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NEURAL NETWORK BASED DATA ANALYSIS FOR CHEMICAL SENSOR ARRAYS

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ABSTRACT

Compact, portable systems capable of quickly identifying contaminants in the field are of great importance when monitoring the environment. In this paper, we examine the effectiveness of using artificial neural networks for real-time data analysis of a sensor array. Analyzing the sensor data in parallel may allow for rapid identification of contaminants in the field without requiring highly selective individual sensors. We use a prototype sensor array which consists of nine tin-oxide Taguchi-type sensors, a temperature sensor, and a humidity sensor. We illustrate that by using neural network based analysis of the sensor data, the selectivity of the sensor array may be significantly improved, especially when some (or all) the sensors are not highly selective.

Keywords: neural network, sensor array, environmental monitoring, sensor selectivity.

1 INTRODUCTION

One of the missions of the Pacific Northwest Laboratory is to examine and develop new technologies for environmental restoration and waste management at the U.S. Department of Energy's Hanford Site[1] (a former

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plutonium production facility). Enormous amounts of hazardous waste were generated during more than 40 years of plutonium production at the Hanford Site. There is an estimated 1700 waste sites distributed around the 1400 square kilometers (560 square miles) of southeastern Washington state (USA) that comprise the Hanford Site. This waste includes nuclear waste (e.g., fission products), toxic chemical waste (e.g., carbon tetrachloride, ferrocyanide, nitrates, etc.), and mixed waste (combined radioactive and chemical waste). The current mission at the Hanford Site is environmental restoration and waste management.

As part of this mission, the Pacific Northwest 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. The objective of our research is to demonstrate the potential information processing capabilities of the neural network paradigm in sensor analysis.

A difficult problem in identifying contaminants in the field is the need for highly sensitive and selective sensors, which are often expensive and sometimes difficult to achieve.[2] This led to research on sensor arrays compromising a set of sensors whose responses are collectively analyzed.[2–4] When a sensor array is analyzed in parallel, more analytes can be identified than by relying separately on the individual sensors.[3]

The use of artificial neural networks (ANNs) for analyzing sensor data allows for real-time parallel processing of the data. Artificial neural networks are widely used in data processing applications where real-time data analysis and information extraction are required. One advantage of the neural network approach is that most of the intense computation takes place during the training process. Once the ANN is trained for a particular task, operation is relatively fast. Real-time classification of unknown samples mainly involves simple matrix manipulation and application of look-up tables (activation function). Thus, unknown samples can be rapidly identified in the field.

2 SENSOR DATA ANALYSIS

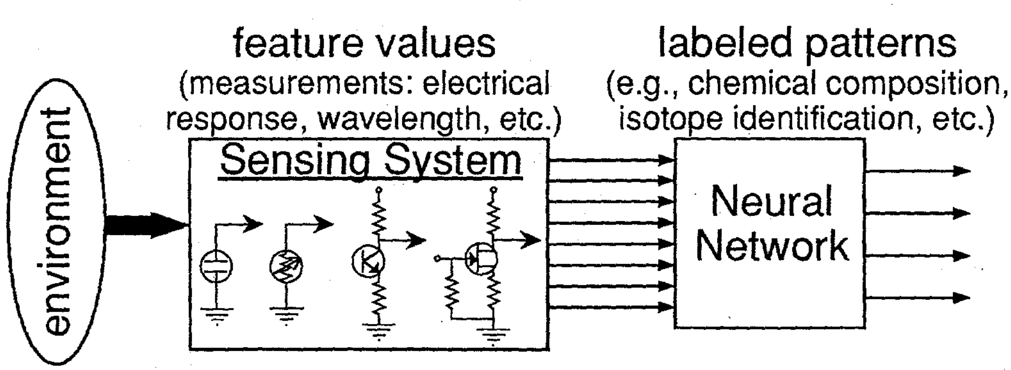

Figure 1: Sensor system combined with an ANN

There are many real-time (rapid response) and remote sensing applications that require an inexpensive, compact, and automated system for identifying an object (e.g., target, chemical, isotope). Such a system can be built by combining a sensor array with an ANN. A generic system is shown in Figure 1.

The quantity and complexity of the data collected by sensor arrays can make conventional analysis of data difficult. ANNs, which have been used to analyze complex data and for pattern recognition, could be a better choice for sensor data analysis. A common approach in sensor analysis is to build an array of sensors, where each sensor in the array is designed to respond to a specific analyte. With this approach, the number of sensors must be at least as great as the number of analytes being monitored. When an ANN is combined with a sensor array, the number of detectable analytes is generally greater than the number of sensors.[3] A sensor array is composed of several sensing elements, where each element measures a different property of the sensed sample. Each object (e.g., target, chemical, isotope) presented to the sensor array produces a signature or pattern characteristic of the object. By presenting many different objects to the sensor array, a database of signatures can be built up. From this database, training sets and test sets are generated. These sets are collections of labeled patterns (signatures) representative of the desired identification mapping. The training sets are used to configure the ANNs. The goal of this training is to learn an association between the sensor array patterns and the labels representing the data.

When a chemical sensor array is combined with an automated data analysis system (such as an ANN) to identify vapors, it is often referred to as an artificial or electronic nose.[4] Several researchers have developed electronic noses that incorporate ANNs for use in applications including monitoring food and beverage odors,[5–7] analyzing fuel mixtures,[8] quantifying individual components in gas mixtures,[9] and environmental monitoring.[10] Several ANN configurations have been used in electronic noses including backpropagation-trained, feed-forward networks; Kohonen's self-organizing networks; Boltzmann machines; and Hopfield networks.[11] This paper extends the work by Keller *et al.*[10] in the area of environmental monitoring. We here examine some aspects relating to identifying mixtures of analytes.

3 A PROTOTYPE CHEMICAL VAPOR SENSING SYSTEM

This system consists of an array of nine tin-oxide gas sensors, a humidity sensor, and a temperature sensor to examine the environment. Although each sensor is designed for a specific chemical, each responds to a wide variety of chemical vapors. 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. In the initial studies, the backpropagation algorithm was used to train the ANN to provide the correct analysis of the presented chemicals.

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.[12] The humidity sensor (Sensor 10: NH-02) and the temperature sensor (Sensor 11: 5KD-5) are used to monitor the conditions of the experiment and are also fed into the ANN.

An ANN was constructed as a multilayer feedforward network and was trained with the backpropagation of error algorithm[13] by using a training set from the sensor database. The network has one hidden layer with four hidden units. The activation function for the hidden units as well as the output units is the logistic sigmoid function $g(s) = (1 + e^{-s})^{-1}$. The training set consists of 177 patterns which corresponds to five household chemicals: acetone, ammonia, isopropanol alcohol, lighter fluid, and vinegar. We used another category, "none," to denote the absence of all chemicals except those normally found in the air. This resulted in six output categories from the ANN. Figure 2 illustrates the network layout.

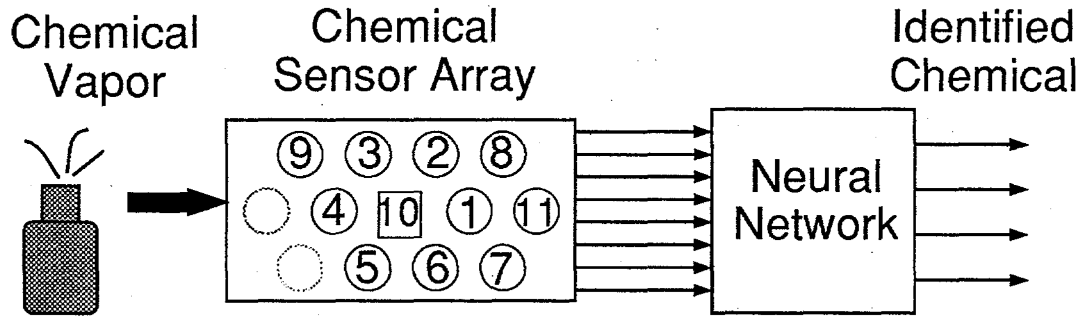

Figure 2: ANN used to identify household chemicals.

During operation, the sensor array "smells" a vapor, the sensor signals are digitized and fed into a 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 a few seconds.

4 DISCUSSION AND CONCLUSIONS

Figures 4 and 5 illustrate the responses of the sensors and the ANN classification for a variety of test chemicals presented to the network (shown in Figure 3). The network was able to correctly classify the test samples, with 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 which have different concentrations of the analytes. This allowed the network 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.

These results demonstrate the pattern recognition capabilities of the neural network paradigm in sensor analysis, especially when the individual sensors are not highly selective. Besides, the prototype presented here has several advantages for real-world applications including compactness, portability, real-time analysis, and

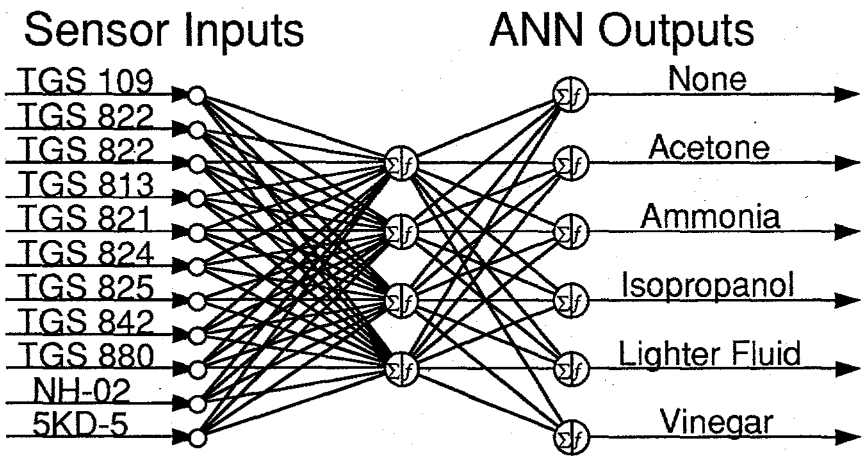

Figure 3: Network Structure

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 Laboratory is available in the World Wide Web (WWW) pages of the Environmental Molecular Sciences Laboratory.
URL: http://www.emsl.pnl.gov:2080/docs/cie/neural/

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6 REFERENCES

[1] B. G. Levi, "Hanford Seeks Short- and Long-term Solutions to its Legacy of Waste," *Physics Today,* vol. 45, no. 3, pp. 17–21, March 1992.

[2] S. J. Patrash and E. T. Zellers, "Characterization of Polymeric Surface Acoustic Wave Sensor Coatings and Semiempirical Models of Sensor Responses to Organic Vapors," *Anal. Chem.*, vol. 65, pp. 2055–2066.

[3] B. S. Hoffheins, "Using Sensor Arrays and Pattern Recognition to Identify Organic Compounds," *MS-Thesis,* The University of Tennessee, Knoxville, TN, 1989.

[4] 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, no. 5, pp. 446–451, May 1990.

[5] T. Moriizumi, T. Nakamoto, and Y. Sakuraba, "Pattern Recognition in Electronic Noses by Artificial Neural Network Models," in *Sensors and Sensory Systems for an Electronic Nose,* J. W. Gardner and P. N. Bartlett, Eds. Amsterdam, The Netherlands, Kluweer Academic Publishers, 1992, pp. 217–236.

[6] A. M. Pisanelli, A. A. Qutob, P. Travers, S. Szyszko, and K. C. Persaud, "Applications of Multiarray Polymer Sensors to Food Industries," *Life Chemistry Reports,* vol. 11, pp. 303–308, 1994.

[7] S. Nathan, "On the Scent of Something Big," *Chemistry and Science,* August 1994, pp. 587.

[8] R. J. Lauf and B. S. Hoffheins, "Analysis of Liquid Fuels Using a Gas Sensor Array," *Fuel,* vol. 70, pp. 935–940, August 1991.

[9] H. Sundgren, F. Winquist, I. Lukkari, and I. Lundström, "Artificial Neural Networks and Gas Sensor Arrays: Quantification of Individual Components in a Gas Mixture," *Measurement Science and Technology,* vol. 2, no. 5, pp. 464–69, May 1991.

[10] P. E. Keller, R. T. Kouzes, and L. J. Kangas, "Three Neural Network Based Sensor Systems for Environmental Monitoring," *IEEE Electro94 Conference,* pp. 378–382, 1994.

[11] S. Haykin, *Neural Networks: A Comprehensive Foundation,* IEEE Press, 1994.

[12] Product literature from Figaro USA, Inc., P.O. Box 357, Wilmette, IL 60091, USA.

[13] D. E. Rumelhart, G. E. Hinton, and R. J. Williams, "Learning Internal Representations by Error Propagation," in *Parallel Distributed Processing: Explorations in the Microstructures of Cognition.* Vol. 1, D. E. Rumelhart and J. L. McClelland, Eds. Cambridge, MA, MIT Press, 1986, pp. 318–362.

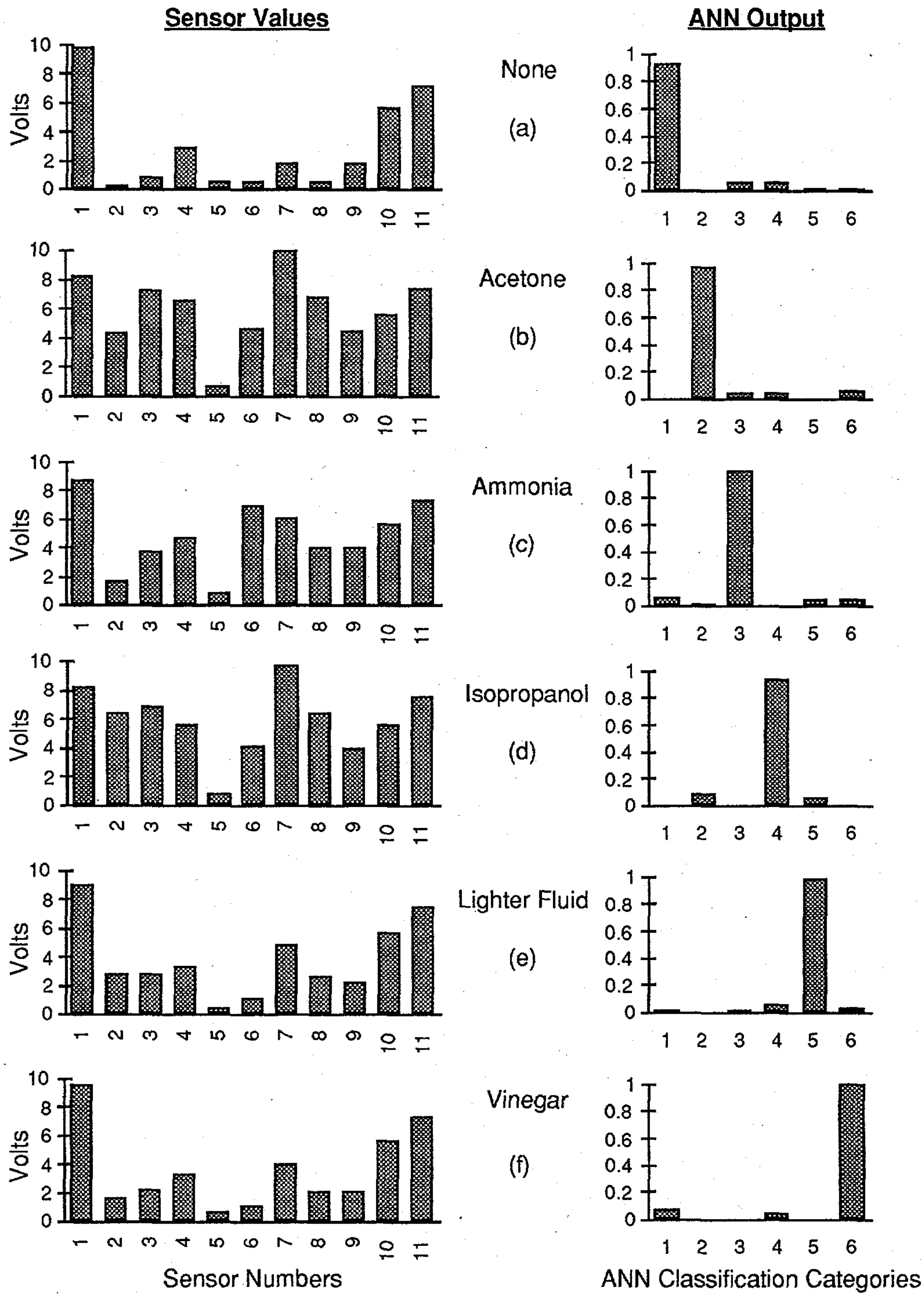

Figure 4: Sample responses and ANN classifications I.

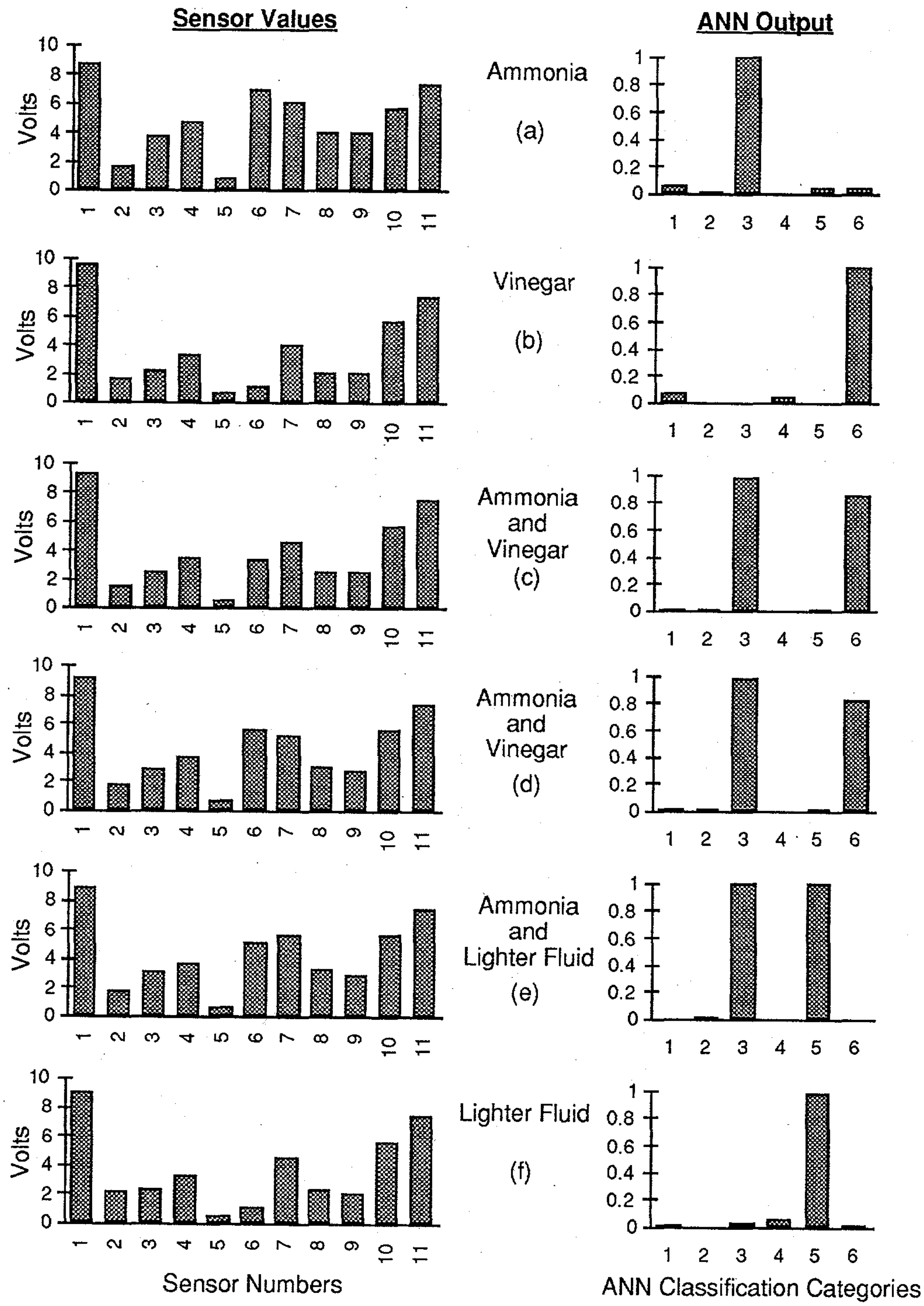

Figure 5: Sample responses and ANN classifications II.