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Neural Networks in The Chemical Industry

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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.

Neural networks can be classified as static (feedforward) or dynamic (recurrent). They can also be classified as employing supervised training or unsupervised or self-organizing training [7]. Their ability to learn from examples is a special characteristic which relates to intelligence. Learning can be regarded as the process of updating the interior layout of the network. Artificial neural networks can be used to extract patterns and detect trends that are either too subtle or too complex to be noticed by humans or other computer techniques. Advantages of artificial neural networks over other modeling techniques include adaptive learning behavior, multivariable pattern recognition capability, good filtering abilities, self-organization, real-time operation, fault tolerance, and the potential for online use.

III. APPLICATIONS

Since neural systems attempt to reflect cognitive processes and behavior, the field is closely related to cognitive and behavioral modeling. Due to the fact ANNs can reproduce and model nonlinear processes, they have found several applications in a wide range of disciplines including system identification and control, quantum chemistry, pattern recognition, medical diagnosis, finance, data mining, machine translation, neurology, and psychology. They have been used in a wide range of applications in the chemical industry such as process control, petrochemicals, oil and gas industry, chemical inventories, chemical reactor, biotechnology, environment, mineral industry, oil mining process, pharmaceutical industry, and polymer industry. The list is long, impressive, and growing rapidly [8].

- **Chemical process control:** Since chemical processes are often characterized by strong nonlinearities, neutral networks are effective tools to model such complex systems. A neural network process control package has been developed to reduce waste and improve product quality. They are also used to perform sensitivity studies, determine process set points, and predict process performance [9]. Some of these neural-network-based control strategies are applied in both online situations and simulation [10].

- **Treatment plant:** ANN provides an effective analyzing and diagnosing tool to understand and simulate the non-linear behavior of a plant. It is used as a valuable performance assessment tool for plant operators and decision makers [11].

- **Petroleum exploration:** Oil companies such as Arco and Texaco are using ANNs to determine the locations of underground oil and gas deposits. The general properties of oil and gas behavior can also be predicted using neural network models [12]. More applications of neural networks in chemistry and chemical engineering can found in reference [13].

IV. LIMITATIONS AND CHALLENGES

While ANNs have several advantages, they are not cure-all. There are many limitations applying neural network computing to industrial chemistry. These include [14]:

(1) Long training times
(2) Large amount of training data
(3) No guarantee of optimal results
(4) No guarantee of 100% reliability

A common criticism of ANN is that they require too much training for real-world operations. In general, chemical processes are complex. The mathematics involved with ANNs are not a trivial matter and they lack generalization. Effective ANNs also require considerable computing resources.

V. CONCLUSION

Basically, artificial neural networks are a family of mathematical models that are based on the human brain functioning. They imitate the way human brain works. They perform favorably in chemical applications and do not require explicit programming by an expert. They offer a promise in solving problems that have been difficult if not impossible to solve so far. The chemical industry has a lot to gain from neural networks because their ability to learn makes them very flexible and powerful for solving complex problems. A lot of information about artificial neural networks can be obtained from Neural Networks, the archival journal of the world's three oldest neural modeling societies (the International Neural Network Society, European Neural Network Society, and Japanese Neural Network Society) and from several books on the subject available at Amazon.com.

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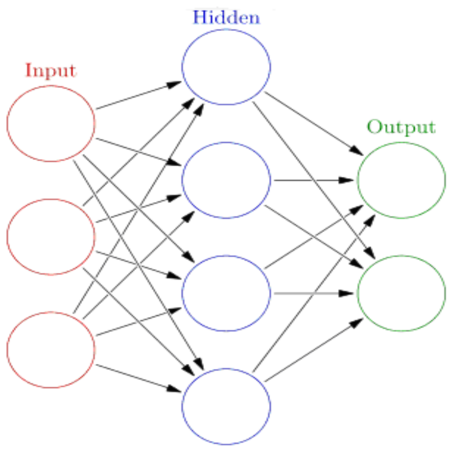

Figure 1. An artificial neural network [5].

Neural Networks. What they are and why they matter. Neural networks are computing systems with interconnected nodes that work much like neurons in the human brain. Using algorithms, they can recognize hidden patterns and correlations in raw data, cluster and classify it, and â€“ over time â€“ continuously learn and improve. History.Â Chemical compound identification. Ecosystem evaluation. Computer vision to interpret raw photos and videos (for example, in medical imaging and robotics and facial recognition). Keywords: Materials science, Engineering, Application, Neural networks, Salient issues, Artificial.Â Neural network models are extremely useful in such circumstances, not only in the study of mechanical properties but wherever the complexity of the problem is overwhelming from a fundamental perspective and where simplification is unacceptable. There are many established theories in materials science and engineering that have been proven empirically through several experiments but are difficult to predict using simple linear and multiple linear regression models: artificial neural networks comes handy in such situations (Ihom, 2014).Â The defence, nuclear and space industries are concerned about the issue of testing and verification. Usually neural networks have to be trained with a representative plant data set before they can generalise to new data and thus can securely be used in a controller. However, building a representative data set for a steel mill typically takes several thousands of strips (i.e. several weeksâ€™ production).Â This procedure results in the post-calculation errors for use of on-line adaptation of the neural network. Thus the networks are capable of forecasting the systematic error component within the framework of post-calculation. The coiler temperature of can be predicted by a hybrid.