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# Infrared Spectra of Liquid Crystal Mixtures and Analysis by Gaussian Radial Basis Functions Techniques

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# INFRARED SPECTRA OF LIQUID CRYSTAL MIXTURES AND ANALYSIS BY GAUSSIAN RADIAL BASIS FUNCTIONS TECHNIQUES

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Abstract We have reported the classification of infrared spectra of binary mixtures of 4-n-nonyl-4'-cyanobiphenyl (9CB) and 4-n-pentylphenyl-trans-4'-pentylcyclohexane-1-carboxylate (5H5) using back propagation networks (BPN)[1]. For the analysis of large sets of data, such as in the cases of infrared spectra of mixtures of 9CB and 5H5, the Gaussian radial basis function networks (RBFN) are better than the BPN. The input neurons represent selected spectral intensities in the range of 1000-40000 wave numbers/cm. The output neurons represent the concentrations of the mixtures, the phases (isotropic, nematic and smectic) at the experimental temperatures. The RBFN correctly classify the phases. The testing for the compositions of some mixtures show improvement over the back propagation networks.

## INTRODUCTION

Artificial neural networks are implementations of computational algorithms that create dynamically data structures that animate some simple functions of human brains. Neural networks are capable of learning patterns and making predictions. They are useful in classifying sets of patterns that may have similarities and dissimilarities. In molecular spectroscopy, such as in the infrared molecular spectroscopy, a spectrum indicates structural motions of the constituent molecules. Since these molecular motions take place in some thermodynamic environment, the phase properties of these substances are related to the molecular properties. Using neural networks, we may be able to extract properties of liquid crystals from experimental data that the experiments can not provide directly.

In the case of liquid crystal mixtures, infrared spectra obtained at different temperatures and compositions show differences in spectral densities and the relative positions of the lines. Phase diagram and spectra of the liquid crystal mixtures, 9CB and 5H5, are reported[2]. In Figure 1, we show a spectrum adapted from the paper.

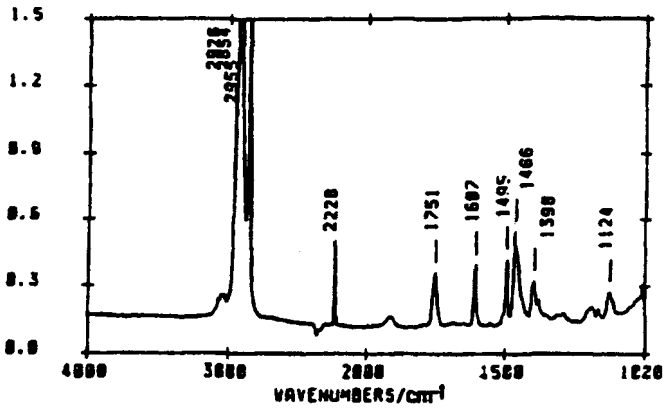


FIGURE 1. Infrared Spectrum of the mixture, 90%(weight) of 9CB and 10%(weight) of 5H5 at 27°C

It shows the spectrum for the mixture 90% of 9CB and 10% of 5H5 (by weight) at 27°C (smectic-A). A spectrum (not shown here) of the same mixture at 60°C (nematic) is quite different . We constructed artificial neural networks to classify the infrared spectra of these mixtures.

## RADIAL BASIS FUNCTION NETWORKS

For the classification of the infrared spectra, we constructed several radial basis function networks (RBFN). It consists of input neurons for relative spectral intensities. The output neurons represent some phase properties of the liquid crystal mixtures. Unlike back propagation neural networks (BPN), there are no hidden layers. Instead, each network has a single layer of special neurons. Dynamically, each of these neurons are represented by radial basis functions of Gaussian forms. When the neural network is learning or testing, the information from the input pattern vector passes through these neurons. They have these characteristics: 1) the location vector of the dynamic center is stored as weight form the input layer to the radial basis neuron, 2) a distance measure to determine how far an input vector is from the center, usually of Euclidean distance, 3) a

transfer function which determines the output of the radial basis neuron by mapping the output of the distance function.

RBFN network is a feed forward network. The output of a pattern is a function f(x) of only the distance between an input vector and the stored center. That is, $f(x) = P(\| x - c \|)$. The architecture of the RBFN is shown in Figure 2.

In practice, the pattern units are defined as

$$I_k = \| \mathbf{X} - c_k \| = \text{square root } [E_i^N( X_i - c_{ki})^2]$$

where $E_i^N$ is summation over index i=1 to a max. number N. The Gaussian transfer function in this case is

$$v_k = \exp[(I_k - R^2)/(s_k^2)],$$

where $s_k$ is the sigma (the standard deviation associated with Gaussian function). The learning for the pattern consists of using a cluster algorithm that determines the value of $c_k$ and the nearest neighbor heuristic for determining the $s_k$. Typically, a gradient descent algorithm is used to determine the weights from the radial basis neuron to the output layer. The implementation of these dynamically mechanisms basically constitute the RBFN tools.

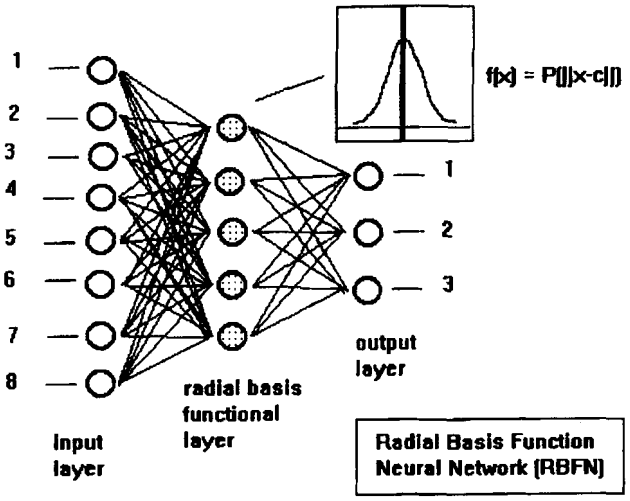


FIGURE 2. The graphical representation of a Radial Basis Function Network (RBFN) with 8 input neurons and 3 output neurons

In a previous study, we show that BPN are capable of classifying the liquid crystal mixtures. For this study, we placed focus on the spectra of the mixtures in smectic phases. We selected a few spectral patterns and used them to train the RBFN. We made use of a neural network development system [NeuralWorks Professional II Plus]. For the experiments, the number of input neurons were varied from 10 to 100 and the output neurons were varied from 2 to 5. These neural experiments were intended to find if semi-quantitative results could be obtained. An example of the working RBFN, the controls and instruments are shown in Figure 3. At the beginning, the spectral data from the input neurons are sent to the radial basis neurons. The clustering algorithm implemented determines the cluster radius positions. As more data are received, the cluster positions are updated. The radial basis neurons send data to the output neurons in accordance with the transfer function. This process is the primary task in the training of the network. The accuracy, convergence and iteration of the whole process are planned and controlled.. The result is a trained network. This trained network is used to test (consult) other spectral patterns in the set.

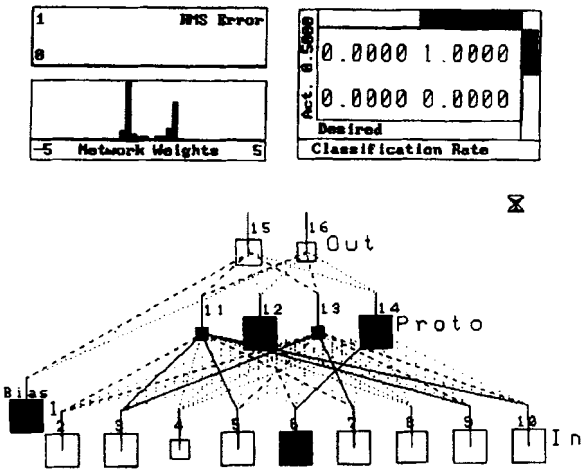


FIGURE 3. An Experimental RBFN and instruments for the analysis of Infrared Spectra of the Liquid Crystal Mixtures.

## SUMMARY OF RESULTS

We varied the input neurons from 9 to 100 and output neurons from 2 to 5. The training were carried out using these values of these parameters: linear coefficient from 0.3 to 0.15, momentum values from 0.2 to 0.4, mapped transfer around 2000, and the iterations from 2000 to 20000. The training accuracies are brought down to 0.0001, which is considered to be quite adequate. In most cases, the root-mean square values of error reduced to low level within 1000 iterations. The results are summarized below.

1. The training time and iteration values are larger when the number of input neurons are large. The convergence to the desired accuracy is attained fairly well in most cases.
2. The training time and iteration values are small when the number of input neurons is small. However, the accuracy is not impaired much. As an example, the concentration of 10% in 9CB of 5H5 is predicted as 21% for 9 input neurons and 2 output neurons.
3. The spectral values used to train the RBFN need not be in sequential spectral order. However, the number of neurons in all pattern units need be the same for all training epochs. Larger number of training sets are highly desirable for better results. These neural networks seem to tolerate bad data in the sets. Although experimental accuracy is usually not that critical, consistency of data usually is.

We constructed radial basis function neural networks to classify infrared spectra of liquid crystal mixtures. The neural networks were able to predict semi-qualitative values of concentrations of the components in the liquid crystal mixtures. For better results, more data patterns are needed. The choice of training algorithms play an important role in these applications of neural networks.

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