DEVELOPMENT OF NEURAL NETWORK TRAINING METHODOLOGY FOR MODELING NONLINEAR SYSTEMS WITH APPLICATION TO THE PREDICTION OF THE REFRACTIVE INDEX

THESIS

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ABSTRACT

Artificial Neural Networks (ANN) constitute a set of powerful mathematical tools which belong to Artificial Intelligence (AI) techniques and have the ability to model an unknown non-linear system using input-output data only (Haykin, 1999). This technique is called "black box", where our system is represented by a black box where only input and output signals are visible, whereas no information from within the box is available: i.e. we do not know the specific mechanism that governs the system.

Depending on the way that the neurons are interconnected we distinguish several neural network architectures; the most popular ones are: Feedforward Neural Networks (FFN), Recurrent Neural Networks (RNN), Kohonen neural networks and Radial Basis Function (RBF) neural networks. The latter form a special neural network architecture which is characterized by two main advantages: The simplicity of its structure, and the speed of the learning algorithms it employs.

The procedure during which the neural networks learn the relation between the input and the output is called training. The RBF network training procedure is divided into two phases. In the first phase, the structure of the network is determined. In the second phase, the parameters of the network which are related to the synaptic weights between the hidden nodes and the nodes of the output layer are calculated using the method of linear regression (Leonard & Kramer, 1991, Powell, 1987). The typical RBF training methodology which is being used in the determination of the structure

of the network, i.e. in the calculation of the hidden node centers is an iterative procedure called the *k*-means algorithm (Darken & Moody, 1990, Macqueen, 1967, Moody & Darken, 1989). This algorithm exhibits two basic drawbacks: It is unable to automatically select the proper number of RBF hidden node centers and it requires high computational times.

In order to overcome the aforementioned problems, a new algorithm was introduced in a recent publication, which determines the structure of the network depending on a fuzzy partition of the input space (Sarimveis et al., 2002). This method called the fuzzy means algorithm presents several advantages over the typical RBF training methodologies and has been proved to be more efficient in non-linear system modeling. The algorithm starts with a fuzzy partition of the input space, and then selects the structure and the centers of the network in only one step, requiring only one pass from the training examples, while it completes the training procedure in very limited computational times.

In this work, we employ a variation of the fuzzy means algorithm called the non-symmetric fuzzy means algorithm, which presents the same advantages with the symmetric one but has more flexibility, which results in better networks in terms of accuracy and/or network complexity. By training RBF neural networks with the fuzzy means algorithm, we can model any non-linear system using only input-output data from it.

A system that would be rather difficult to model using first principle equations is the problem of predicting the refractive index. The refractive index is a fundamental physical property of substance with great importance that is not limited only to an optical context, since it is directly related to electrical, magnetic, thermal, etc properties. For example, the refractive index can be used in order to identify a particular substance, to confirm its purity, or to measure its concentration.

In this work, we trained RBF neural networks with the non-symmetric fuzzy means algorithm, using as inputs experimental data like wavelength, temperature and concentration in order to model the refractive index of several substances (Alexandridis et al., 2011). To be more specific, we studied two cases involving the prediction of the refractive index of two semiconductor material crystals (silicon and germanium) and a water-ethanol mixture.

For the case of silicon and germanium, the objective was to predict the refractive index for each semiconductor crystal using as inputs the wavelength and temperature (Frey et al., 2006). The RBF models trained with the non-symmetric fuzzy means algorithm presented more satisfying results, compared not only to other neural network training methodologies but also to empirical equations that were built solely for this purpose. Figure 1 shows a three-dimensional plot of the surface predicted by RBF network trained with the non-symmetric algorithm, together with the experimentally measured data points, where we can see that the experimental values are pretty close to the predictions. The importance of the produced model is significant, since it provides us with a nomograph that can be used to identify the refractive index for every combination of wavelength and temperature, while the measurements are restricted to a few specific values of wavelength and temperature.

Employing a similar process to the case of silicon, we trained RBF models with the non-symmetric fuzzy means algorithm for the case of germanium. Once more the non-symmetric algorithm outperformed the other neural network training algorithms and the empirical equations.

In order to demonstrate the generic nature of the neural network approach, we tested a different case, examining the prediction of the refractive index for a two-component mixture comprising of ethanol and water. The study of the refractive index for this two-component mixture is rather interesting since it follows a non-linear mixing rule (Rioboo et al., 2009). For this case, we trained neural network models that can predict the refractive index of an ethanol-water mixture, using as inputs the

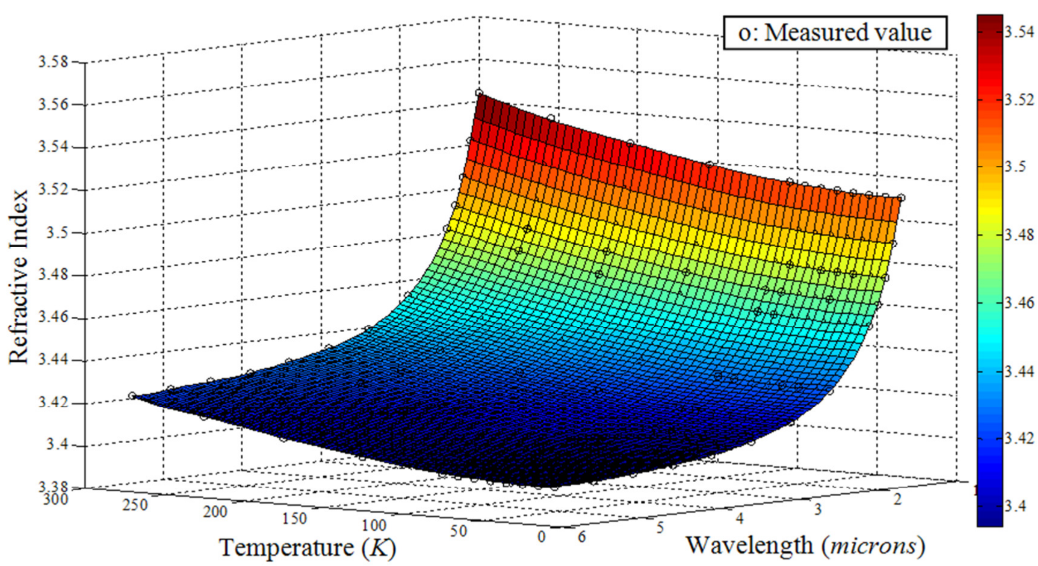

Figure 1. Nomograph based on RBF network predictions for Silicon.

mixture concentration in water and the temperature. Figure 2 shows the surface plot of the refractive index predicted by the network versus the concentration and temperature, together with the experimentally measured data points. It can be seen that the surface produced by the RBF network approximates the measured data with great accuracy.

In all the cases we examined, the results showed that the produced neural network models provide an accuracy of several decimal places that in most cases is rather close to the measurement accuracy. Due to the generic nature of neural networks, they can be applied to similar cases for any kind of material, modeling the effect of various parameters affecting the refractive index.

Results from this work were submitted for publication to the scientific journal *Materials Science and Engineering: B*.

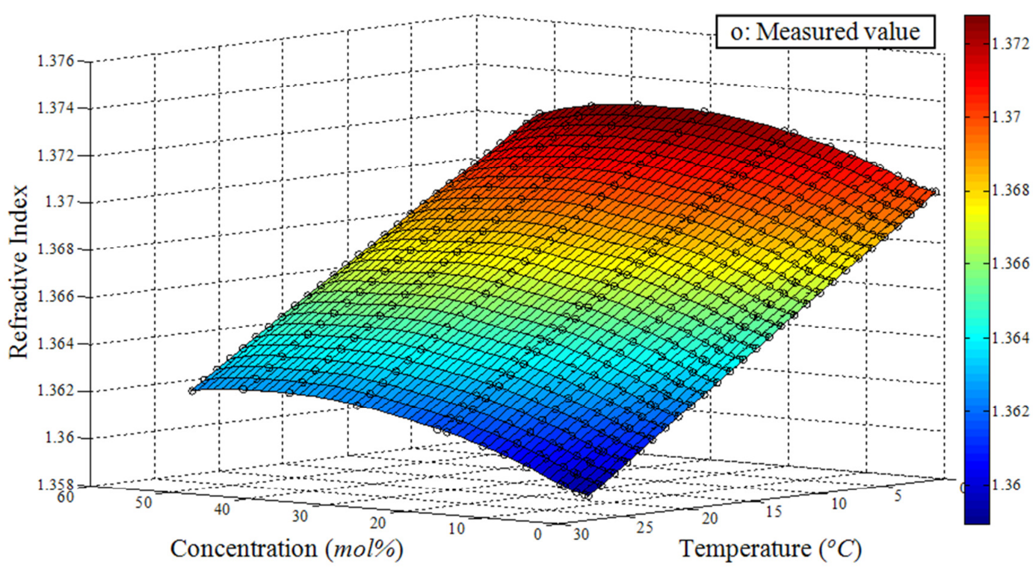

Figure 2. Nomograph based on RBF network predictions for Ethanol-Water.

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