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Artificial Neural Networks Used to Predict Electrical Properties of Polymers

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Abstract

The ability to predict properties of molecules prior to their synthesis can be of great importance in optimizing their design. Substantial savings in time as well as cost can be achieved if some desired properties can be predicted prior to the synthesis of the molecule. The outer orbitals of a molecule are primarily responsible for many different properties of the molecules. These outer orbital parameters can be utilized by an intelligent computing system like an Artificial Neural Network to extract necessary knowledge about the properties of the molecule. An Artificial Neural Network was trained to extract electrical parameters of several polymers. The former was then tested using a number of molecules set aside (not used in training) solely for this purpose.

Introduction

The ability to predict physical, chemical and biological properties of molecules is of great value in optimizing their design, modification and processing. Both time and cost of synthesis can be saved if the properties of the molecules are predicted accurately prior to their synthesis.

In the present day approach, a molecule is designed and optimized first using different types of quantum mechanical calculations. The molecule is then physically synthesized in the laboratory before its properties can be tested. If the test for the properties fails, the entire molecule is generally discarded. This means a total waste of time and money for the synthesis stage. This new approach attempts to optimize the entire process and uses artificial intelligence techniques to predict the required properties from the quantum mechanical calculations.

It is well known that the outer orbitals of a molecule are the most active ones and are primarily responsible for the major chemical, physical and biological properties of the molecule. It was, thus, assumed that some extremely useful information might be embedded in various molecular orbital parameters that can readily be obtained usingthe well known SCF-MO quantum mechanical calculations. These calculations were performed on the available molecules using ab initio Self-Consistent Field - Molecular Orbital (SCF-MO) calculations (Darsey et al., 1993; Soman et al., 1995).

In the next stage, an Artificial Neural Network (ANN) was trained on different properties of different sets of molecules relating the quantum mechanical parameters obtained in the previous stage. These neural networks were tested using, a number of molecules set aside (not used in training) solely for this purpose.

Methodology

Artificial Neural Networks.--The fundamental processing element of a neural network is a neuron. This building block of human awareness encompasses a few general capabilities. Basically, a biological neuron receives inputs from other sources, combines them in some way, performs a generally nonlinear operation on the result, and then outputs the final result. But currently, the goal of artificial neural networks is not the grandiose recreation of the brain. On the contrary, neural network researchers are seeking an understanding of nature's capabilities for which people can engineer solutions to problems that have not been solved by traditional computing.

To do this, the basic units of neural networks, the artificial neurons, simulate the four basic functions of natural neurons. Currently, neural networks are the simple clustering of primitive artificial neurons. This clustering occurs by creating layers which are then connected to one another. How these layers connect is the other part of the "art" of engineering networks to resolve real world problems.

Although there are useful networks which contain only one layer, or even one element, most applications require networks that contain at least the three normal types of lay-

ers - input, hidden, and output (Fig. 1). The layer of input neurons receives the data either from input files or directly from electronic sensors in real-time applications (Mitra and Darsey, 1995). The output layer sends information directly to the outside world, to a secondary computer process, or to other devices such as a mechanical control system. Between these two layers can be many hidden layers. These internal layers contain many of the neurons in various interconnected structures. The inputs and outputs of each of these hidden neurons simply go to other neurons (Baba, 1989; Chui, 1992).

Table 1.

Dieelectric Constants

Name of Polymer	Observed Data	Predicted Data	Error %
Poly(tetrafluoroethylene)	2.00	1.87	6.50
Polyisobutylene	2.23	2.32	-4.00
Polyethylene	2.30	2.19	4.80
Polypropylene	2.30	2.41	-4.80
Polyisoprene	2.40	2.37	1.70
Polybutadiene	2.51	2.44	2.80
Polysiloxane	3.04	2.87	5.60
Poly(vinyl acetate)	3.50	3.39	3.10
Poly(methyl methacrylate)	3.60	3.06	15.0
Poly(oxymethylene)	3.70	2.54	31.4
Polyacrylonitrile	6.50	4.12	36.6
Poly(vinyl alcohol)	7.80	3.25	58.3
Poly(vinylidenefluoride)	8.40	3.04	63.8

Fig. 1. Architecture of an Artificial Neural Network with one hidden layer.

In most networks each neuron in a hidden layer receives the signals from all of the neurons in a layer above it, typically an input layer. After a neuron performs its function it passes its output to all of the neurons in the layer below it, providing a feedforward path to the output.

Once a network has been structured for a particular application, that network is ready to be trained. To start this process the initial weights are chosen randomly. Then, the training, or learning, begins. There are two approaches to training - supervised and unsupervised. Supervised training involves a mechanism of providing the network with the desired output either by manually "grading" the network's performance or by providing the desired outputs with the inputs (Crooks, 1992). In unsupervised training where the network has to make sense of the inputs without outside help. The vast bulk of networks utilize supervised training.

Artificial Neural Networks for the Prediction of Dielectric Constant of Polymers.--A multilayered backpropagation network was designed to achieve this goal. The network had three layers - the input layer with 31 input nodes (30 eigenenergies and dipole moment for each polymer), the output layer with one output node (corresponding to the property predicted dielectric constant) and a hidden layer with eight nodes.

Results and Discussion

The eigenenergies of the lowest 15 unoccupied molecular orbitals, the 15 highest occupied molecular orbitals and the dipole moment of each polymer were obtained by using quantum mechanical calculations Gaussian 86 and 92 programs. STO-3G* was used as the basis set and POP=REGULAR was used as a keyword. The dielectric constants of polymers used in this study were obtained from the literature (Brandrup and Immergut, 1975).

Out of the available 14 conductive polymers, 13 were used for training and one was left for testing or to validate the training. In the next run, a different set of 13 polymers was used for training, and the remaining polymer was used for testing. A total of 14 sets of training was conducted in this manner and the results have been presented in Table 1 and Fig. 2. As observed from table 1, 9 out of 14 polymers, which have smaller dielectric constants, had less than 10% error in the prediction of the dielectric constants. Figure 1 presents

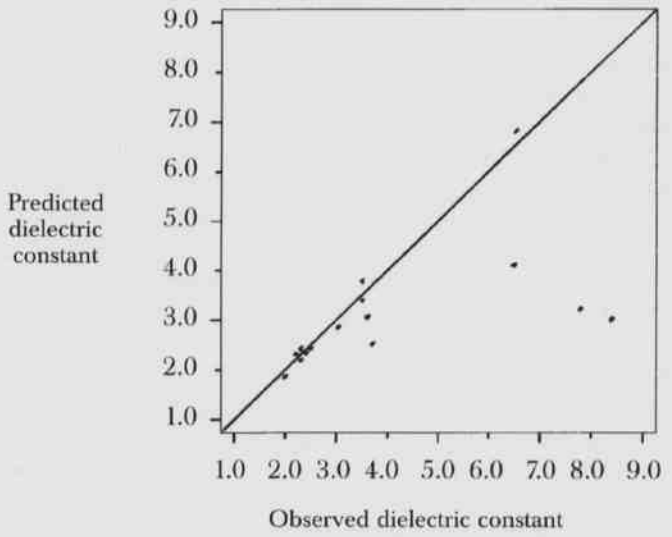

Fig. 2. Correlation between the actual values of dielectric constants and the values predicted by the Artificial Neural Netowrk.

the same information. However, when the dielectric constant data was large, the percent error was also getting large. The reason for this, we feel, was the small number of compounds tested. If you don't provide enough information to train the network, it won't learn properly.

Conclusions

So far the results obtained from using neural networks are good enough to justify further work on making a better association between molecular orbital and the electric properties of polymers. In particular efforts should be made to increase the number of polymers in the dataset and also to include a wider range of dielectric constants.

A combination of quantum mechanical and artificial intelligence techniques has been applied in this work to predict the dielectric constant of conductive polymers. If the process of prediction becomes more reliable, the technique can lead to substantial savings in time and cost. This technique might, as well, be tried on other electrical and non-electrical properties of both polymeric and non-polymeric materials.

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