Use of Artificial Intelligence in Designing Dyes, Chemical Auxiliaries, Polymers, and Textile Fibers

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Abstract

The first phase of this research project involves the integration of fuzzy entropies (used in the context of measuring uncertainty and information) with computational neural networks. An algorithm for the creation and manipulation of fuzzy entropies, extracted by a neural network from a data set, is being designed and implemented. Advantage is being taken of the learning capability of the neural network to manipulate fuzzy entropies for classification and recognition processes. The neural network is being used to find patterns in terms of structural features and properties that correspond to a desired level of activity in various classes of molecules, such as azo dyes. Each molecule is described by a set of structural features, a set of physical properties and the strength of some activity under consideration. After developing an appropriate set of input parameters, the neural network is trained with selected molecules, then a search is carried out for compounds that exhibit the desired level of activity.

High level molecular orbital and density functional techniques are being employed to establish databases of various molecular properties required by the neural network approach. We are making extensive use of the Spartan (Wavefunction, Inc.) and GAUSSIAN (Gaussian, Inc.) molecular modeling packages for these calculations.

Introduction

This project focuses on the use of recent developments in the field of artificial intelligence (AI), including genetic algorithms, neural networks, and fuzzy logic, to aid in the development of novel, state-of-the-art dyes, chemical auxiliaries, fibers, and polymers which are of commercial importance to the U.S. textile industry. Where appropriate, modern molecular orbital (MO) and density functional (DF) techniques are being employed to establish the necessary databases of molecular properties to be used in conjunction with the AI approach.

For the first four months of this project we have concentrated on: 1) using molecular modeling to establish databases of various molecular properties required as input for our neural network approach; and 2) designing and implementing a fuzzy neural network architecture suitable to process these databases.

Molecular Modeling

Properties of various molecules of interest to the textile industry are being established using density functional calculations at the BP/DN** computational level. This approach uses non-local corrections for the functional according to the method of Becke and Perdew [1-3]. The DN** numerical basis set is very flexible and includes polarization functions on all the atoms [4]. Complete geometry optimization with no constraints are performed on all the molecules in this project.

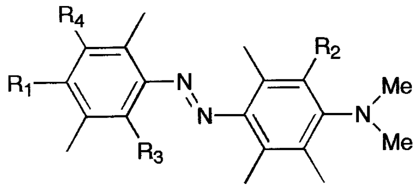
We decided to concentrate initially on azo dyes which account for more than 50% of the commercial dye market. One advantage of azo dyes is that they have been studied more than any other class of dyes, and a significant amount of experimental data currently exists on them [5]. This experimental data serves as a check on the results of our calculations, and also augments our database. It should be mentioned that the toxicological results of Freeman and coworkers [6] have been very useful in this regard.

A selection of the azo benzene compounds for which we have completed geometry optimizations at the BP/DN** level are shown schematically in Figure 1. Studies on approximately 40 azo derivatives have been completed to date. We are currently performing calculations on various conformations of the side-chains in many of those molecules to increase the probability that we have found the global minima on the potential energy surfaces. We are calculating a variety of molecular properties, including dipole moments, HOMO and LUMO energies, and charge distributions. In Figures 2 and 3 we show samples of the graphical data obtained from our calculations for 4-amino-3-methoxyazobenzene.

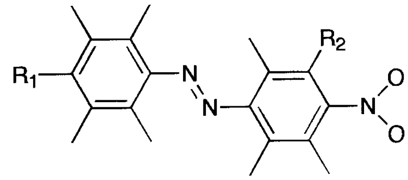
Artificial Intelligence (AI)

In the last several years there has been a large and energetic upswing in research efforts aimed at synthesizing fuzzy logic with computational neural networks in the emerging field of soft computing in AI. The enormous success of commercial applications (primarily by Japanese companies), which are dependent to a large extend on soft computing technologies, has led to a surge of interest in these techniques for possible applications throughout the US textile industry.

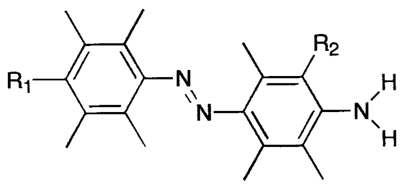
The marriage of fuzzy logic with computational neural networks has a sound technical basis, because these two approaches generally attack the design of “intelligent” systems from quite different angles. Neural networks are essentially low level, computational algorithms that offer good performance in dealing with large quantities of data often required in pattern recognition and control. Fuzzy logic, introduced in 1965 by Zadeh [7], is a means for representing, manipulating and utilizing data and information that possess non-statistical uncertainty. Thus, fuzzy methods often deal with issues such as reasoning on a higher (i.e., on a semantic or linguistic) level than do neural networks. Consequently, the two technologies often complement each other: neural networks supply the brute force necessary to accommodate and interpret large amounts of data and fuzzy logic provides a structural framework that utilizes and exploits these low level results.



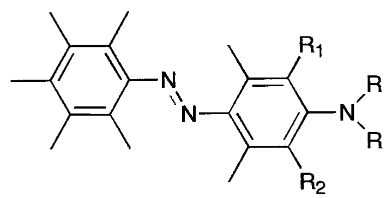
R1	R2	R3	R4
H	H	H	H
NO_2	H	H	H
H	H	HCO_2	H
H	H	H	Me



R1	R2
H	H
H	OMe
NH_2	H
NO_2	H
CHO	H
NC	H
F	H
SO_3H	H



R1	R2
H	H
H	OMe
H	OPr
H	OnBu
H	OCH_2CH_2OH
OH	H
SO_3H	H
SO_3Na	H
NO_2	H



R	R1	R2
H	H	H
Me	H	H
Pr	H	H
nBu	H	H
Me	Me	Me

Figure 1. Selected azo benzene derivatives for which BP/DN** optimizations have been performed.

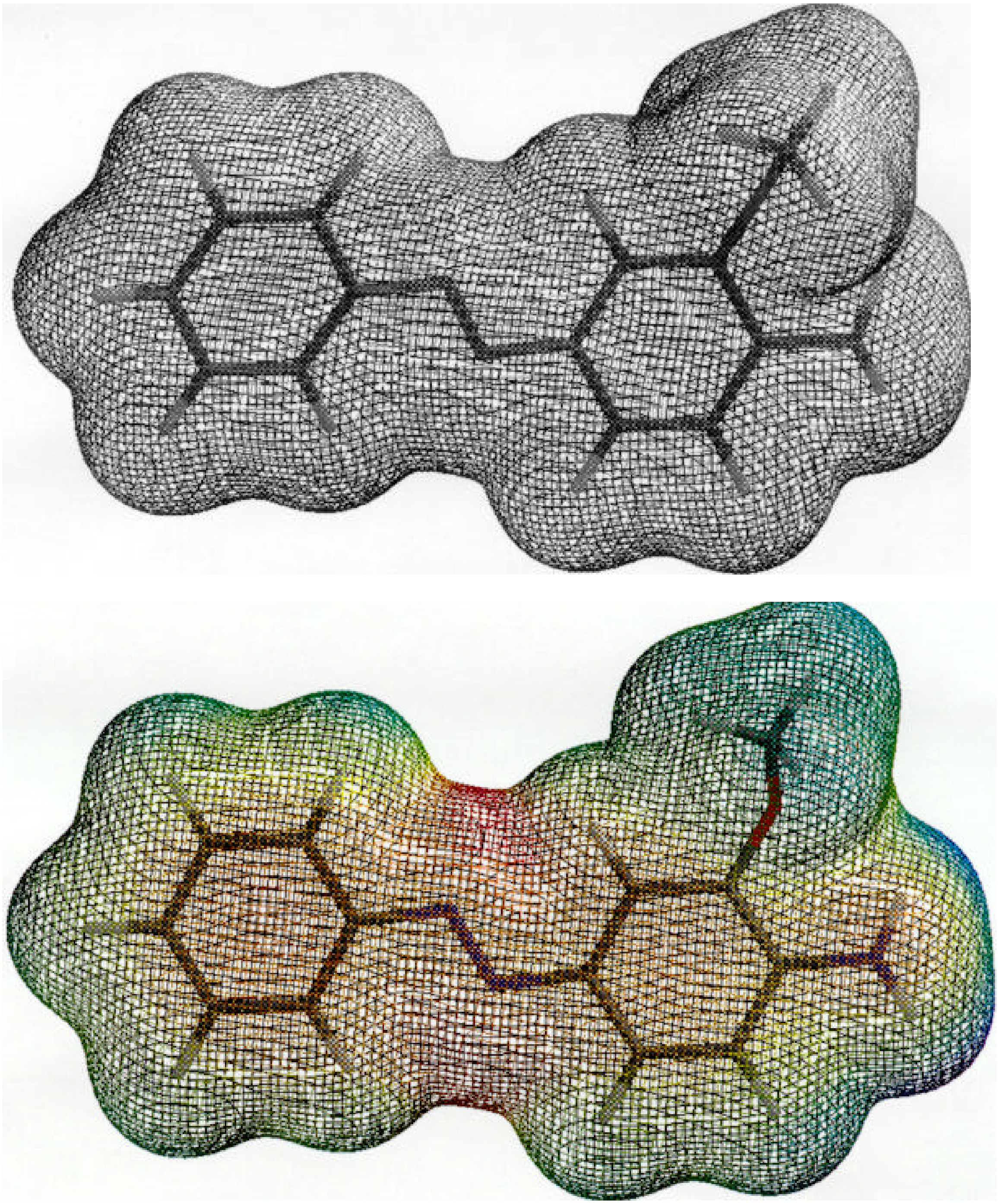


Figure 2. The density (top, 0.002 electrons/au^3), and the electrostatic potential superimposed on the density (bottom) for 4-amino-3-methoxyazobenzene.

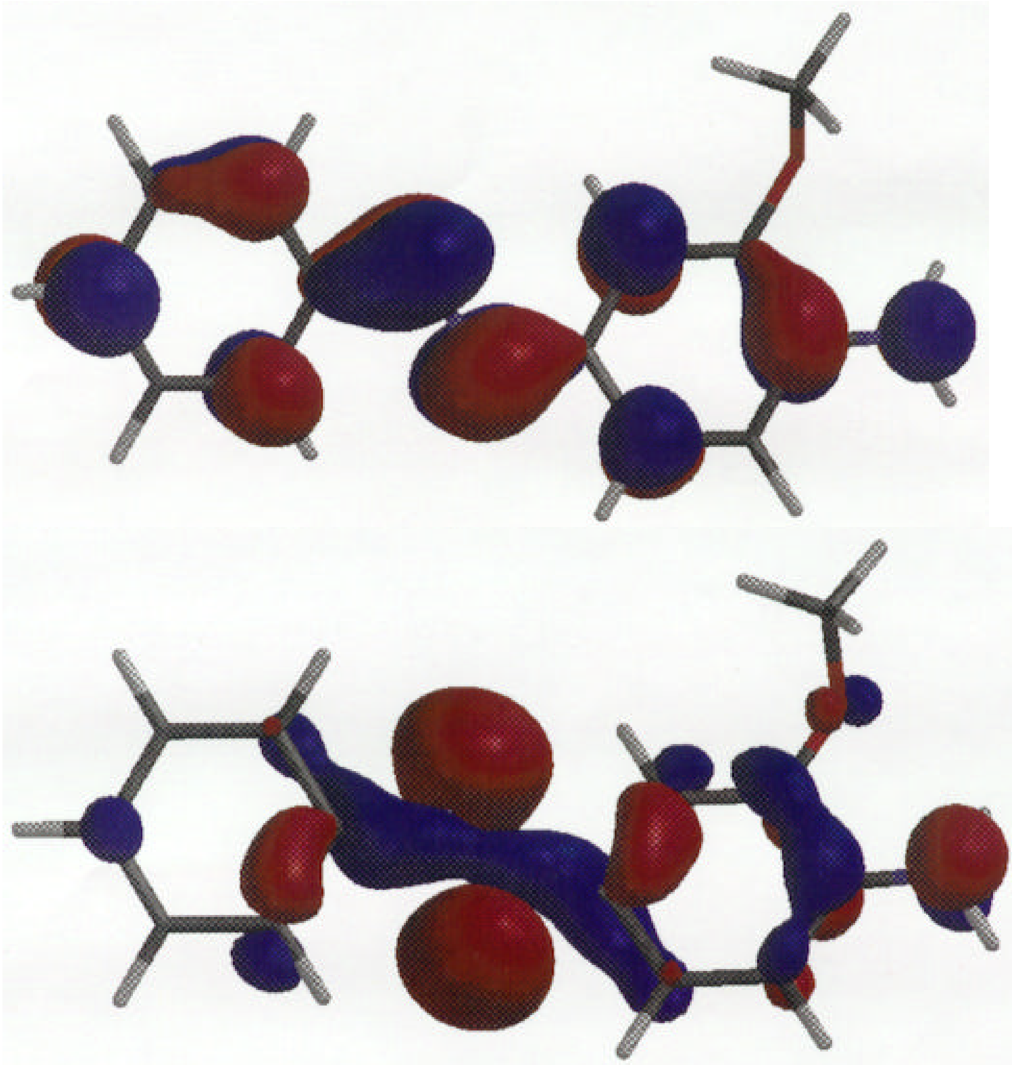


Figure 3. The LUMO (top) and HOMO (bottom) of 4-amino-3-methoxyazobenzene.

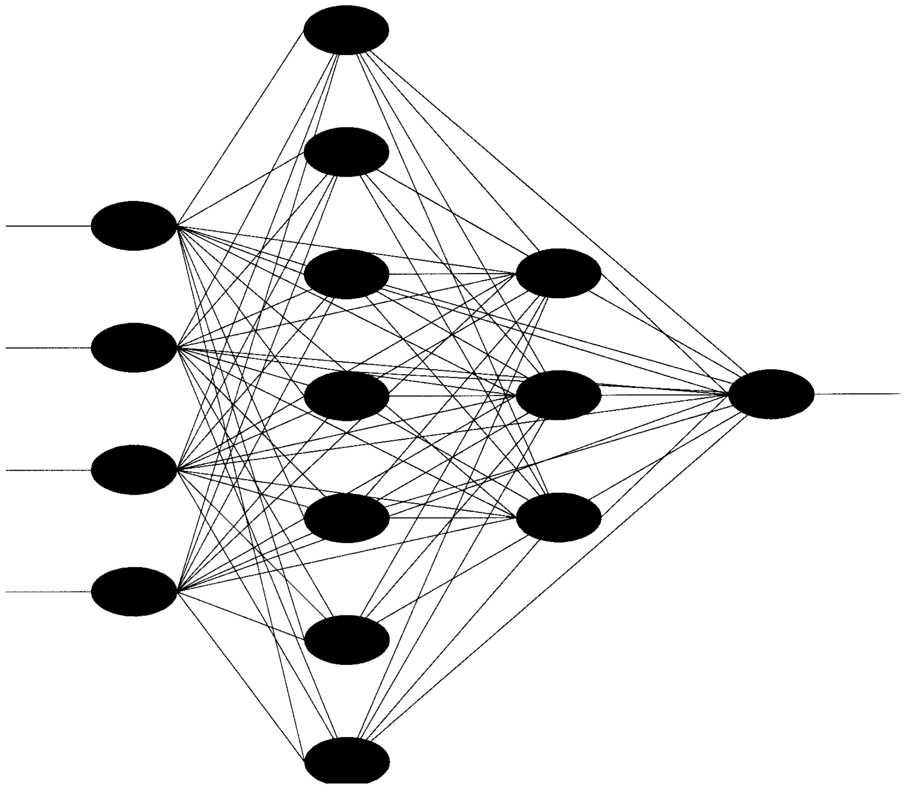
It has been shown that either technology can be used as a "tool" within the framework of a model based on the other. As the neural network is well known for its ability to represent functions, and the basis of every fuzzy model is the membership function, so the natural application of neural networks in fuzzy models has emerged to provide good approximations to the membership functions that are essential to the success of the fuzzy approach.

This research is concerned with the integration of fuzzy logic and computational neural networks. Therefore, an algorithm for the creation and manipulation of fuzzy membership functions, which have previously been learned by a neural network from some data set under consideration, is being designed and implemented. In the opposite direction we should be able to use fuzzy tree architecture to construct neural networks and take advantage of the learning capability of neural networks to manipulate those membership functions for classification and recognition processes. In this research, membership functions are used to calculate fuzzy entropies for measuring uncertainty and information. That is, the amount of uncertainty regarding some situation represents the total amount of potential information in this situation. The reduction of uncertainty by a certain amount (due to new evidence) indicates the gain of an equal amount of information.

A general method of how to generate fuzzy subsets from numerical data and rank them was previously developed by the principal investigator [8], and is being used in this project. The proposed fuzzy neural network algorithm shows a way in which neural network technology can be used as a "tool" within the framework of a fuzzy set theory. Generating membership functions with the aid of a neural network has been shown to be an extremely powerful and promising technology. Our hybrid fuzzy neural algorithm is a building block towards combining the two soft computing paradigms. It allows for a self-generation of a feed-forward network architecture suited for a particular problem.

The main features and advantages of the proposed algorithm are: 1) it is a general method of how to use numerical information, via neural networks, to provide good approximations to the membership functions; 2) it is a simple and straightforward quick-pass build-up procedure, where no time-consuming iterative training is required, resulting in much shorter design time than most of neural networks; 3) there is a lot of freedom in choosing the membership functions; this provides flexibility for designing systems satisfying different requirements; and 4) it performs successfully on data where neither a pure neural network nor a fuzzy system would work perfectly.

To determine the effectiveness of the proposed algorithm, the performance was evaluated on a database of molecular properties involving some azo dyes. We are working on determining the appropriate input parameters which can be used to predict various properties. As a simple example, using only the detailed BP/DN** geometry of some azo dyes, in conjunction with experimental toxicological data, the network has been able to learn and differentiate between mutagenic and non-mutagenic dyes. We expect the fuzzy neural network to predict the mutagenic nature of other chemical structures. The resulting neural network architecture, for the example mentioned above, is shown in Figure 4. Figure 5 depicts fuzzy entropy values at all hidden nodes for the generated neural network.



Input: geometry properties

Hidden layers (corresponding to entropy)

Output: decision (Y/N)

FEED-FORWARD NEURAL NETWORK ARCHITECTURE

Figure 4. The resulting neural network architecture for indication of mutagenicity/carcinogenicity.

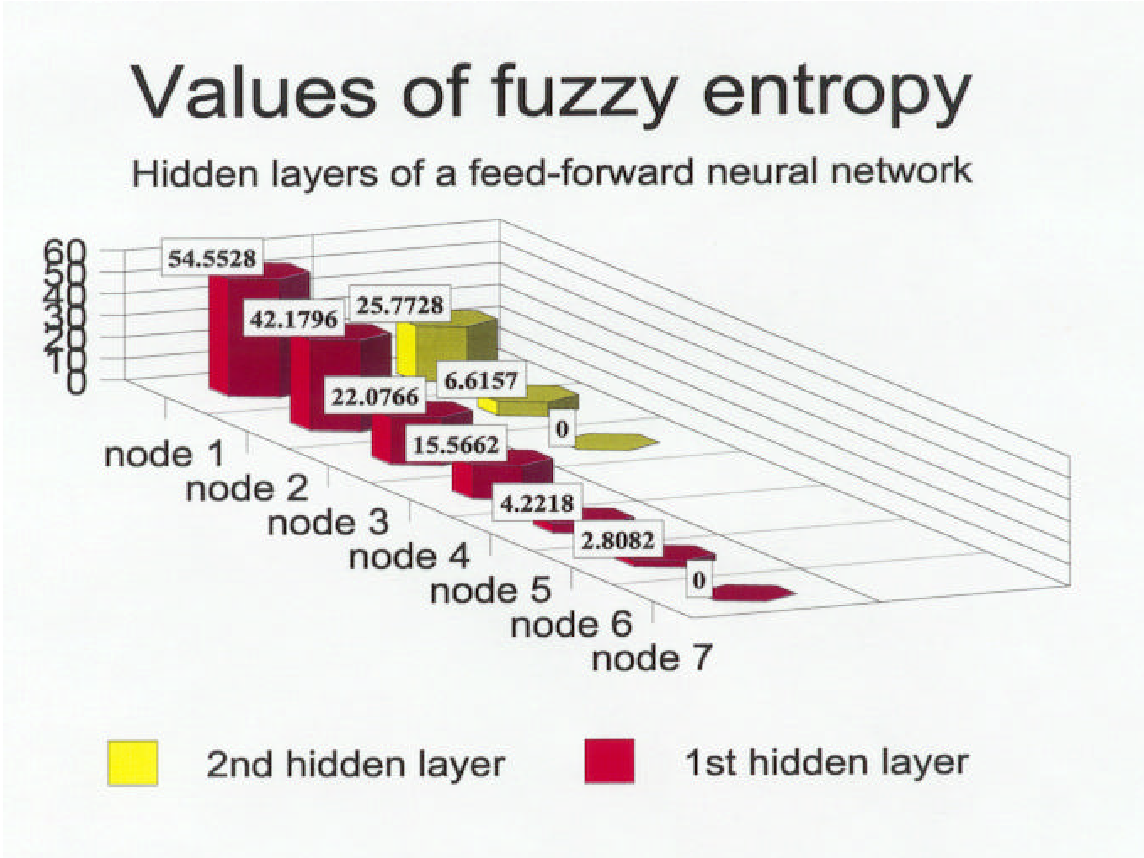


Figure 5. Fuzzy entropy values at hidden nodes for the neural network shown in Figure 4.

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