ARTIFICIAL NEURAL NETWORKS FOR E-NOSE ^{1.} T.Rajthilak, ^{2.} M.Sasikumar

ABSTRACT:

Neural networks have seen an explosion of interest over the last few years. The primary appeal of neural networks is their ability to emulate the brain's pattern-recognition skills. The sweeping success of neural networks can be attributed to some key factors. The paper explicates the features of neural networks and also enlightens how neural networks are being successfully applied across an extraordinary range of problem domains, in areas as diverse as finance, medical, engineering, physics etc...

Electronic nose is a new and promising technology which is rapidly becoming a valuable tool for the organoleptic evaluation of food parameters related to taste and smell and could replace human sensory panels in quality control applications, where the objective, rapid and synthetic evaluation of the aroma of many specimens is required. An electronic nose is generally composed of a chemical sensing system (e.g., sensor array or spectrometer) and a pattern recognition system (e.g., artificial neural network). We are developing electronic noses for the automated identification of volatile chemicals for environmental and medical applications. In this paper, we briefly describe neural networks, electronic nose & show some results from a prototype electronic nose.

1. INTRODUCTION:

All the electronic noses developed so far are based on the same working principle: an array of chemical sensors mimicking the olfactory receptors, matched with a suitable data processing method, allows to retrieve quantitative and qualitative information on the chemical environment. A sensor comprises a material whose physical properties vary according to the concentration of some chemical species. These changes are then translated into an electrical or optical signal which is recorded by a device. Contrary to physical senses some aspects of the human taste and olfaction physiological working principle are still unclear. Because of these intrinsic difficulties toward the understanding of the nature of these senses, only sporadic research on the possibility of designing artificial olfactory systems was performed until the end of the eighties.

1.1 Why use neural networks?

Neural networks, with their remarkable ability to derive meaning from complicated or imprecise data, can be used to extract patterns and detect trends that are too complex to be noticed by either humans or the computer techniques. A trained neural network can be thought of as an "expert" in the category of information it has been given to analyze. This expert can then be used to provide projections given new situations of interest and answer "what if" questions.

Other advantages include:

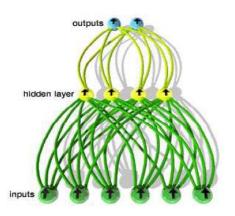
I. Adaptive learning: An ability to learn how to do tasks based on the data given for training or initial experience.

2. *Self-Organization:* An ANN can create its own organization or representation of the information it receives during learning time.

3. Real Time Operation: ANN computations may be carried out in parallel, and special hardware devices are being designed and manufactured which take advantage of this capability.

1.2 Architecture of neural networks:

The commonest type of artificial neural network consists of three groups, or layers, of units: a layer of "input" units is connected to a layer of "hidden" units, which is connected to a layer of "output"



units. (See Figure) The activity of the input units represents the raw information that is fed into the network. The activity of each hidden unit is determined by the activities of the input units and the weights on the connections between the input and the hidden units. The behavior of the output units depends on the activity of the hidden units and the weights between the hidden and output units. This simple type of network is interesting because the hidden units are free to construct their own representations of the input. The weights between the input and hidden units determine when each hidden unit is active, and so by modifying these weights, a hidden unit can choose what it represents. We also distinguish single-layer and multi-layer architectures. The single-layer organization, in which all units are connected to one another, constitutes the most general case and is of more potential computational power than hierarchically structured multi-layer organizations. In multi-layer networks, units are often numbered by layer, instead of following a global numbering.

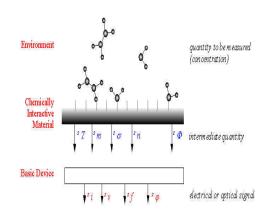
1.3 Pattern Recognition:

An important application of neural networks is pattern recognition. Pattern recognition can be implemented by using a feed-forward neural network that has been trained accordingly. During training, the network is trained to associate outputs with input patterns. When the network is used, it identifies the input pattern and tries to output the associated output pattern. The power of neural networks comes to life when a pattern that has no output associated with it, is given as an input. In this case, the network gives the output that corresponds to a taught input pattern that is least different from the given pattern.

2. How does an electronic nose work?

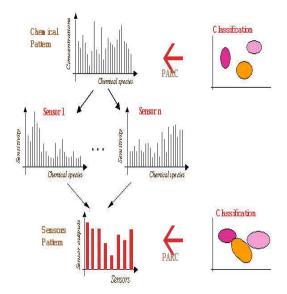
The two main components of an electronic nose are the sensing system and the automated pattern recognition system. The sensing system can be an array of several different sensing elements (e.g., chemical sensors), where each element measures a different property of the sensed chemical, or it can be a single sensing device (e.g., spectrometer) that produces an array of measurements for each chemical, or it can be a combination. Each chemical vapor presented to the sensor array produces a signature or pattern characteristic of the vapor. By presenting many different chemicals to the sensor array, a database of signatures is built up. This database of labeled signatures is used to train the pattern recognition system. The goal of this training process is to configure the recognition system to produce unique classifications of each chemical so that an automated identification can be implemented.





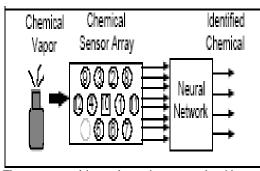
The quantity and complexity of the data collected by sensors array can make conventional chemical analysis of data in an automated fashion difficult. One approach to chemical vapor identification is to build an array of sensors, where each sensor in the array is designed to respond to a specific chemical. With this approach, the number of unique sensors must be at least as great as the number of chemicals being monitored. It is both expensive and difficult to build highly selective chemical sensors. A chemical compound is identified by a pattern of the outputs given by the different sensors, thanks to pattern recognition methods.

Artificial neural networks (ANNs), which have been used to analyze complex data and to recognize patterns, are showing promising results in chemical vapor recognition. When an ANN is combined with a sensor array, the number of detectable chemicals is generally greater than the number of sensors. Also, less selective sensors which are generally less expensive can be used with this approach. Once the ANN is trained for chemical vapor recognition, operation consists of propagating the sensor data through the network. Since this is simply a series of vector- matrix multiplications, unknown chemicals can be rapidly identified in the field. Electronic noses that incorporate ANNs have been demonstrated in various applications. Some of these applications will be discussed later in the paper. Many ANN configurations and training algorithms have been used to build electronic noses including back propagation-trained, feed-forward networks; fuzzy ART maps; Kohonen's self-organizing maps (SOMs); learning

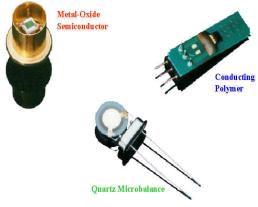


Vector quantizes (LVQs); hamming networks; Boltzmann machines; and Hopfield networks.

Figure illustrates the basic schematic of an electronic nose.



The sensors used in an electronic nose can be either mass transducers (such as Quartz microbalanz or QMB) or chemo-resistors (based on metal-oxides or conducting polymers); some arrays comprise both types of sensors.Currently extensive research is being carried out on the exploitation of metallo-porphyrins as coating material for QMB: the main feature of such sensors is the dependence of the sensing properties (selectivity and sensitivity) on the nature of the substituents of the porphyrin. This flexibility makes this class of compounds of interest for electronic nose applications.



2.1 PROTOTYPE ELECTRONIC NOSE:

One of our prototype electronic noses, shown in Figure 2, is composed of an array of nine tin oxide vapor sensors, a humidity sensor, and a temperature sensor coupled with an ANN. Two types of ANNs were constructed for this prototype: the standard multilayer feed-forward network trained with the back propagation algorithm and the fuzzy ART map algorithm. During operation a chemical vapor is blown across the array, the sensor signals are digitized and fed into the computer, and the ANN (implemented in software) then identifies the chemical. This identification time is limited only by the response time of the chemical sensors, which is on the order of seconds. This prototype nose has been used to identify common household chemicals by their odor.



Figure 2: Photograph of the prototype electronic nose

Figure 3 illustrates the structure of the ANN. The nine tin-oxide sensors are commercially available, Taguchi-type gas sensors. (Sensor 1, TGS 109; Sensors 2 and 3, TGS 822; Sensor 4, TGS 813; Sensor 5, TGS 821; Sensor 6, TGS 824; Sensor 7, TGS 825; Sensor 8, TGS 842; and Sensor 9, TGS 880). Exposure of a tin-oxide sensor to a vapor produces a large change in its electrical resistance. The humidity sensor (Sensor 10: NH-02) and the temperature sensor (Sensors 11: 5KD-5) are used to monitor the conditions of the experiment and are also fed into the ANN.

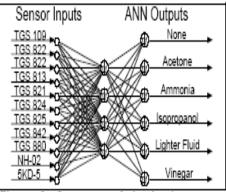
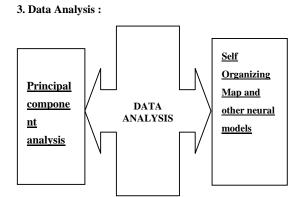


Figure 3: Structure of the backpropagation ANN used in the prototype to identify household chemicals

Although each sensor is designed for a specific chemical, each responds to a wide variety of chemicals. Collectively, these sensors respond with unique signatures patterns) to different chemicals. During the training process, various chemicals with known mixtures are presented to the system. By training on samples of various chemicals, the ANN learns to recognize the different chemicals.

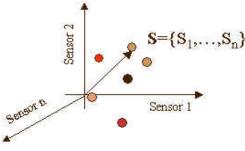


$$\begin{aligned} \mathbf{X}_{tm} = \mathbf{U}_{tm} \cdot \mathbf{S}_{mmi} \mathbf{V}_{mm} = \\ (\mathbf{u}_{1}, \dots, \mathbf{u}_{m}) \begin{pmatrix} \mathbf{s}_{1} & 0 & \dots & 0 \\ 0 & \mathbf{s}_{2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \mathbf{s}_{m} \end{pmatrix} \cdot (\mathbf{v}_{1}, \dots, \mathbf{v}_{m}) \end{aligned}$$

vectors \mathbf{v} are the base of the PC space, vectors \mathbf{u} are the projection of experimental data in the PC space scalars \mathbf{s} are the singular values, they are considered as a measure of the particular contribution to the systematic variance of the respective principal component.

3.1 Principal component analysis:

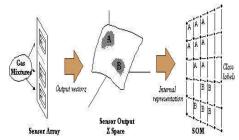
The data of an electronic nose experiment are represented in a multidimensional space (the sensor space), whose dimension is equal to the number of sensors in the array. A single measure is an ndimensional vector.



Let **X** be the data matrix, and let us consider the Singular Value Decomposition of **X**:

vectors \mathbf{v} are the base of the PC space, vectors \mathbf{u} are the projection of experimental data in the PC space scalars \mathbf{s} are the singular values, they are considered as a measure of the particular contribution to the systematic variance of the respective principal component.

3.2 Self Organizing Map and other neural models: SOM belongs to the category of competitive learning methods and is based on unsupervised learning. This last aspect means that the SOM algorithm does not require any additional information but the sensors output. SOM is a network formed by N neurons arranged as the nodes of a planar grid.



4. Applications for Neural Networks:

Neural networks are applicable in virtually every situation in which a relationship between the predictor variables (independents, inputs) and predicted variables (dependents, outputs) exists, even when that relationship is very complex and not easy to articulate in the usual terms of "correlations" or "differences between groups." A few representative examples of problems to which neural network analysis has been applied successfully are:

- * Detection of medical phenomena
- * Stock market prediction.
- * Monitoring the condition of machinery.
- * Industrial process control.
- * data validation
- * target marketing

4.1 Electronic Noses for Medicine:

Because the sense of smell is an important sense to the physician, an electronic nose has applicability as a diagnostic tool. An electronic nose can examine odors from the body (e.g., breath, wounds, body fluids, etc.) and identify possible problems. Odors in the breath can be indicative of gastrointestinal problems, sinus problems, infections, diabetes, and liver problems. Infected wounds and tissues emit distinctive odors that can be detected by an electronic nose. Odors coming from body fluids can indicate liver and bladder problems. Currently, an electronic nose for examining wound infections is being tested at South Manchester University Hospital. A more futuristic application of electronic noses has been recently proposed for telesurgery. While the inclusion of visual, aural, and tactile senses into telepresent systems is widespread, the sense of smell has been largely ignored. An electronic nose will potentially be a key component in an olfactory input to telepresent virtual reality systems including telesurgery. The electronic nose would identify odors in the remote surgical environment. These identified odors would then be electronically transmitted to another site where an odor generation system would recreate them.

5. Conclusion:

The computing world has a lot to gain from neural networks. Their ability to learn by example makes them very flexible and powerful. Furthermore there is no need to devise an algorithm in order to perform a specific task; i.e. there is no need to understand the internal mechanisms of that task. Perhaps the most exciting aspect of neural networks is the possibility that some day 'conscious' networks might be produced. There are a number of scientists arguing that consciousness is a 'mechanical' property and that 'conscious' neural networks are a realistic possibility.

ANNs are used experimentally to implement electronic noses. Electronic noses have several potential applications. The electronic nose would identify odours in the remote surgical environment. These identified odours would then be electronically transmitted to another site where a door generation system would recreate them. Because the sense of smell can be an important sense to the surgeon, telesmell would enhance telepresent surgery. The major differences between electronic noses and standard analytical chemistry equipment are that electronic noses

(1) Produce a qualitative output

(2) Can often be easier to automate

(3) Can be used in real-time analysis.

Further work involves in comparing neural network sensor analysis to more conventional techniques, exploring other neural network paradigms, and evolving the preliminary prototypes to field systems. Finally, I would like to state that even though neural networks have a bright prospective we will only get the best of them when they are integrated with computing, AI, fuzzy logic and related subjects.

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