

ELECTRONIC NOSES AND THEIR APPLICATIONS

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ABSTRACT

Electronic/artificial noses are being developed as systems for the automated detection and classification of odors, vapors, and gases. 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 an electronic nose, show some results from a prototype electronic nose, and discuss applications of electronic noses in the environmental, medical, and food industries.

INTRODUCTION

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.

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 [1]. 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 backpropagation-trained, feed-forward networks; fuzzy ARTmaps; Kohonen's self-organizing maps (SOMs); learning vector quantizers (LVQs); Hamming networks; Boltzmann machines; and Hopfield networks. Figure 1 illustrates the basic schematic of an electronic nose.

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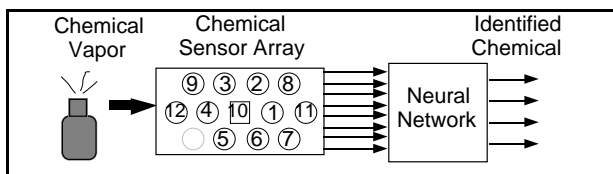


Figure 1: Schematic diagram of an electronic nose

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 backpropagation algorithm and the fuzzy ARTmap algorithm [2]. 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 [3].

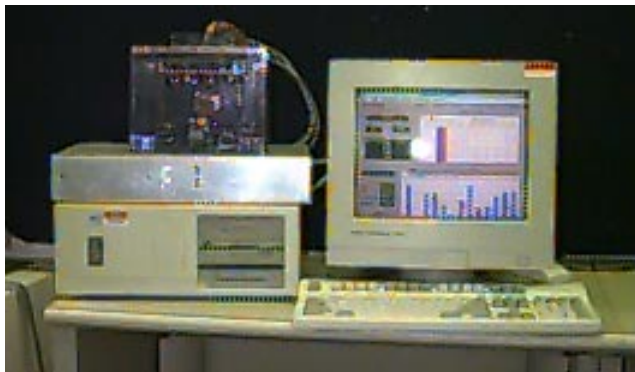


Figure 2: Photograph of the prototype electronic nose

Figure 3 illustrates the structure of the ANN. The nine tin-oxide sensors are commercially available Taguchi-type gas sensors obtained from Figaro Co. Ltd. (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.

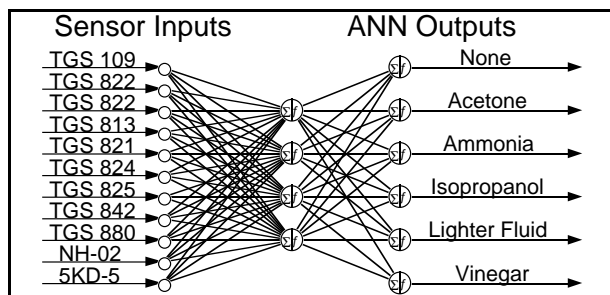


Figure 3: Structure of the backpropagation ANN used in the prototype to identify household chemicals

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.

This prototype nose has been tested on a variety of household and office supply chemicals including acetone, ammonia, ethanol, glass cleaner, contact cement, correction fluid, iso-propanol, lighter fluid, methanol, rubber cement and vinegar. For the results shown in the paper, five of these chemicals were used: acetone, ammonia, isopropanol, lighter fluid, and vinegar. Another category, "none" was used to denote the absence of all chemicals except those normally found in the air which resulted in six output categories from the ANN. Table 1 lists the training parameters for one backpropagation and one fuzzy ARTmap network.

Backpropagation	
Architecture:	11-11-6 feedforward
Activation:	Logistic Sigmoidal
Learning Rate:	0.10
Momentum:	0.90
No. of Epochs:	1369
Fuzzy ARTMap	
Training Vigilance:	0.98
Testing Vigilance:	0.80
No. of Epochs:	3

Table 1: ANN training parameters

Both networks were trained using randomly selected sample sensor inputs. The ANNs used here were not trained to quantify the concentration level of the identified analytes, but were trained with samples with different concentrations of the analytes. This allowed the ANN to

generalize well on the test data set. Performance levels of the two networks were basically equivalent ranging from 89.7% to 98.2% correct identification on the test set depending on the random selection of training patterns. Table 2 summarizes one set of network performances for novel sensor inputs.

Num Train	Num Test	Input Substance	% Correct	
			BP	FA
67	28	None	96.4	96.4
75	22	Acetone	100	100
64	14	Ammonia	100	100
93	28	Isopropanol	92.9	100
5	3	Ammonia & Isopr.	00.0	66.7
106	25	Lighter Fluid	100	96.0
74	27	Amm. & Lighter Fluid	100	92.6
66	21	Vinegar	81.0	95.2
68	26	Ammonia & Vinegar	92.3	76.9
1	2	Isopropanol & Vinegar	00.0	00.0
619	196	Totals	92.9	93.4

Table 2: ANN performance for backpropagation (BP) and fuzzy ARTmap (FA)

Figures 4 and 5 illustrate the responses of the sensors and the ANN classification for a variety of test chemicals presented to the ANNs. The ANN was able to correctly classify the test samples with only small residual errors.

While the ANN used here was not trained to quantify the concentration level of the identified analytes, it was trained with samples with different concentrations of the analytes. This allowed the ANN to generalize well on the test data set.

From the responses of the sensors to the analytes, one can easily see that the individual sensors in the array are not selective (Figure 4). In addition, when a mixture of two or more chemicals is presented to the sensor array, the resultant pattern (sensor values) may be even harder to analyze (see Figure 5: c, d, and e). Thus, analyzing the sensor responses separately may not be adequate to yield the classification accuracy achieved by analyzing the data in parallel.

ELECTRONIC NOSES FOR ENVIRONMENTAL MONITORING

Enormous amounts of hazardous waste (nuclear, chemical, and mixed wastes) were generated by more than 40 years of weapons' production in the U.S. Department of Energy's weapons' complex. The Pacific Northwest National Laboratory is exploring the technologies required to perform environmental restoration and waste management in a cost effective manner. This effort includes the development of portable, inexpensive systems capable of real-

time identification of contaminants in the field. Electronic noses fit this category.

Environmental applications of electronic noses include analysis of fuel mixtures [4], detection of oil leaks [5], testing ground water for odors, and identification of household odors [3]. Potential applications include identification of toxic wastes, air quality monitoring, and monitoring factory emissions.

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 [6].

A more futuristic application of electronic noses has been recently proposed for telesurgery [7]. 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.

ELECTRONIC NOSES FOR THE FOOD INDUSTRY

Currently, the biggest market for electronic noses is the food industry [8]. Applications of electronic noses in the food industry include quality assessment in food production [9], inspection of food quality by odor, control of food cooking processes [10], inspection of fish, monitoring the fermentation process, checking rancidity of mayonnaise, verifying if orange juice is natural, monitoring food and beverage odors [11], grading whiskey, inspection of beverage containers, checking plastic wrap for containment of onion odor, and automated flavor control [12] to name a

few. In some instances electronic noses can be used to augment or replace panels of human experts. In other cases, electronic noses can be used to reduce the amount of analytical chemistry that is performed in food production especially when qualitative results will do.

DISCUSSION

In this paper we discussed electronic noses, a prototype system that identifies common household chemicals, and applications of electronic noses in the environmental, medical, and food industries. 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, and (3) can be used in real-time analysis.

REFERENCES

- [1] B.S. Hoffheins, *Using Sensor Arrays and Pattern Recognition to Identify Organic Compounds*. MS-Thesis, The University of Tennessee, Knoxville, TN, 1989.
- [2] G.A. Carpenter, S. Grossberg, N. Markuzon, J.H. Reynolds, and D.B. Rosen, "Fuzzy ARTMAP: A Neural Network Architecture for Incremental Supervised Learning of Analog Multidimensional Maps," *IEEE Transactions on Neural Networks*, vol. 3, 698 -713.
- [3] P.E. Keller, R.T. Kouzes, and L.J. Kangas, "Three Neural Network Based Sensor Systems for Environmental Monitoring," *IEEE Electro 94 Conference Proceedings*, Boston, MA, 1994, pp. 377-382.
- [4] R.J. Lauf and B.S. Hoffheins, "Analysis of Liquid Fuels Using a Gas Sensor Array," *Fuel*, vol. 70, pp. 935-940, 1991.
- [5] H.V. Shurmur, "The fifth sense: on the scent of the electronic nose," *IEE Review*, pp. 95-58, March 1990.
- [6] K. Pope, "Technology Improves on the Nose As Science Tries to Imitate Smell," *Wall Street Journal*, pp. B1-2, 1 March 1995.
- [7] P.E. Keller, R.T. Kouzes, L.J. Kangas, and S. Hashem, "Transmission of Olfactory Information for Telemedicine," *Interactive Technology and the New Paradigm for Healthcare*, R.M. Satava, K. Morgan, H.B. Sieburg, R. Mattheus, and J.P. Christensen (ed.s), IOS Press, Amsterdam, 1995, pp. 168-172.
- [8] A.M. Pisanelli, A.A. Qutob, P. Travers, S. Szysko and K.C. Persaud, "Applications of Multi Array Polymer Sensors to Food Industries," *Life Chemistry Reports*, vol. 11, pp. 303-308, 1994.
- [9] "Going the nose one better," *Food Engineering*, November 1994.
- [10] A. Almeida, "Neural network in oven prevents overcooking," *The Institute*, pp. 3, Nov. 1994.
- [11] J.W. Gardner, E.L. Hines, and M. Wilkinson, Application of Artificial Neural Networks to an Electronic Olfactory System. *Measurement Science and Technology*, vol. 1, 1990.
- [12] T. Moriizumi, T. Nakamoto, and Y. Sakuraba, "Pattern Recognition in Electronic Noses by Artificial Neural Network Models," *Sensors and Sensory Systems for an Electronic Nose*. Kluwer Academic Publishers, J.W. Gardner and P.N. Bartlett (ed.s), Amsterdam, The Netherlands, 1992, pp. 217-236.

These results from the prototype electronic nose demonstrate the pattern recognition capabilities of the neural network paradigm in sensor analysis, especially when the individual sensors are not highly selective. In addition, the prototype presented here has several advantages for real-world applications including compactness, portability, real-time analysis, and automation. Further work will involve comparing neural network sensor analysis to more conventional techniques, exploring other neural network paradigms, and evolving the preliminary prototypes to field systems.

Information on ANN developments at Pacific Northwest National Laboratory is available on the World Wide Web at:

<http://www.emsl.pnl.gov:2080/docs/cie/neural/>

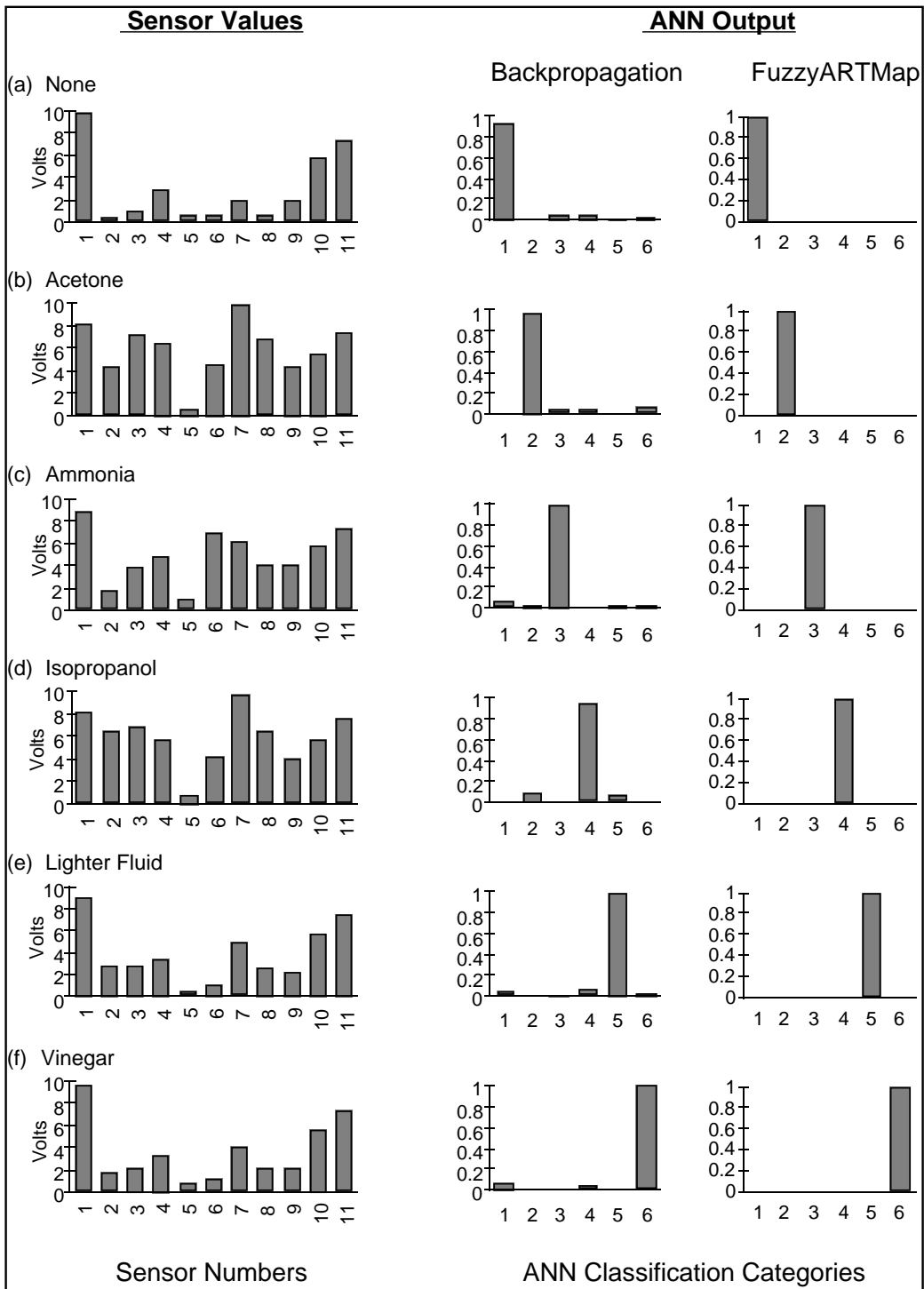


Figure 4: Sample responses and ANN classifications. Sensor numbers and ANN classification categories correspond to those found in Figure 3.

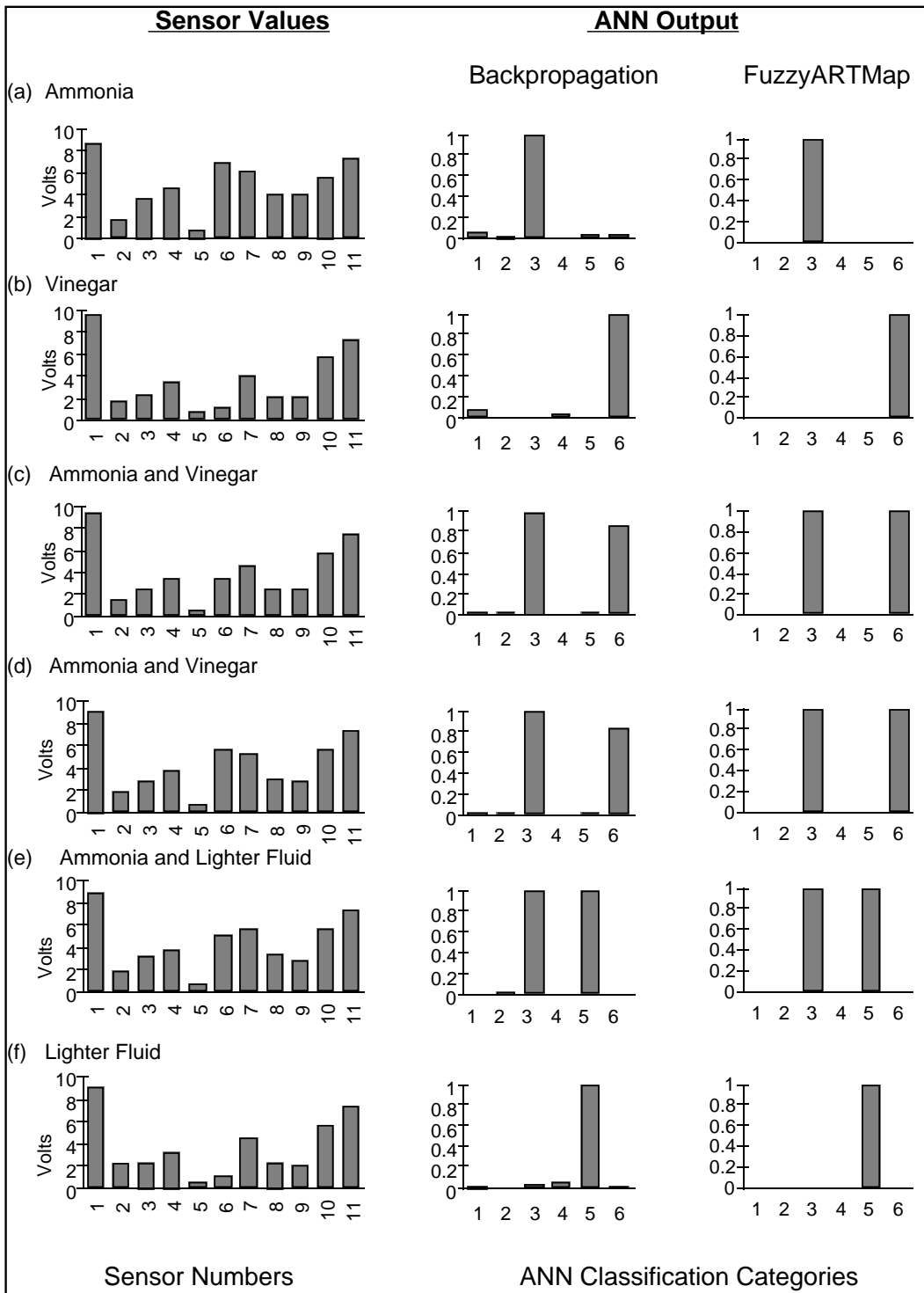


Figure 5: Sample responses and ANN classifications. Sensor numbers and ANN classification categories correspond to those found in Figure 3.