

Neural Networks in The Chemical Industry

Matthew N. O. Sadiku¹, Sarhan M. Musa¹, and Osama M. Musa²

¹Roy G. Perry College of Engineering Prairie View A&M University
Prairie View, TX 77446

²Ashland Inc, Bridgewater, NJ 08807

ABSTRACT: An artificial neural network (ANN) is an information processing construct inspired by the manner in which the brain processes information and were originally developed to mimic the learning process of the human brain. They have been increasingly used in the chemical industry for data analysis, process control, pattern identification, identification of drug targets, and the prediction of several physicochemical properties. This paper provides a brief introduction on neural networks and their applications to the chemical industry.

KEY WORDS: artificial neural networks, chemical industry, chemical engineering, modeling

I. INTRODUCTION

Artificial neural networks (ANNs) (also called perceptron networks, connectionist systems or neurocomputers) are designed to mimic the complexities of the brain functions in an effort to capture the amazing learning capabilities of the human brain. They may be regarded as a sort of parallel processor designed to imitate the way the brain accomplishes tasks [1]. They provide a wide range of powerful new techniques for solving problems in diverse chemical engineering applications. Due to their simplicity, ANNs are a promising tool for simulating the highly interdependent variables of complex manufacturing processes. The idea of ANNs was inspired by the structure of the human brain and by an envy of what the brain can accomplish. The 1980s witnessed a resurgence of interests in ANNs. This interest was due to the development in new algorithms and VLSI. The field of neural networks and the development of neural network tools have expanded unbelievably in the past years [2]. Engineering systems are generally less complex than the brain. Various chemical processes can be described by relatively straightforward mathematical functions. Chemometrics is widely employed to solve complex chemical problems via the use of large data sets which contain embedded implicit relationships through the construction of composite, generally linear, response relationships. ANN is a non-traditional chemometric tool for providing accurate solutions to complex, non-linear problems. ANNs can be viewed as non-linear models that can represent input-output data, classify data, and recognize patterns within data. ANNs can solve practical complex tasks in a number of applications that should be of interest to chemists and chemical engineers [3]. The main advantage of ANNs is their ability to represent complex input-output relationships.

II. CHARACTERISTICS OF ANN

An artificial neural network is an interconnection of nodes, similar to the network of neurons in a brain, working in unison to solve specific problems. The interconnections of the nodes are called synapses. ANN is a mathematical tool whose functioning is inspired by that of the human brain. Thus, an ANN basically consists of nodes (or neurons), connections (axons and dendrites) between nodes, connection weights (synapses) and thresholds. It contains an input layer, an output layer, and one or more hidden layers [4].

Different types of artificial neural networks are available: (1) support vector machine (SVM), (2) self-organization map (SOM), (3) multilayer perceptron (MLP). Typically, neurons are organized in layers. The neurons act as nonlinear processing elements within the network. Signals travel from the first (input), to the last (output) layer, possibly after traversing the layers multiple times. The number of neurons in the input and output layers are fixed based on the number of inputs and outputs. As shown in Figure 1 [5], the neurons are generally grouped into three different types of layers [6]:

- Input layer: whose number of nodes depends on input variables
- Output layer: whose number of nodes is equal to the number of predicted variables
- Hidden layer: situated between the first two layers.

Artificial neural networks acquire knowledge during a learning process and that knowledge is stored in the synaptic weights of the connections.

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