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Pattern recognition for sensor array signals using Fuzzy ARTMAP

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ABSTRACT

A Fuzzy ARTMAP classifier for pattern recognition in chemical sensor array was developed based on Fuzzy Set Theory and Adaptive Resonance Theory. In contrast to most current classifiers with difficulty in detecting new analytes, the Fuzzy ARTMAP system can identify untrained analytes with comparatively high probability. And to detect presence of new analyte, the Fuzzy ARTMAP classifier does not need retraining process that is necessary for most traditional neural network classifiers. In this study, principal component analysis (PCA) was first implemented for feature extraction purpose, followed by pattern recognition using Fuzzy ARTMAP classifiers. To construct the classifier with high recognition rate, parameter sensitive analysis was applied to find critical factors and Pareto optimization was used to locate the optimum parameter setting for the classifier. The test result shows that the proposed method can not only maintain satisfactory correct classification rate for trained analytes, but also be able to detect untrained analytes at a high recognition rate. Also the Pareto optimal values of the most important parameter have been identified, which could help constructing Fuzzy ARTMAP classifiers with good classification performance in future application.

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1. Introduction

There are different types of poisonous gases or vapors in the environment, which have harmful effects on human health. One class of examples is volatile organic compounds (VOC). Their detection and identification are extremely important. Many types of chemical sensors have been reported for identification of VOCs. One example is chemiresistive sensor array, which is usually employed to acquire signals for different analytes such as VOCs and other toxic gases [1–5]. A sensor array has different response profiles or patterns to different VOCs. Its signals thus can be used to analyze and classify vapors with statistical or nonparametric intelligent methods.

To classify different VOCs, training for the classification model is usually necessary. For certain VOCs, all the relevant information, e.g., sensor signal, along with its corresponding class, is needed for obtaining classification models during the training stage. Especially when new VOCs are added, retraining for original and new VOCs is generally needed with current reported approaches. In addition, although various classification methods have been applied to classify VOCs, most of them only focus on identifying trained VOCs. There are few reports on the detection of untrained VOCs.

Fuzzy ARTMAP [6] is a constructive neural network model developed upon Adaptive Resonance Theory (ART) and Fuzzy set theory [6–10], which allows knowledge to be added during training if necessary. It avoids discarding the previous knowledge or model and spares repeating the whole training process. The Fuzzy ARTMAP classifier's continuous online learning capability greatly facilitates the dynamic changing of the classifier's knowledge base. The learning and forecasting mode of the Fuzzy ARTMAP system can function alternatively. Thus, the Fuzzy ARTMAP classifier is competent for working in a dynamic environment that is subjected to the presence of new vapor. For example, the Fuzzy ARTMAP classifier can always recognize new vapors, and learn to classify them by changing its structure and parameters without retraining for the original trained vapors. Because of Fuzzy ARTMAP system's self-organizing scheme, it does not need pre-determination of many parameters, e.g., some structure parameters; that is not the case for most traditional ANNs. For example, in multi-layer perceptrons (MLPs), the amount of its hidden layer(s), and the number of nodes in hidden layer(s) must be decided before training. Also, the training of the Fuzzy ARTMAP classifier is very fast compared with Back Propagation (BP) neural networks. In addition, a Fuzzy ARTMAP classification system based on the knowledge of several known or trained vapors can detect the presence of a new or untrained vapor. This function can alert to the presence of a potential threat from a new vapor in a dynamic environment.

To date, there are many studies and successful applications of Fuzzy ARTMAP in the pattern classification field [11–15]. However,

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based on the authors' best knowledge, there are no reports using Fuzzy ARTMAP to identify the untrained analytes from sensor array responses. Instead, most current classifiers applied in this area have no capability to identify untrained new vapors. In addition, analysis of the effect of some important parameter toward the classification system was presented. Pareto optimization method was applied to analyze variation of classification performance corresponding to the change of vigilance parameter's value. The Pareto optimization analysis identified the general near optimal value of initial vigilance parameter. That provides some hint for constructing parameter set of Fuzzy ARTMAP classifier in similar application.

In this paper, the Fuzzy ARTMAP classifiers are applied to analysis of the responses of a chemiresistor sensor array with different nanostructured sensing materials [3–5] to a set of VOCs, namely vapors generated from organic solvents, benzene (Bz), hexane (Hx), p-xylene (Pxy), and toluene (Tl). The sensing array materials consist of (1) NDT-linked nanoparticles (NDT-$Au_{2\,nm}$), (2) PDT-linked nanoparticles (PDT-$Au_{2\,nm}$), (3) MUA-linked nanoparticles (MUA-$Au_{2\,nm}$), (4) MHA-linked nanoparticles (MHA-$Au_{2\,nm}$), (5) MPA-linked nanoparticles (MPA-$Au_{2\,nm}$) [1–4]. NDT: 1,9-nonanedithiol (HS–$(CH_2)_9$–SH), PDT: 1,5-pentadithiol (HS–$(CH_2)_5$–SH), MUA: 11-mercaptoundecanoic acid (HS–$(CH_2)_{10}$–CO_2H), MHA: 16-Mercaptohexadecanoic acid (HS–$(CH_2)_{15}$–CO_2H), and MPA: 3-mercaptopropanoic acid (HS–$(CH_2)_2$–CO_2H), were used as received (Aldrich). From the four vapors, three are alternatively selected as known vapors to the classifier viz. the Fuzzy ARTMAP. This classifier will then be trained to learn the above three selected vapors. The fourth vapor is considered a new vapor to the classification model. Partial data for the chosen known vapors are employed to build a PCA model, and the main PC variables are then served as input to train the Fuzzy ARTMAP classifier. The remaining data for the trained vapors and complete set of data for untrained vapor together constitute the testing data set. The new PC scores from testing data are then calculated from the previously built PCA model. After transformation, the adjusted PCs are fed to Fuzzy ARTMAP classifier to test the classification performance. Finally, the Pareto optimization method is applied to analyze the relationship between parameter setting and performance of Fuzzy ARTMAP system.

2. Experiment

Sensor-response measurements were performed using a customized interdigitated microelectrode (IME) device, which has 300 pairs of platinum electrodes of 5 μm width and 5 μm spacing on glass substrate (100-nm thick). The thickness of the coating of molecularly linked nanoparticle thin film was below or close to the finger thickness. Details about the preparation of molecularly linked nanoparticle thin film assembly were described previously [2,4]. Briefly, the thin films were prepared via "exchanging–crosslinking–precipitation" route. The reaction involved an exchange of linker molecule (NDT, PDT, MUA, MHA, MPA) with the gold-alkanethiolates, followed by crosslinking and precipitation via either Au S bonding at both ends of NDT or PDT, or hydrogen bonding at the carboxylic acid terminals of MUA, MHA or MPA. The platinum-coated IME devices were immersed into the solution of the mixed nanoparticles and thiols at room temperature, and solvent evaporation was prevented during the film formation. The thickness of the thin films grown on the surface of the substrates was controlled by immersion time [2,4].

A computer-interfaced multi-channel multimeter (Keithley, Model 2700) was used to measure the lateral resistance of the nanostructured coating on IME. The resistance and frequency measurements were performed simultaneously with computer control. All experiments were performed at room temperature, $22 \pm 1\,^{\circ}C$. N_2 gas (99.99%, Progas) was used as reference gas and as diluent to change vapor concentration by controlling mixing ratio. The gas flow was controlled by a calibrated Aalborg mass-flow controller (AFC-2600). The flow rates of the vapor stream were varied between 5 and 50 mL/min, with N_2 added to a total of 100 mL/min. The vapor generating system followed the standard protocol [6b]. The vapor stream was produced by bubbling dry N_2 gas through a bubbler of the vapor solvent using the controller to manipulate vapor concentration [2,4].

The measured resistance (R) values were expressed as relative differential resistance change $\Delta R/R_i$ for the evaluation of the vapor sorption responses. ΔR is the difference between the maximum and minimum values in the resistance response and R_i is the initial resistance of the film [2,4].

3. Classification methodology

The following schematic diagram (Fig. 1) depicts the general classification procedure in this study. The original responses from sensor arrays are preprocessed and the principal component analysis method is applied to extract feature vectors. Through PCA, the dimension of signal is reduced, and the noise in original signals could be eliminated to some extent. The feature vectors are then projected into range [0,1] and serve as the input to Fuzzy ARTMAP classifier, which can identify the both trained and untrained vapors. Normalization and complimentary coding are important steps to get appropriate input for Fuzzy ARTMAP system. The performance of classifier is tested by classifying the new data from both trained and untrained vapors.

The classification results are also been analyzed by multiple objective optimization method. In this study, Pareto optimization is implemented to identify optimal parameter set for Fuzzy ARTMAP classifiers. For different parameter settings of Fuzzy ARTMAP classifiers, there is a trade-off between successful classification rate for trained and untrained vapors. When there is a change in the value of a decision variable or parameter in certain direction, one objective, e.g., one correct classification rate, will increase, while the other objective will show some deterioration. Since the two objectives could not reach their global optima simultaneously, a multi-objective optimization technique is employed to identify a Pareto optimal set.

3.1. Principal component analysis

Principal component analysis is a multivariate analysis method which transforms a set of correlated variables into a set of uncorrelated variables. Assuming there are p variables in original data X, i.e. $X = (x_1,\ldots,x_p)$, PCA forms p linear combinations [16]:

$$\begin{aligned}
\mathrm{PC}_1 &= w_{11}x_1 + w_{12}x_2 + \cdots + w_{1p}x_p \\
\mathrm{PC}_2 &= w_{21}x_1 + w_{22}x_2 + \cdots + w_{2p}x_p \\
&\vdots \\
\mathrm{PC}_p &= w_{p1}x_1 + w_{p2}x_2 + \cdots + w_{pp}x_p
\end{aligned}$$

$$w_{i1}^2 + w_{i2}^2 + \cdots + w_{ip}^2 = 1 \quad i = 1, \ldots, p$$

$$w_{i1}w_{j1} + w_{i2}w_{j2} + \cdots + w_{ip}w_{jp} = 0 \quad \text{for all } i \neq j \tag{1}$$

where new variables $\mathrm{PC}_1, \mathrm{PC}_2, \ldots, \mathrm{PC}_p$ are p principal components (PCs). The first principal component, PC_1, accounts for the maximum variance in the original data; and PC_2, the second principal component, accounts for maximum variance that has not been accounted for, by the first PC, etc. [16]. The weight of the jth original variable for the ith PC is w_{ij}.

The PCA method can reserve most information in the original data while at the same time eliminate a certain amount of

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