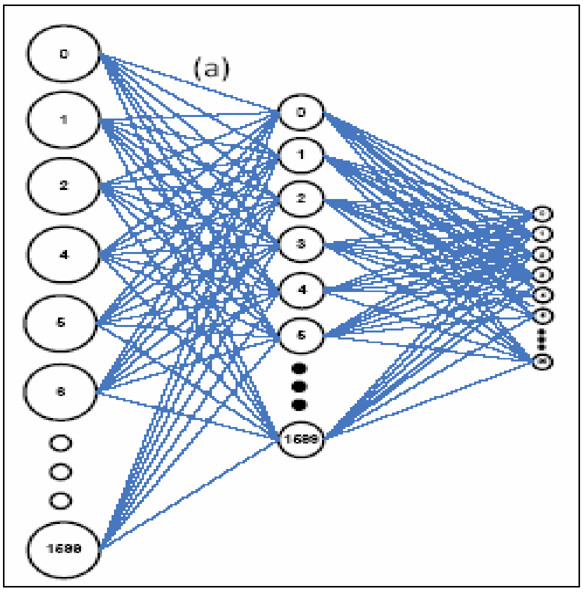

Figure 3: The representation of the chemical ring recognition neural network using the ordinary method.

Another experiment which is based on the number of black pixels at each row and the number of black pixels at each column has been tries. The number of inputs for the neural network is based on the formula Nc + Nr, where Nc is the number of columns in the grid and Nc is the number of columns in the grid. Each input node corresponds to a row represents the number of black pixels at that row. Similarly, each input node corresponds to a column represents the number of black pixels at that column. This method reduces dramatically the number of inputs. Again this method gave a worse result than the first one. The system performance didn't exceed 1%.

A third experiment is used to improve the performance. This method is based on drawing a horizontal midline cutting the image from point (0,20) to (40,20) (look at Fig. 4), so we can calculate the number of lines that the midline crossed, and use these calculations in classification , but the idea failed . The idea failed because, the number of lines cuts by the midline may differ from writer to another. (Look at Fig. 5) writer A at left, and writer B at right) the number of lines that the midline cut by writer A (4) but the number of lines that the midline cut by writer B (5).

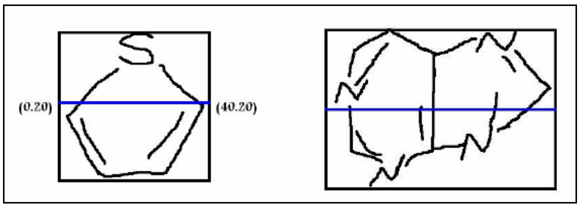

Figure 4: A midline cut at (0,20) and (40,20)

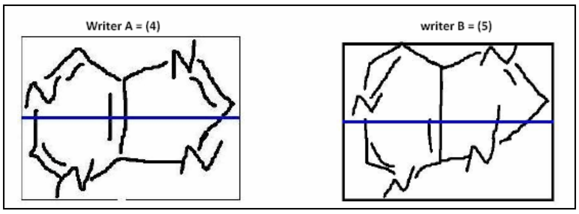

Figure 5: The position of cut line may give a different result for the same shape.

2.1. THE CLASSIFIER-RECOGNIZER APPROACH

The main idea of this approach is to use two phases, the first phase is a classifier while the second phase is a recognizer. Fig. 6 represents the general structure of the proposed solution. We used three variations for the same concepts which we shall discuss in the following subsections with comparative study among their results.

2.1.1 Whole Image Recognizer

This approach is to use the character above the rings. This would help us to classify the rings into four classes "class O, class N, class S and class Others ". The method says that there are two phases the image must pass through. The first one includes one neural network that does the classification process (we call it classifier neural network); it classifies the image to one out of the four classes, and then sends it to the second phase. This neural network doesn't take the whole image, but just takes the horizontal upper part of the image (40 X 15) pixel (see Fig. 7), and by this we can use the features of the shapes, this neural network will just determine the image for any class.

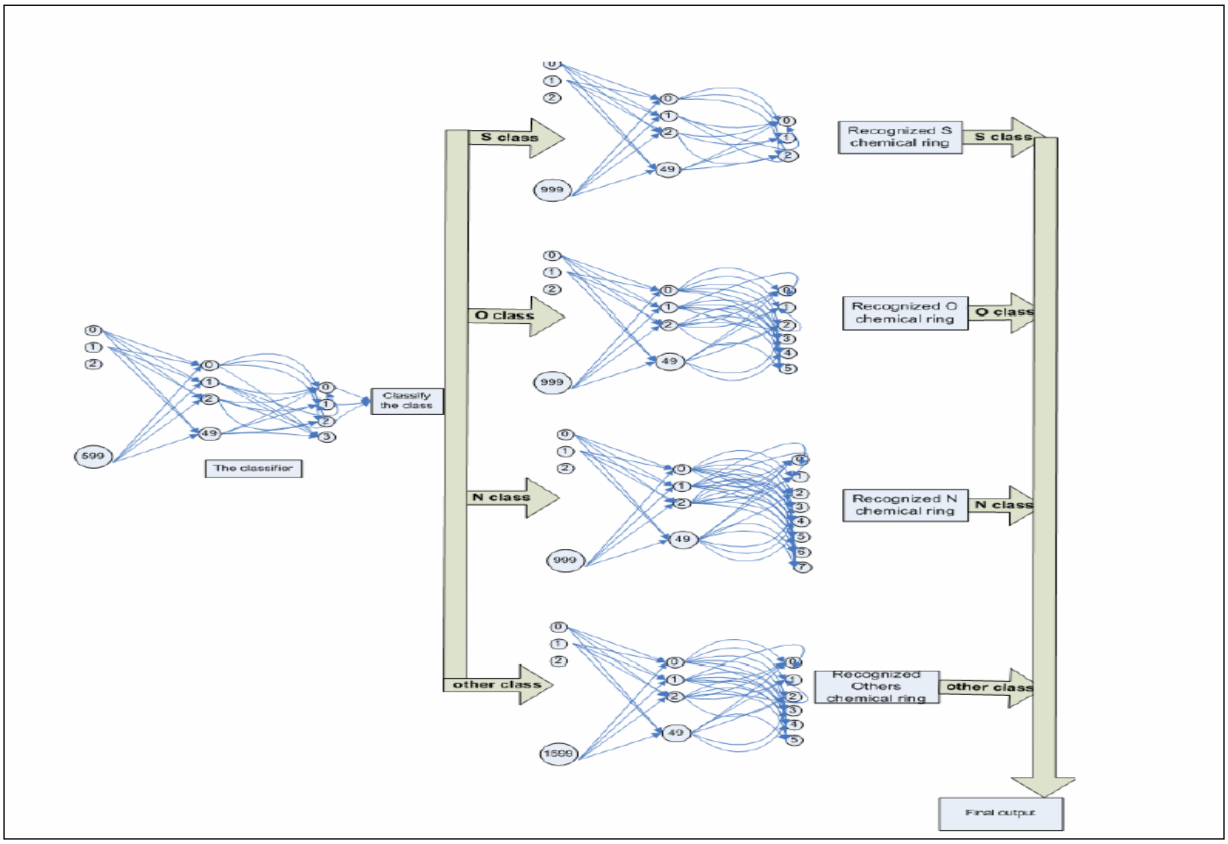

Figure 6: The general proposed structured which is composed of two phases, the classifier phase and recognition phase.

The second phase consists of four Neural Networks (we call each neural network as recognizer), every one represents one class. The input of the recognizer is the whole ring based on the class obtained in the classifier Neural Network.

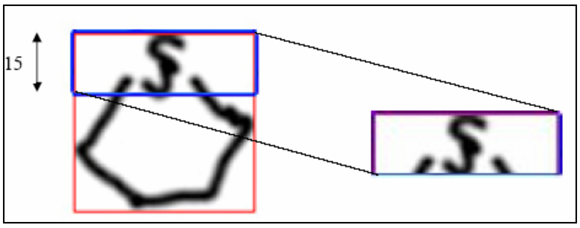

Figure 7: The upper part of the image is taken in the classifier phase.

2.2 WHOLE IMAGE RECOGNIZER WITH HALF SIZE GRID.

Following the whole image recognizer approach and to decrease the number of inputs in the neural network, odd rows of the inputs are only considered, which means instead of using 1600 pixels as inputs, we use 800 pixels (20 x 40). This surely will decrease the computation time. Fig. 8 shows a shape after and before resizing. In the recognition face, the whole ring is entered as input to its class neural network.

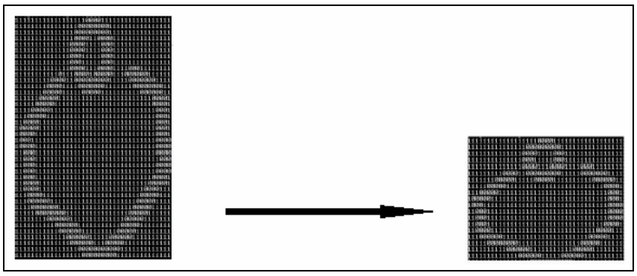

Figure 8: Only odd number of rows were used to improve the cost of time.

2.3 LOWER PART IMAGE RECOGNIZER WITH HALF SIZE GRID.

Following the same approach used in the whole image recognizer with half size grid and to increase the performance of the system as we shall see in the results section, instead of using the whole ring in the recognition phase, the lower part of the image is only considered as inputs for the “S, O and N” recognizers. The “others” class will still have the whole ring as inputs. This is done due to close similarities of the rings in the same class. Fig. 9 shows the strategy used in the Lower part image recognizer with half size grid.

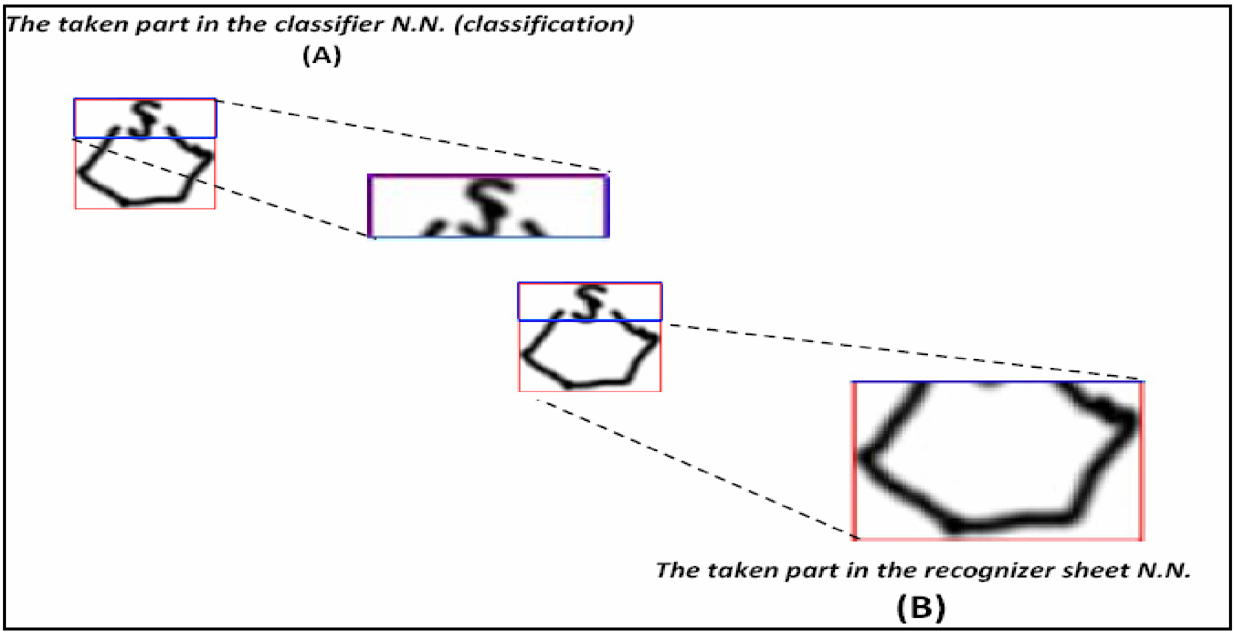

Figure 9: A. shows the part taken for classification phase. B. Shows the part taken for recognition phase.

2.2 THE RECOGNITION CYCLE.

The recognition of any chemical ring will include the following steps:

1. Convert the image to monochrome : In this step the image is converted to monochrome bitmap.
2. Grid/Image scaling: In this step the drawing grid should be converted to 40x40. This means if the user draws in a grid of 60x50 (the used portion for drawing could be 50X40) , 50x 30 or 30x20, all must be converted to 40x40 grid.
3. Bound the Shape/Ring: All the shapes have to be of one size after scaling the grid to 40X40. In this stage the image (shape/ring) itself is scaled to be of 40x40. This means all the images will be 40X40.
4. Enter the bit pattern matrix to the classifier neural network (the upper part only after making the upper cut line cross) and find to which class does the entered ring belong.
5. Based on the class obtained in step 4, enter the lower part of the ring to the corresponding recognizer neural network in case of “N, S or O classes, and the whole ring in case of “others” class.

It is to be noticed that during training, for every neural network either classifier or recognizer, the training will be independent. This means each neural network is trained separately from others.

3. THE PRODUCED SOFTWARE

The produced software is called chemical pattern recognition. It is very simple to use with a user friendly interface. The user can train the system if he wishes to do so or can upload the trained neural nets using the software attached XML files. After training or uploading the databases, the user can enter the ring to be recognized through a node pad, scanner or Photoshop software. Fig.10 shows the main interface.

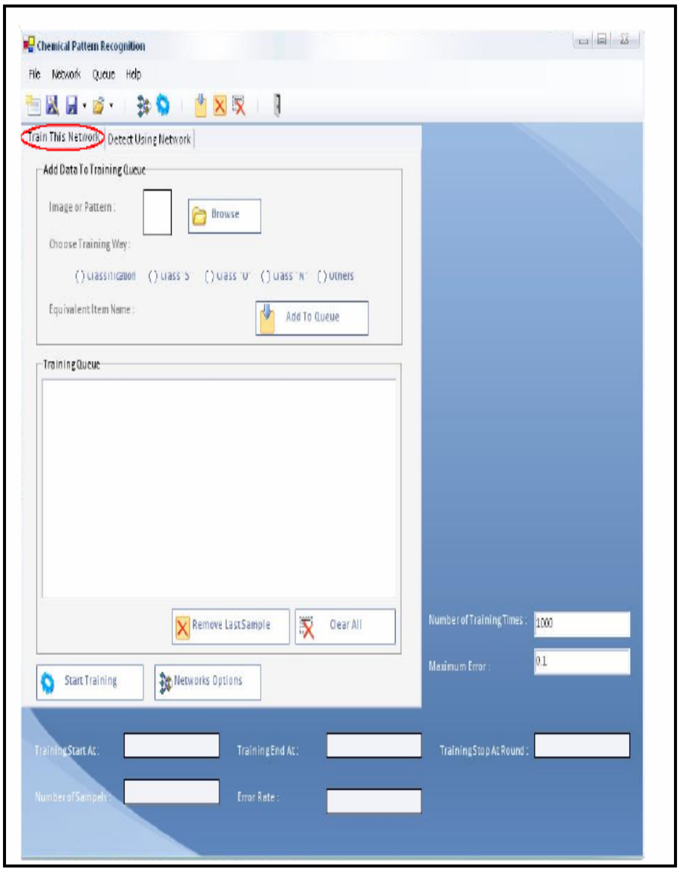

Figure 10: The main interface of the chemical ring recognition software.

It is to be noticed that the user can stop the training through the number of epochs or based on a certain error ratio. Fig. 11 shows a training step for a set of chemical rings retrieved from a queue.

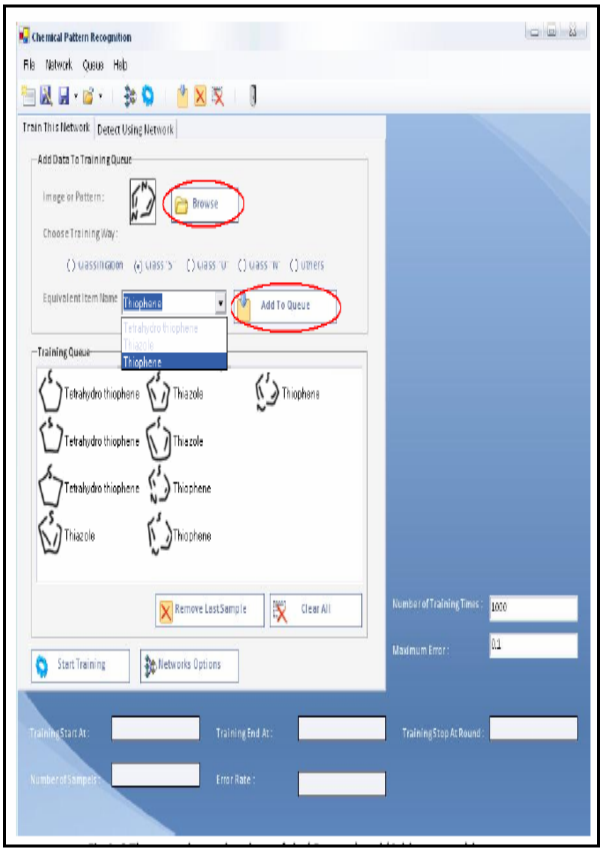

Figure 11: a training step for a set of chemical rings retrieved from a queue.

4. RESULTS

In this section, we shall present, discuss and compare the results obtained using all the three proposed variations of The Classifier-Recognizer Approach. Table 1 shows the index name of the methods used and the corresponding method names. The index names will be used instead of the names of the methods in all the remaining tables. Table 2 contains the results of the training samples for the three methods.

Table 1: The used methods with their corresponding index names.

Index Name	**Method Name**
First	whole image recognizer
Second	whole image recognizer with half size grid
Third	lower Part image recognizer with half Size grid.

Table 2: The results of the training samples applied on the three methods.

Training information					Testing information	
Method Index	N. samples	N. iteration	Hidden layer	Training time (Hour)	Error (%)	Performance (%)
First	1500	1000	50	~53	13.0 %	87.0%
Second	1500	1000	50	~41	9.0%	91.0%
Third	1500	1000	50	~35	6.0%	94.0%

The number of training samples is 1500 distributed as 300 for S class, 400 for N class, 400 for O class and 400 for others class. It is to noticed that the best performance during the training is the lower part image recognizer with half Size grid, with error of 6.0%. Moreover, the training time is still best for the same method. This is due to the less number of inputs comparing to the first and second methods (only half size shape and lower part inputs for recognizers). The training performance results are for all over the system performance regardless of the ring type. Fig. 12 shows the performance for "S" class recognizer during the training. Fig. 13 shows the performance for "N" class recognizer during the training phase. Fig. 14 shows the performance for "O" class recognizer during the training phase where Fig. 15 shows the performance for "others" class recognizer during the training phase.

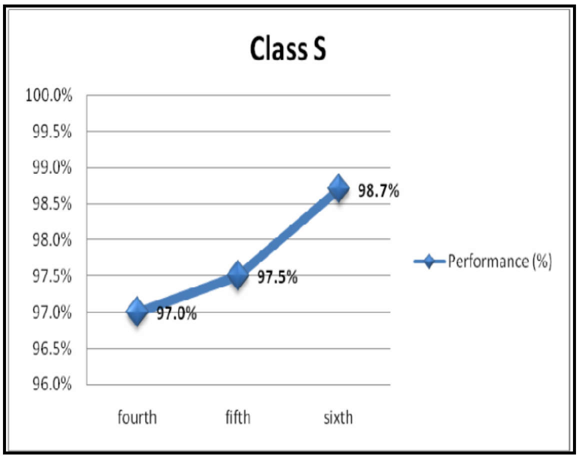

Figure 12: The recognizer performance for "S" class

rings during training.

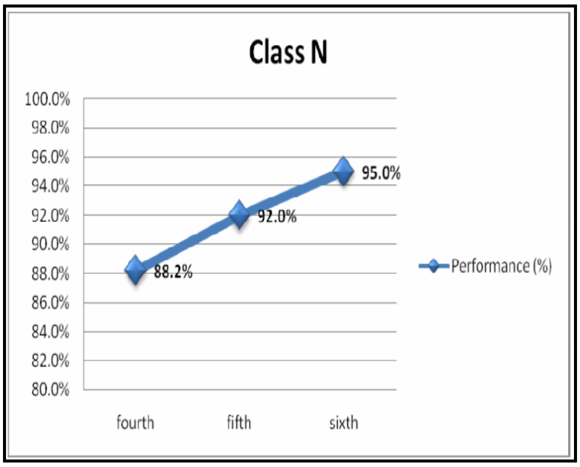

Figure 13: The recognizer performance for "N" class rings during training.

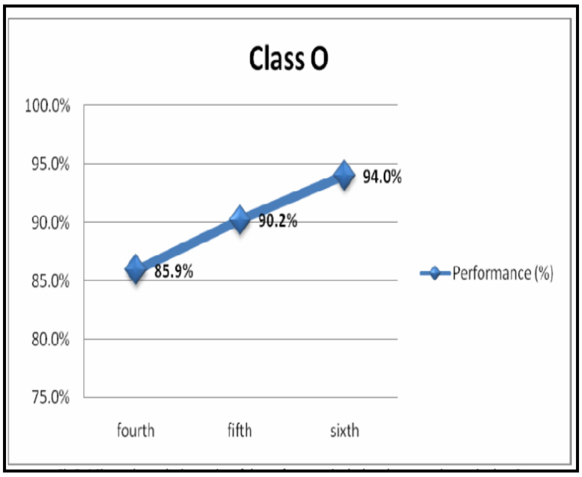

Figure 14: The recognizer performance for "O" class rings during training.

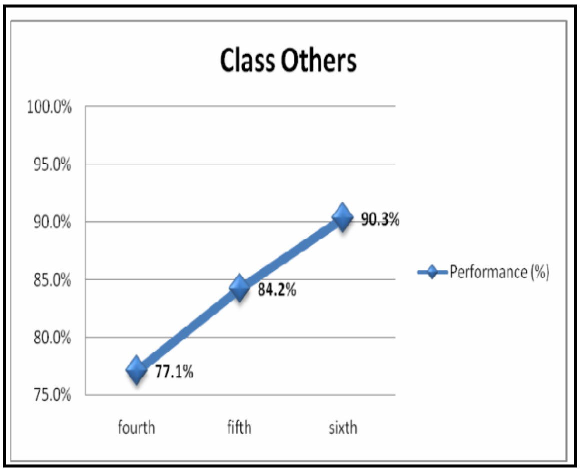

Figure 15: The recognizer performance for "others" class rings during training.

It is to be noticed that the third method is better than the other two methods in all the ring recognizers. It is also to be noticed that the performance of the three methods for the recognition of class "others" is less than their performance with other ring recognizers. This is due to the complexity and similarity of the rings involved in the "others" class.

Table 3 shows the results of the testing performance for the classifier phase for the lower Part image recognizer with half Size grid . The number of tested samples is 1150.

Table 3: This table shows the performance of classifier phase during testing.

Classifier				
The name of class	N. samples	True samples	Performance (%)	Error (%)
Class "S"	150	150	100.00%	0.00%
Class "O"	300	296	98.67%	1.33%
Class "N"	400	391	97.75%	2.25%
Class "Others"	300	293	97.67%	2.33%

It is clear that the classifier phase has a very high performance for all the rings. The "S" class has no error, while other classes has marginal errors. It is to noticed that the training of the classifier phase is separated from the recognizer phase. Table 4 shows the performance of the same testing samples for the recognition phase.

Table 4: This table shows the performance of the recognizers during the testing phase.

Recognition				
The name of class	Testing samples	True samples	Performance (%)	Error (%)
Class "S"	150	147	98.00%	2.00 %
Class "O"	300	289	96.33%	3.67 %
Class "N"	400	386	96.50%	3.50 %
Class "Others"	300	279	93.00%	7.00 %

It is to be observed that the results of training is still similar to the results obtained for testing. The third method still has the best performance, but it is important to notice that the third method for testing the class "others" has a better performance than the training where during the training the performance is 90.3% and the performance during testing is 93.0%. This could be due to the less number of tested samples than that of the training samples, and the nature of the tested samples in terms of handwritten. The performance results of the tested samples for “O” class and “N” class are almost close to the performance results obtained for training. The overall system performance is 94.0% which has been taken from various runs for testing the system .

5 CONCLUSIONS

In this research we have designed and developed a method to recognize handwritten heterocyclic chemical rings using Neural Networks. Several experiments and adjustments have been performed until a method which we call “Lower Part Image Recognizer with Half Size Grid” has been adopted. The used approach is based on two phases, classification phase and recognition phase. In the classification phase, a Neural Network to classify the chemical ring based on its upper portion is used. Four classes are specified, S, N, O and Others. In the second phase, for each class, a Neural Network to recognize the chemical ring is used. In the recognition phase, the lower part of the ring is considered for recognition. Moreover, the size of the ring is made as half size of the original size. This will make the computation time much less due to the smaller number of inputs to the neural networks. The performance of the used approach was very high where it reached to about 94%. The performance results was compared with other two methods (two variations) results. These two methods are “Whole Image Recognizer” and “Whole Image Recognizer with Half Size Grid”. The performance results was significant in favor of “Lower Part Image Recognizer with Half Size Grid”. The future work is applying our approach/other approaches to capture all the chemical rings. Moreover, checking the possibility of our approach to other handwritten recognition problems.

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