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ARTIFICIAL NEURAL NETWORK APPLICATIONS IN ELECTROCHEMISTRY — A REVIEW

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Artificial neural network is an information processing system with analytical capabilities. It offers an alternative to mathematical regression for analyzing complex data sets. This technique is primarily software based and finds applications wherever automation is required. It is being used for chemical and electrochemical research also. This paper reviews the recent trend and possible applications in electrochemistry.

Keywords : Neural networks; Back propagation model; Applications in electrochemistry

INTRODUCTION

Artificial Neural Networks (ANN), a nascent branch of computer science, already started finding a place in electrochemistry as in the case of many areas of science. Pattern recognition and voice recognition, the two important branches of artificial intelligence solely depend on ANN. The applications of ANN are as important and necessary as numerical computation or consultation based expert systems for the growth of electrochemistry. The range of applications is so wide and varies from the simple cyclic voltammetry to the advanced corrosion prediction. A brief description about ANN and a review of its applications in electrochemistry are presented below.

Artificial Neural networks

A neural network is an information processing system and consists of a large number of very simple highly interconnected processors called neurodes. These neurodes perform in a manner that is analogous to the most elementary functions of the biological neuron (of brain). The neurodes are connected to each other by a large number of weighted links, over which signals can pass. Each neurode may receive one or more input signals but it produces only one output signal. ANNs exhibit surprising number of brain's characteristics. They learn from experience, generalize from previous examples to new ones, and abstract essential characteristics from inputs containing irrelevant data. ANNs can modify their behaviour in response to their environment. Shown a set of inputs (and desired outputs if available), they self adjust to produce consistent responses, based on the training they received. A wide variety of training algorithms have been developed. Fig 1 illustrates the physical connections of a typical neural network.

Training is an important and fundamental step in neural networks. In the process of training the network learns to recognize and interpret similar types of signals. This particular property is exploited in many fields to achieve automation.

A wide variety of ANNs were proposed starting from the simplest one called perceptron, which consists of a single layer of neurodes. The back propagation neural network is the most popular one. This has got multiple layers of neurodes, the first layer is called the input layer, the last one is called output layer and the remaining are called hidden layers.

The ANNs are further classified into two broad categories viz. supervised learning model and self-organization model (unsupervised) depending on the way they learn. Back propagation model falls under supervised learning category. It works somewhat similar to the common iteration method. For a given input signal, the output of the network is compared with the desired result and the error is fed back (back propagated), simultaneously making changes to the connection weights till the error is minimized. A large number of inputs whose results are known are required, to train a network. Once a network is trained successfully to perform a task, it can be utilized to do same/similar type of job in a much faster automated way and in this process also the network learns further. Several classic books on neural networks have been published by various authors [1-3].

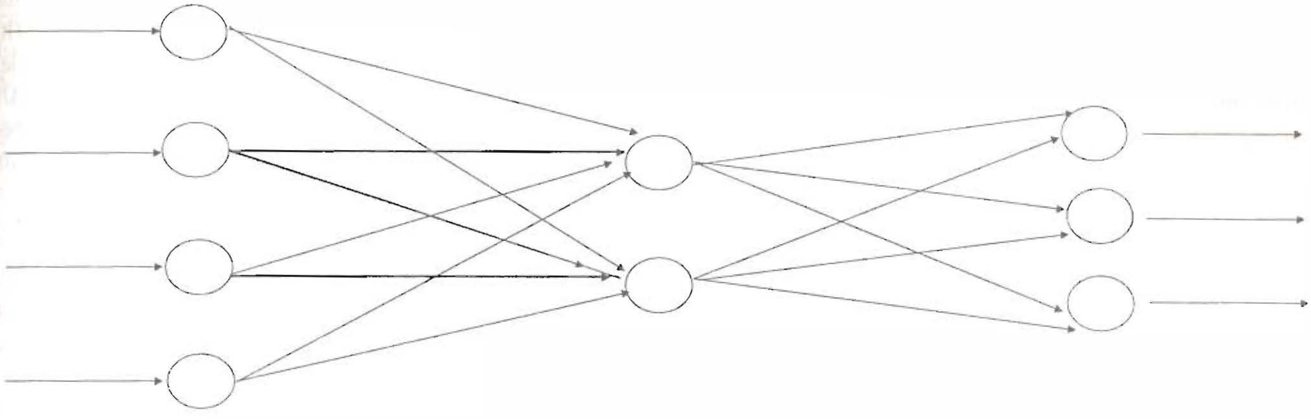

Fig. 1: Physical connections of a typical multilayer neural network

Applications

Electrochemical applications of ANN include corrosion prediction, inhibitor design, automatic pipeline inspection, analysis of electrochemical impedance data., electrochemical polymerization, electrochemical sensors, stripping voltammetric analysis, battery cell performance etc. Apart from these specific applications, there are numerous papers on ANN applications to chemistry (and related to analytical chemistry and electrochemistry) appeared in the literature [4-7]. Spectral analysis (IR, NMR) finds a prominent role in ANN. Thermal analysis [8], particle size distribution [9], non-selective gas sensors [10], phase diagram [11], estimation of kinetic analytical parameters [12], predicting solubility are some of the other related applications.

Stripping voltammmetry

Lastres et al [13] studied the use of neural networks in solving interferences caused by formation of intermetallic compounds in anodic stripping voltammetry. The software developed for this purpose allows one to construct neural networks of virtually any type of architecture and train it automatically using the backpropagation method. The ability of neural networks for addressing interferences arising from interactions with the hanging mercury drop electrode is demonstrated for the Cu-Zn binary system.

Zinc and copper are two elements which mutually interfere with each other in stripping analysis. The cause is the formation of a Zn-Cu intermetallic compound in the mercury film, which affects both Cu & Zn analyses. Chow et al [14] applied the backward error propagation ANN in a novel approach for the determination of correct Zn in the presence of Cu using potentiometric sripping analysis. This performed well in determining the correct Zn concentration in the sample when provided with the stripping times of Zn & Cu and the Cu concentration (determined by shifting the plating potential to a lower value to prevent the zinc being plated onto the Hg film electrode). The unknown Zn concentration was determined by following an initial period of network exposure to a set of experimental data, which were used as examples of the required input/ouput data mapping.

Chan et al [15] also used ANN for processing of stripping analysis responses for identifying and quantifying heavy metals in the presence of intermetallic compound formation. The networks were shown to be capable of (i) correlating voltammetric responses with individual heavy metals in complex mixtures, (ii) determining the relationship between responses and concentrations and (iii) rapidly determining concentrations of individual components from mixtures once trained. Using simulated data, modeled after complex interactions experimentally observed in samples containing Cu & Zn, it has been demonstrated that networks containing three layers of neurons can be trained to calculate concentrations under a variety of complicated situations. The authors have trained the network to simultaneously determine concentrations of four metals (Cu, Pb, Cd and Zn) in a concentration range where all responses were complicated by intermetallic compound formation (1-500 ppb).

Corrosion

Corrosion is one of the active areas of research in electrochemistry. Rosen and Silverman [16] applied ANN to predict corrosion from polarization scans. Here the ANN is made to recognize certain relationships in potentiodynamic polarization scans 'to predict if crevice corrosion, pitting, and general corrosion are possible concerns. They used 87 polarization scans to train the network using back propagation model. The input variables are passive current density, repassivation potential, pitting potential, current density at scan reversal and potential at anodic-to-cathodic transition.

Crevice corrosion, like other modes of localized corrosion, is a stochastic process which should be treated using probability laws and concepts. Crevice corrosion of stainless steels and related alloys in near neutral chloride containing environment is a very widespread form of localized corrosion in industrial plants where sea water is a common coolant medium and the complexity gives rise to many types of potentially dangerous crevice corrosion. The complexity of the processes occurring during the onset and development of crevice corrosion and the poor reliability of the available test methods led to the development of artificial intelligent systems to probe this phenomena. Trasatti and Mazza [17] developed a neural network to rapidly predict and study the crevice corrosion in alloys in chloride containing environments. The predictions of the ANN are in reasonable agreement with those expected on the basis of reported field experience.

A neural network based automatic pipeline inspection system was developed by Suna and Berns [18]. Neural network was successfully used for the study of inhibitors by several workers [19,20]. It has also been used for the forensic analysis of car paints from IR spectra [21] as well as for the online real time measurement of coating thickness [22].

Sensors

A wide variety of sensors are used in electrochemical research. Conducting polymers such as polypyrrole and polyaniline present a new class of organic polymers that are capable of molecular interactions and being able to interact, chemically or electrochemically with the species of interest for detection. Problems exist due to the dynamic nature of the polymers thereby mitigating against their successful application as novel sensors. Talaie and Romagnoli [23] examined these problems through the introduction of a new series of integrated artificial intelligence/conducting polymer based sensor. In this type of sensors analytical responses, which look irreversible and non producible, are combined by an ANN trained computer by which reproducible output, based on the created model and pattern by the computerized system can be predicted.

Talaie et al [24] designed an ANN based conducting polymer biosensor for the detection of trace concentrations of formate. The data collected (current signals) from amperometric detection of the polypyrrole formate biosensor were transferred into an ANN trained computer for modeling and prediction of output. This method was found to have advantages of being more selective and more accurate over conventional methods. ANN was applied to real time operation of conducting polymer sensor also [25]. This method is capable of creating different patterns and models based on an on-line data collection from a multichannel A/D device. Depending on the inputs, the ANN creates best possible patterns, based on selected parameters, to classify the type of ions existing in the operational environment.

Choi et al [26] investigated the characteristic patterns of adsorption-desorption of alcohols on lipids using quartz crystal microbalance. The characteristic parameters were deduced from the retardation of adsorption and the frequency change. A neural network pattern recognition system was employed to analyse the response curve and hence to carryout chemical identification. Kinetic determination of organic vapour mixtures with single piezoelectric quartz crystal sensor using artificial neural networks and partial least squares was carried out by Xing and He [27]. From the adsorption and desorption curves of analytes, which had somewhat differences in shape, frequency shifts from ten time windows were taken as inputs for two chemometric methods, partial least squares and ANN. The prediction was better for ANN.

An integrated ANN based conducting polymer pH sensor has also been reported [28]. Endres et al [29] developed a neural network based thin film SnO_2 sensor system for the simultaneous detection of CO and NO_2.

Quality classification of grain using an array of electrochemical sensors combined with pattern recognition by neural network approach was carried out by Stetter et al [30]. The authors recorded signals from four sensors for four different catalyst temperatures in order to generate 16 signals for each grain odor sample. The 16 sensor signals were treated as a 16-dimensional vector or pattern of responses that was characteristic of the odor sample. The patterns for different grain odor samples were compared using both nearest neighbour analysis and a commercial neural network simulation program.

Other applications of ANN include battery performance study and electrolytic cell control. Young et al [31] studied the feasibility of using neural network technique for performance predictions of long-string energy storage systems. They found that in a long-string lead acid peak-shaving battery, it was possible to select 70% of high performance cells, without any false selections from the low-performance cells and it was possible to identify nearly 96% of the poor performance cells with none of the high-performance cells mis-selected. Hence this method can be adopted as a routine one for maintenance of battery systems. A somewhat similar type of intelligent control of the feeding of aluminum electrolytic cells using neural networks was also developed [32]. To be efficient, the control of alumina feeding of the electrolytic cell must be based on cell resistance, alumina concentration and cell state. Most control schemes now in use are based on cell resistance only and not explicitly tied to concentration nor to cell state. This results in the cell operating at non optimal concentrations, and cell efficiency is diminished. To overcome this, a learning vector quantization type of neural network was built and trained to recognize cell state. Knowing the state of the cell and its resistance, concentration can be estimated using predetermined regression functions. The decision criteria for the control logic are then consequently adopted. A closed loop control scheme is thus obtained. This flexible and intelligent character of the neural control can provide a considerable advantage as compared to the standard control.

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