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Sensors and Actuators B 69 (2000) 248–252

SENSORS AND ACTUATORS B CHEMICAL

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Odor discrimination using adaptive resonance theory

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Received 4 October 1999; accepted 22 February 2000

Abstract

The paper presents two neural networks based on the adaptive resonance theory (ART) for the recognition of several odors subjected to drift. The neural networks developed by Grossberg (supervised and unsupervised) have been used for two different drift behaviors. One in which the clusters end up to overlap each other and the other when they do not. The latter case is solved by unsupervision, which is useful to track the moving clusters and possibly discover new odors autonomously.

Keywords: Olfaction; Adaptive resonance theory; Fuzzy logic; Parameter drift

1. Introduction

System identification in the field of intelligent gas sensors is mainly concerned with the determination of the input–output mapping in highly dynamic conditions. Several methods have been applied to learn the mapping by predicting the relative output, but few of them try to solve the parameter drift problem. In an electronic nose there are several interfering inputs: operating temperature of the sensor and the relative humidity of the odor. Long-term drift is more often associated with the contamination of the sensor material. Parameter drift sometimes makes the clusters overlap each other and have an irregular shape. Artificial neural networks have been extensively implemented to solve this problem, since they present the following characteristic: on-line learning, fault tolerant, parallel computation, the ability to deal with noise and non-linearity of the sensor response, blind identification (unsupervised learning) in which the knowledge of the input of the system is not available or not sufficient.

Supervised methods such as the back-propagation algorithm have been applied but it would not perform well if the clusters overlap. They use gradient search based strategy, which has the drawback of getting trapped in local minima that do not guarantee the correct global classification. Also, convergence requires a huge number of iterations and is highly sensitive to parameter initialization (they do not self-organize).

In Ref. [6], two counteraction methods are proposed: self-organizing maps [7] and system identification by modeling the artificial nose as a dynamic system with an accuracy of 78% and 85%, respectively. In this paper, we present an approach for the recognition of several odors subjected to drift by using neural networks based on the adaptive resonance theory (ART). Two basic architectures have been developed: unsupervised, ART2 [4], and supervised, ART1 [5]. ART2 is used in Ref. [9] to identify individual gas odor using an array of four tin oxide sensors giving good identification results for separate clusters. In general, unsupervised learning perform well when the desired classes are obvious, but makes mistakes otherwise. The mistakes can be corrected with supervision. So far, two different aspects of the parameter drift have been considered: clusters that do not overlap each other and clusters that do.

In the first case, the problem is focused by using the unsupervised architecture, ART2, which will be shown how it is able to track the moving centroids. ART2 incrementally learns and stabilizes analog input patterns presented in an arbitrary order. Furthermore, it will be shown how ART2 classifies odors as supplied by an array of four thin film SnO_2 sensors. It is able to recognize autonomously (in a blind fashion) if an input is novel or familiar without leading to the *plasticity–stability*

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0925-4005/00/$ - see front matter
PII: S0925-4005(00)00502-5

dilemma. The discrimination of the familiar versus novel input pattern presented is the task of the *vigilance parameter*, which defines the granularity of the network.

The latter case cannot be handled with an unsupervised network because the supervised component to incorporate the initial knowledge of the moving centroids is needed. A supervised version of the ART theory that self-organizes its recognition codes called Fuzzy ARTMAP [2] will be presented. It includes learning, pattern recognition and hypothesis testing capabilities plus the adaptive naming, since the architecture is constituted of two components: the unsupervised component (ART2) and the supervised one (ART1). The first attempts to self-organize the recognition codes and to track the readings under drifting and the second learns how to predict its output given the presented input pattern. The transformation of vectors from the input space into the output vectors defines a map that is learned by examples from the correlated (input, output) pairs of sequentially presented vectors.

Section 2 introduces the human olfactory system by finding the area of the brain responsible for the recognition. Section 3 describes two neural classifiers in analogy to the human model, then experimental results and discussions follow.

2. The human olfactory system

Humans can discriminate thousands of odoriferous chemicals and can detect odorants at very low concentrations. The sense of smell (olfaction) is carried out by receptors that lie within the nasal cavity (called the olfactory epithelium) [3]. The olfactory epithelium contains cells, supporting cells and, basal cells. Receptors are bipolar neurons that have a short peripheral process and a long central process. The short peripheral process ends up in several cilia that interact with odorants. The longer central process is an axon that joins others in order to form a bundle which ends up at under the surface of the olfactory bulb (Fig. 1). The olfactory neurons must extend their axons into the central nervous system and continually form synapses with target cells in the olfactory bulb. Cells in the olfactory bulb do not divide and therefore accept new synapses continually. Every 60 days the receptor cells are generated from precursor basal cells. Odorants are presented to the receptor by olfactory binding proteins. The protein also protects olfactory neurons from exposure to excessively high concentration of odorants.

In the visual system, three cone pigments are sufficient to discriminate the myriad of hues. The discovery of a large family of potential olfactory receptors suggests that hundreds of receptors, each recognizing a single or a few odorants, enable us to detect a wide range of odorants. It is not yet known if a single olfactory neuron has multiple receptors, nor how narrowly tuned a given receptor is to individual odorants.

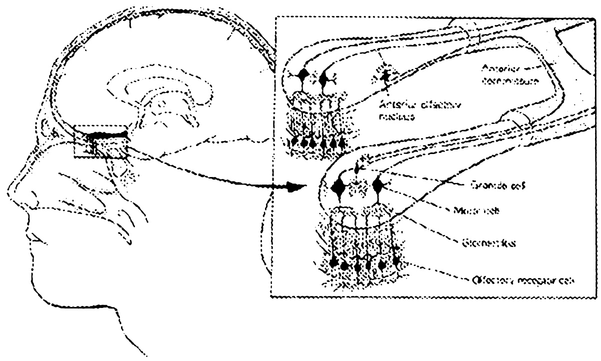


Fig. 1. Olfactory receptors in the nasal cavity project to the olfactory bulbs. Olfactory bulbs are connected to each other by the anterior commissure (adapted from Ref. [3]).

Response to specific odorants occurs throughout the epithelium and it has been shown that specific areas are more sensitive to an odorant than others. For example, butanol best activates neurons in the anterior regions of the mucosa. When the stimulus intensity is increased, it is possible to activate previously silent olfactory receptors in and around the area of high sensitivity (it will change the overall-firing pattern). The axons of the olfactory neurons terminate into the olfactory bulb. Here they synapse with the dendrites of the mitral cells and tufted cells, in specialized area called the glomeruli. The axon of mitral and tufted cells project in the olfactory tract and synapse on neuron in five separate regions of the olfactory cortex: the anterior olfactory nucleus which connects the two olfactory bulb; the olfactory tubercle; the pyriform cortex, the main olfactory discrimination region; the cortical nucleus of the amygdala and the ethorinal area which in turns projects to the hippocampus. Unlike the visual system, where afferent stimuli are organized in a topographic manner, there is no strict relationship between the arrangement of the projection of the olfactory neurons in the olfactory bulb and the regions of the mucosa from which they originate. Therefore, the olfactory bulb must be able to interpret different signals from the same subregion as different odors. This is because each receptor responds to a number of different odors, making several spatial patterns of response in the sheet of receptor under the mucosa. Therefore, the olfactory glomeruli with the synaptic connections onto mitral, tufted and periglomerular dendrites represent the “level of input processing”. The control of the outputs from the olfactory bulb to the olfactory cortex represents the “level of output control”. A part of the olfactory cortex, called the *pyriform cortex* would function as an associative memory network [10], having the ability to identify conjunctions of odor components that make up complex odors. Ref. [1] proposed the idea that the interactions between the olfactory bulb and the olfactory cortex result in a form of hierarchical clustering for storage and recognition of complex odors.

3. ART2 and Fuzzy ARTMAP

The general ART2 model [4] has an input layer and an output layer. The former is called *comparison field* (F_1) and matches each input pattern with its memory patterns (*prototypes*). The output layer is called *category representation field* (F_2) and chooses (with a winner-take-all strategy) the prototype nearest to the input pattern. The F_1 and F_2 fields interact with each other through weighted bottom-up and top-down connections W (the long-term *memory* LTM) called *adaptive filters*. Short-term memory (STM) is contained in the N and M neurons of F_1 and F_2, respectively. Neurons are activated when the input pattern is presented to the input field, giving rise to an internal activity pattern of nodes $x=(x_1, \ldots, x_N)$ contained in F_1 which represent STM. The network attempts to classify the pattern into one of the available categories based on its similarity with the associated prototypes. This is accomplished by activating the F_2's nodes that compete through a *winner-take-all* strategy. Each node calculates its bottom-up activation

$$T_i(x) = \frac{|\boldsymbol{w}_i \cap x|}{\alpha + |\boldsymbol{w}_i|} \qquad i = 1, \ldots, M,$$

where $|\cdot|$ is the squared norm operator, $\boldsymbol{w}_i$ is the weight vector of category i, α is a network parameter. The node J with the highest internal activity supplies the recognition code $T_J = \max\{T_i | i = 1, \ldots, M\}$. Subsequently, F_2 propagates the winner's internal activity through top-down weights to F_1, where it is matched with the input pattern. Their similarity must satisfy the equation:

$$\frac{|\boldsymbol{w}_J \cap I|}{|I|} \geq \rho,$$

where ρ is called *vigilance parameter* and fixes the threshold for resonance. If the condition is satisfied, the network updates its weights as follow:

$$\boldsymbol{w}_J^{\mathrm{new}} = \eta\left(\boldsymbol{w}_J^{\mathrm{old}} \cap x\right) + (1-\eta)\boldsymbol{w}_J^{\mathrm{old}}.$$

Otherwise, a reset signal is sent to F_2 and the active neuron J is inhibited from competing on the following iterations of the same input. The process continues until the input pattern is classified or no matches are found. In the latter case, a new neuron with a suitable recognition code is inserted in the network.

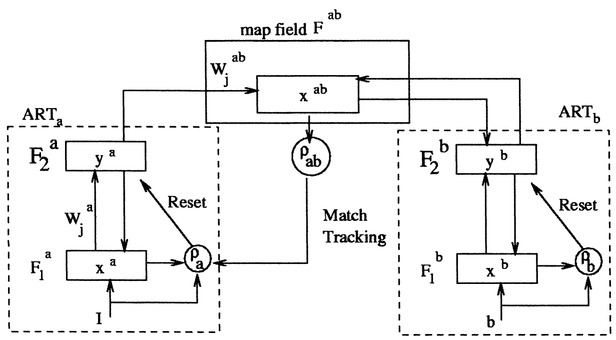


Fig. 2. Fuzzy ARTMAP architecture. When a prediction by $\mathrm{ART_a}$ is not met by $\mathrm{ART_b}$, then an inhibition of a map field is carried out and the vigilance ρ_{a} is adjusted accordingly.

The second neural classifier used in this paper is the Fuzzy ARTMAP architecture, constituted by a Fuzzy ART component[1] ($\mathrm{ART_a}$) and an ART1 component [5] (for binary input $\mathrm{ART_b}$) as shown in Fig. 2. The two components are linked together via an inter-ART module F^{ab} called a *map field*. The map field performs predictive association between categories and to realize the match-tracking rule, increasing ρ_{a} in response to a mismatch at $\mathrm{ART_b}$. The map field is activated when one of the $\mathrm{ART_a}$ or $\mathrm{ART_b}$ categories is active, that is:

$$\boldsymbol{x}^{\mathrm{ab}} = \begin{cases} y^{\mathrm{b}} \cap \boldsymbol{w}_J^{\mathrm{ab}} & \text{if the } J\text{th } F_2^{\mathrm{a}} \text{ node is active and } F_2^{\mathrm{b}} \text{ is active} \\ \boldsymbol{w}_J^{\mathrm{ab}} & \text{if the } J\text{th } F_2^{\mathrm{a}} \text{ node is active and } F_2^{\mathrm{b}} \text{ is inactive} \\ y^{\mathrm{b}} & \text{if } F_2^{\mathrm{a}} \text{ is inactive and } F_2^{\mathrm{b}} \text{ is active} \\ 0 & \text{if } F_2^{\mathrm{a}} \text{ is inactive and } F_2^{\mathrm{b}} \text{ is inactive.} \end{cases}$$

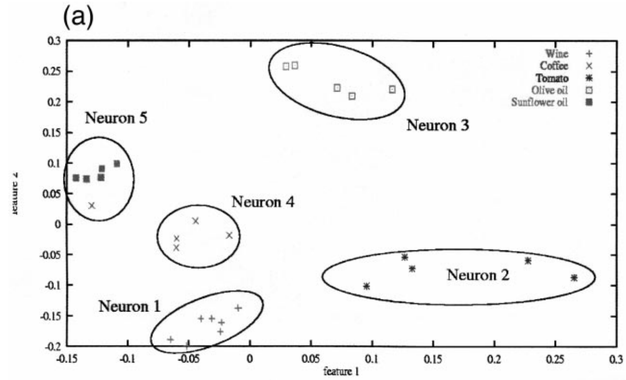
The match tracking rule must obey $|\boldsymbol{x}^{\mathrm{ab}}| < \rho_{\mathrm{ab}}|y^{\mathrm{b}}|$ to recognize the current activated map with the presented input I. The initial map field weights are $\boldsymbol{w}_{jk}^{\mathrm{ab}}(0) = 1$, and during resonance with the ART_a category J active, $\boldsymbol{w}_J^{\mathrm{ab}}$ approaches the map field vector $\boldsymbol{x}^{\mathrm{ab}}$. Once J learns to predict the $\mathrm{ART_b}$ category K, that association is permanent (i.e. $\boldsymbol{w}_{JK}^{\mathrm{ab}} = 1$ for all time).

4. Results

In the first experiment, the unsupervised architecture ART2 is used. The active layers of the array consist of pure and doped SnO_2 thin films prepared by means of sol–gel technology. Pd, Pt, Os, and Ni were chosen as doping elements starting from different precursors of the preparation of the modified films. The films, whose thickness was about 100 nm, were deposited on alumnia substrates supplied with interdigitated electrodes and platinum heater, by the spin coating technique at 3000 rpm, dried at 80°C and heat treated in air at 600°C. After deposition, the sensors were mounted onto a TO8 socket and inserted in the test chamber.

The data set is composed by four dimensional vector readings of several odors: wine, tomato, olive oil, sunflower oil and coffee. Fig. 3a shows the classification results with the Sammon's mapping onto a 2D graph [8]. Since the clusters are spread out, unsupervised architec-

[1] The fuzzy ART algorithm is mainly based on the ART2 algorithm described above, by substituting the "∩" operator with the "*min*" fuzzy operator. The complete dynamics of the network can be found in Ref. [2].



(b)

ρ	% correct matches	# of epochs
0.98	98	15
0.99	92	18
0.5-0.90	63	7-10

Fig. 3. (a) Classification with ART2 architecture. Ellipses correspond to the ART2 classifications, and the patterns to the true values; (b) accuracy results of different vigilance parameters ρ with the same data set.

tures are particularly useful for discovering new odors. It is interesting to observe the self-organization property of the networks, ordering the neurons in a counterclockwise fashion. As shown in Fig. 3, ART2 fails to identify the sunflower oil in place of the coffee's odor, which is occupied by the neuron 4.

The second experiment was carried out by considering a different data set and using Fuzzy ARTMAP, in which the parameter drift makes the identification process harder. The data set[2] is derived from an array of 15 sensors used to detect five different gases for a period of 45 days. This data set is subjected to parameter drift making the readings difficult to be identified and thus the clusters difficult to be separated. The measurements are made by determining the response of each sensor to the five gases (1-propanol, 2-propanol, 2-butanol, 1-butanol, and water) in rotation. Fig. 4a presents the 4400 total readings by considering 880 readings for each gas (the representation has been limited to the two features of the three extracted by the method of principal component analysis). To train the network, the first 2400 readings have been considered. Next, the network has been tested with the remaining 2000 readings which are strongly subjected to noise. The results show an error of 27% over that data set, whereas can be seen in Fig. 4b, the clusters overlap each other. Some readings, like those of the 2-propanol, fall into the cluster of 1-propanol and the water, making the classification impossible

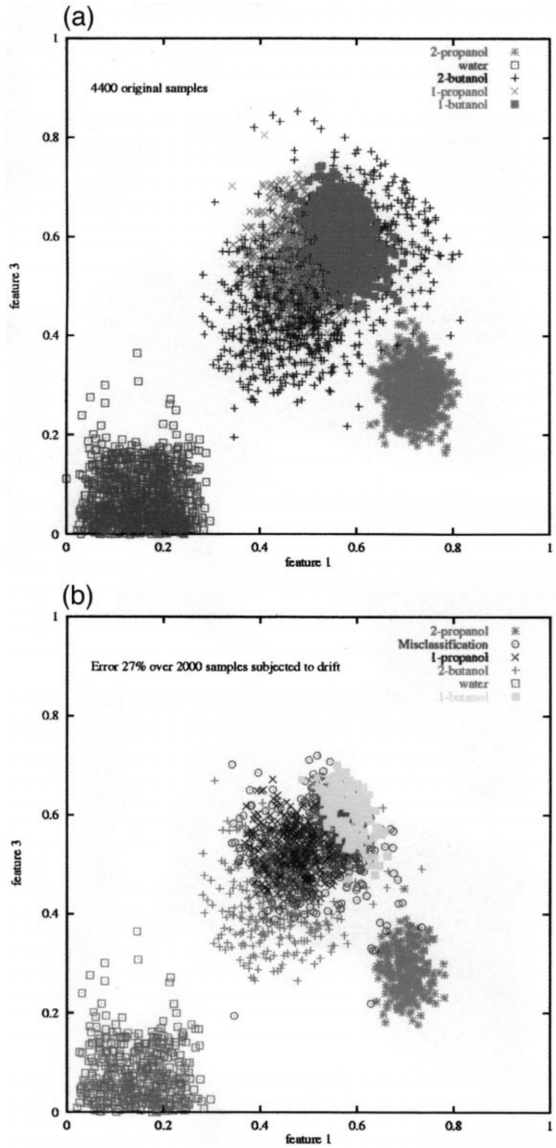


Fig. 4. (a) True values of the 4400 readings; (b) test of the Fuzzy ARTMAP network by using the last 2000 readings.

at least with this predictive methods. Results of this last experiment are reported in Table 1.

Table 1
Results using the Fuzzy ARTMAP architecture of the experiment shown in Fig. 4 for the vigilance parameter of the map field $\rho_{ab} = 0.1$. Smaller values of vigilance ρ_b of the supervised component allows the unsupervised component ART_a to create more categories

ρ_a	ρ_b	Number of epochs	% Correct matches	No. ART_a nodes
0.87	0.1	14	73	483
0.93	0.2	11	70	592
0.94	0.9	7	68	396
0.0	0.6	10	72	448

[2] Note that the data set for this case has been taken from the literature.

5. Conclusions

In this paper, we have presented two different ways of handling the parameter drift problem: clusters that never overlap each other and clusters that do. An unsupervised method (ART2) has been applied in order to track the moving clusters and preserving the stability and the plasticity of the system. In the case where the clusters overlap, the supervision (Fuzzy ARTMAP) component is necessary to reduce uncertainty.

The identification of odors subject to drifted data need to be explored by a method that autonomously adapts its internal state with sensor response changes. This means that a neural-based approach able to retrain its knowledge base without using a teacher but purely based on its experience is necessary to follow the dynamics of the chemical sensors. In addition, future work will address the first case by including in the neural architecture a state estimator to calculate the position of the centroids while moving, based on the analysis of the initial behavior of each sensor. The latter case could be approached by including the time component in the identification process (for example, a STM realized by recurrent neural network or an instance-based technique) in order to discriminate between different odors that occupy the same region of the feature space.

Acknowledgements

The work was partially supported by the Italian National Research Council (CNR) under the grant "Progetto Finalizzato MADESS 2" and by the Project "FESR subprogram II" of the European Community.

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Biographies

Cosimo Distante received the *Laurea* degree in Computer Science from the University of Bari in 1997. He has been a visiting researcher at the Computer Science Department of the University of Massachusetts at Amherst 1998–1999. Currently, he is a PhD student at the University of Lecce, Italy, and is mainly involved in the pattern recognition field applied to chemical sensor responses, chemical sensors applied to robotics, robot learning and artificial intelligence methods applied to manufacturing.

Pietro Siciliano received his degree in Physics in 1985 from the University of Lecce. He took his PhD in Physics in 1989 at the University of Bari. During the first years of activities, he was involved in research in the field of electrical characterisation of semiconductors devices. He is currently a senior member of the National Council of Research at the Institute for the Study of New Materials for Electronics (IME-CNR), where he has been working for many years in the field of preparation and characterisation of thin film for gas sensor. His interest is now devoted to manufacturing artificial intelligence systems, like electronic nose.

Lorenzo Vasanelli was born in 1947. After the degree in Physics, he was at the Department of Physics of Bari as a lecturer and successively as an Associate Professor of Experimental Physics. Since 1987, he is a full professor of Solid State Physics at the University of Lecce. Since 1994, he is also the Director of the Institute for the Study of New Materials for Electronics of CNR, located in Lecce. His research activity was initially devoted to transport and photoelectronic properties of layered III–VI semiconductor compounds. His interest was successively devoted to structural and electrical properties of thin semiconducting films prepared by sputtering and their applications (solar cells, nuclear detectors, sensors). He has been also involved in some researches about GaAs-based devices.