Artificial Neural Network Electronic Nose For Volatile Organic Compounds

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Abstract

Advanced microsystems that include, sensors, interface-circuits, and pattern-recognition integrated monolithically or in a hybrid module are needed for civilian, military, and space applications. These include: automotive, medical applications, environmental engineering, and manufacturing automation. ASICS with Artificial Neural Networks (ANN) are considered in this paper, with the objective of recognizing air-borne volatile organic compounds, especially alcohols, ethers, esters, halocarbons, NH_3, NO_2, and other warfare agent simulants. The ASIC inputs are connected to the outputs from array-distributed sensors which measure three-features for identifying each of four chemicals. A Specialized Reinforcement Neural Network (RNN) learning approach is chosen for the chemicals classification problem. Hardware implementation of the RNN is presented for 2 μm CMOS process, MOSIS chip. Design implementation and evaluation are also presented.[1]

1 Introduction

Artificial neural networks offer potential advantages in non-parametric pattern recognition, classification, and distinction among multicomponent chemical sensor systems. A generic architecture of an electronic nose is given in [1],[2], where input odors are sensed as analog voltage, current, or resistor values. Sensor output is then converted into digital format and then processed through a sensor processor, an array processor, and a knowledge based system with pattern recognition engine. The pattern recognition engine is trained by updating rules to corelate the output chemical (odor) to a set of input features. The electronic nose output response from an unknown chemical is based on comparison against stored knowledge base data.

Neural network methods for pattern recognition have recently been proposed for use with chemical sensors. Most published research about NN usage for chemical sensing is mainly verified by computers in simulation of supervised back-propagation methods: Niebling in [3] used a multilayer perceptron neural network for problem classification. His simulations showed that neural networks are appropriate for nonlinear signal evaluations, where statistical pattern recognition methods may not be, since neural networks determine their network connections (weights and biases) through training phase.

Fryder et al [4] presented computer simulation results for an electronic nose performance in pattern recognition by using a back-propagation artificial neural network, with a specific calibration gas. Schweizer-Berberich [5] used feedforward back-propagation for training with randomized input patterns. Hong in [6] presented a number of basic component analysis of a gas sensor array with twelve gas samples. The information *might* be used for gas identification using neural networks. In [7] fuzzy arithmetic is used in a back-propagation artificial neural network, this may allow for both quantitative and qualitative chemical sensing.

Increased interest in electronic/microelectronic integrated chemical substance detection and classification is expected in automation process manufacturing, e.g. in process control for VLSI semiconductor wafer fabrication [8], [9], [10], [11]; Consumer and automotive industry recent requirements for active protection of passengers in automotive vehicles from inherent pollutants such as nitric oxides (NO), hydro-

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carbons (HC), and carbon monoxide (CO) [13], [12]; Possible replication of human Olfactory System in an Electronic Nose [1], [2]; Other medical applications, e.g glucose sensors [14]; and environmental control.

The work in this paper presents an Artificial Neural Network (ANN) electronic nose, intended particularly for volatile organic compounds. The electronic nose considers inputs from arrays of conducting polymer (polyaniline and polypyrrole [15]) thin film sensors. Measurements of sensors polymer resistance are used as key features in determining chemical vapors.

2 ANN Approaches

Learning methods in ANNs can be classified as: Supervised learning; Unsupervised learning; and Reinforcement Neural Networks (RNNs). For chemical sensing problems detailed description (Models) of the features is usually difficult or not available. Thus, practical supervised learning is difficult. Chemical sensing arrays can however provide some evaluative knowledge about the features of the different chemicals. Thus, one expect to do better than with unsupervised learning. Consideration of reinforcement learning matches the electronic nose problem need.
RNN is most suitable in situations where there is not enough detailed information available to the network, only right or wrong assessment. Sometimes this type of learning is called "learning with a critic," as opposed to "learning with a teacher" in supervised neural networks [16]. There are several classes of reinforcement learning: (1) Where a specific reinforcement is attached to a specific Input/Output (I/O) association pair; (2) Where the environment is modeled randomly and therefore the reinforcement is expressed probabilistically; and (3) Where the environment is dynamic and the reinforcement is given after a series of consecutive actions. A general block representation for the reinforcement learning is given in Fig. 1. Where the network interacts with its environment and receives a reinforcement signal which could be a scalar or a vector quantity, in response to the network's actions on the environment. The reinforcement signal (ρ_i), at the i^{th} neuron is an indication of the cumulative correct response.

This paper presents a specific RNN algorithm and a VLSI circuit implementation for recognizing four chemicals, each of which is characterized by the percentage change in the resistanse of sensor array as a function of three features.: Temperature; Saturation level; and Sensor exposure time to the analyte/air mixture.

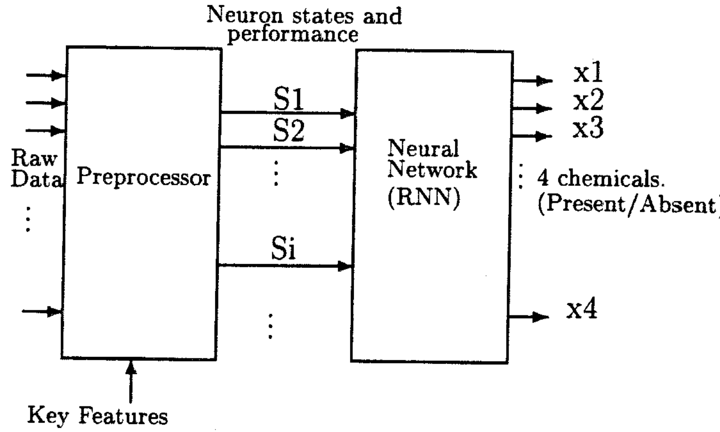

Figure 1: Reinforcement learning: General block representation.

3 RNN Design

In this paper a specialized RNN is developed to classify FOUR different chemicals, based on their distinguishing features. The features composition of each chemical are presented in the form of a TRAINING VECTOR to the NN. The NN system consists of an input layer with FOUR input neurons. The input features vector is multiplied by weights pertaining to each neuron and then passed through a nonlinear element. Each input is evaluated by the network to develop a distribution of reward or penalty signals and to consequently accomplish classification of the chemicals. The synaptic weights will iteretively converge in order to reflect the characteristics of the chemicals. The network outputs conform to the appropriate type of chemical. A block diagram for the implemented RNN system is depicted in Fig. 2 and Fig. 3 where the change in weights (ΔW_{ij}) is made equal to the reinforcement rate (R_i) (which is a function of a learning rate (η) times the reinforcement signal) multiplied by eligibility (E_{ij}). The learning rate is higher for positive reinforcement (reward) and lower for negative reinforcement (penalty).

$$\Delta W_{ij} = R_i(\eta)E_{ij}. \tag{1}$$

Several algorithms for RNN have been researched and investigated including [17], [18] with only one published implementation using pRAM in [17].

4 Electronic Nose Implementation

The specialized RNN approach is used to classify four volatile compounds: acetone, methanol, benzene and chloroform. The factor g_i in the neurons states,

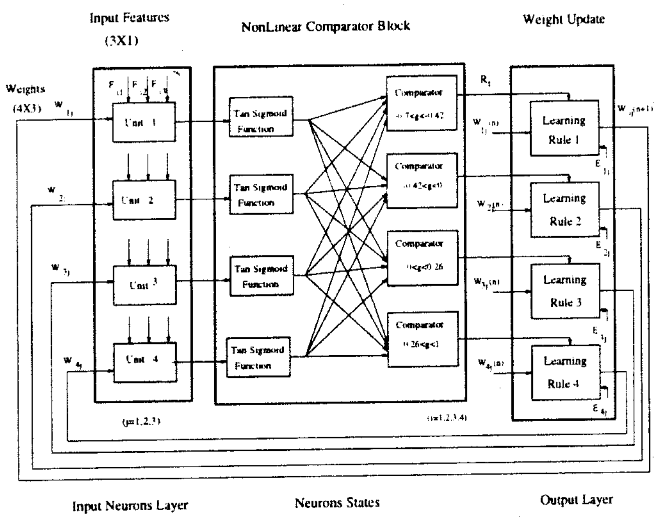

Figure 2: ANN Block diagram for identifying methanol, acetone, benzene, and chloroform based on sensor resistance measurements. Each chemical has 3-features. The learning approach is the specialized RNN.

Fig. 2, is a measure of the percentage change in resistance of the sensor, and R_i is the reinforcement rate. Sensors of spun polypyrrole soluble onto integrated gold electrode arrays (15 μm spacing between electrodes) [15] are assumed, for measuring the percentage changes in resistance after 5-seconds exposure of the sensor to static air saturated with the analyte at room temperature. Conducting polymer thin-film sensors are chosen since each sensor gives a large increase in resistance with different analytes.

With sensors coated with doped polypyrrole and exposed to air saturated with analyte vapor for 5-seconds at room temperature, the percentage change in sensor resistance is given as

$$\Delta R_o = \frac{R - R_o}{R_o}. \qquad (2)$$

For the considered chemicals: Methanol (with $\Delta R_o = -o.7$), Acetone (with $\Delta R_o = -o.42$), Benzene (with $\Delta R_o = 0.26$), and Chloroform (with $\Delta R_o = 1$).

Matrix formulation and supporting MATLAB simulation of the specialized approach are given by the author in [19]. The considered features for chemical classification are: Temperature, Saturation level, and Sensor exposure time to the analyte/air mixture.

Published practical gas sensors include: Highly sensitive flammable gas detector [20]; Semiconductor gas sensor array of 4-elements for SnO_2 [12]; Sensors for detecting NO and CO traces [13]; Sensors for recognizing two vapors; and Glucose sensors using immobilized glucose oxidants with long term stability [14].

5 Summary and Conclusions

In this paper, a novel ANN system is designed and simulated for integrated circuit chip implementation of an electronic nose capable of recognizing Methanol, Acetone, Benzene, and Chloroform. The design may be altered, to be programmable, for recognizing other volatile organic compounds. The inputs to the ANN system are the measurements from the polypyrrole spun integrated electrode sensor arrays. The key features used for identifying the chemical vapors are: temperature; saturation level; and sensor exposure time to the analyte/air mixture. Each feature affect the sensor resistance change differently. Other features may be added at the cost of expanded hardware. Conducting polymer sensors have been used since they give a considerable increase or decrease in resistance with different analytes.

The RNN algorithm and its hardware implementation present a key building block in the development of bionic brain [20], upon testing and verification. The RNN learning approach is generally more robust than traditional statistical methods. All VLSICs are implemented using ORBIT facilities through the MOSIS 2 μm n-well CMOS process.

Totally supervised learning is NOT recommended with chemical-sensors. This could be due to features overlap and incompleteness in measurements. Although unsupervised NN approaches (e.g. SOFM) may still have potential in chemical recognition, the performance of RNN Learning is guided by the reward and penalty which are readily available, based on sensors measurements. Prototype test results will be presented.

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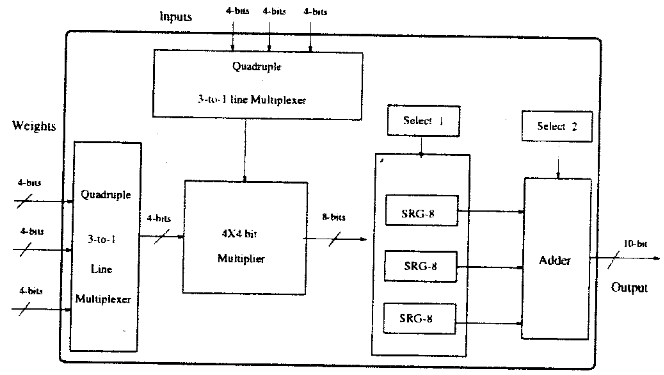

Figure 3: Unit block diagram: Multiplier-Adder Circuit.

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