



Improving gas identification accuracy of a temperature-modulated gas sensor using an ensemble of classifiers

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ABSTRACT

Data processing methods commonly used in conjunction with the array- and quasi-array-based gas identification systems generally include a dimension reduction followed by categorization using a classifier. Here, we have applied an ensemble of classifiers, directly to the high dimensional feature vectors and fused their verdicts by majority voting. The quasi-array investigated is a metal oxide sensor temperature-modulated with different rectangular heating voltage pulses. The experimental database was developed by recording the temporal responses obtained at different conditions to methanol, ethanol and 1-butanol vapors. Features related to each response were extracted by wavelet transform. The classification rates achieved with traditional methods were compared to that obtained using an ensemble of classifiers. The classification rate was improved by majority voting among the classifiers, each trained on different feature subsets, for the classification verdict.

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1. Introduction

The problem of high dimensional data in e-noses, also referred to as “the curse of dimensionality” in statistical pattern recognition, significantly increase the complexity of the classification algorithm, time and memory requirements. Many of the features of the recorded patterns are irrelevant or redundant due to the cross-selectivity of the responses of the array components or the outputs of the virtual components of the virtual array utilized [1]. A simple strategy to reduce the number of features is to select a subset of the available features, feature subset selection (FSS). The goal of FSS is to find an optimal subset of features that maximizes prediction or classification accuracy. An exhaustive search of all possible subsets of features will guarantee that the optimal subset is found. However, this is computationally impractical even for a moderate number of features. The performance of different sensors and feature selection methods have been studied by various researchers in the electronic nose community [2–5], but the potential improvement in classification through feature fusion by ensemble-based approach [6–8] has not been a topic in research. While the feature selection seeks to find an optimal subset of features, the goal of classifier ensembles is to combine the outputs of diverse classifiers to achieve optimal accuracy. This approach generally belongs to

the multiple classifier systems which are explained in detail in the following section.

The responses of a chemoresistor temperature-modulated with a heating voltage waveform contain significant amount of information related to the nature of the prevailing analyte in the background atmosphere [9–12]. Different voltage waveforms, such as staircases, pulse trains, sinusoids, and step functions have been applied to the microheater of these sensors resulting in different success levels in analyte recognition by utilization of a single classifier [13–17]. Traditionally, a dimension reduction is carried out on the features of the recorded response patterns, and the classifier is trained based on the training database comprising all the low dimension features.

Here, we demonstrate the significance of using an ensemble of classifiers, in the categorization of gases using an operating temperature modulated gas sensor for the first time. A generic tin oxide-based gas sensor is temperature modulated with six different rectangular heating voltage pulses. The responses obtained are introduced to an ensemble of six classifiers, each trained on different feature subsets, for classification. The obtained classification rate is compared with those achieved with traditional processing methods utilizing a single classifier trained on all the recorded feature database.

2. Multiple classifier systems

Combining multiple classifiers to achieve higher accuracy is one of the foremost research areas in machine learning. It is known under various names, such as multiple classifier systems, classifier

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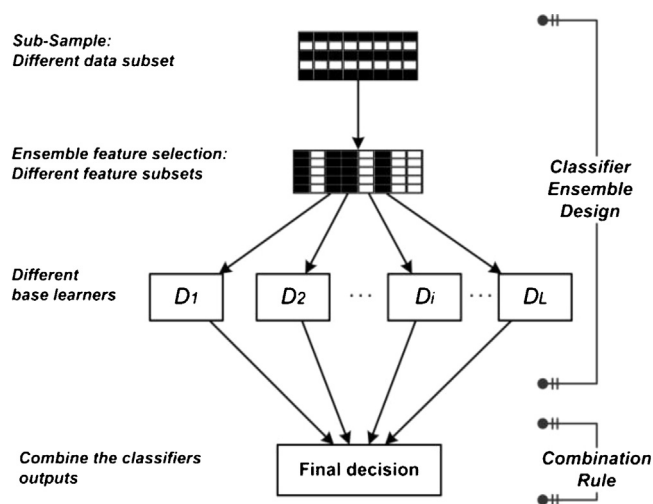


Fig. 1. The structure of a multiple classifier system.

ensemble, committee of classifiers, and classifier fusion. Multiple classifier systems can generate more accurate classification results than each of the individual classifiers [18]. In such systems, as shown in Fig. 1, the classification task can be solved by integrating different classifiers, leading to better performance. However, the ensemble approach depends on the assumption that single classifiers make errors on different samples, known as classifier diversity [19]. The intuition is that if each classifier makes different specific errors, then the total errors can be reduced by an appropriate combination of these classifiers. There are three general approaches to create an ensemble of classifiers. The most straightforward approach is using different learning algorithms for the base classifiers or variations of the parameters of the base classifiers. For example, different initial weights or different topologies of a series of neural network classifiers can be utilized as different base classifiers. Another approach is using different training sets to build different base classifiers. Such sets are often obtained from the original training set by re-sampling techniques [20,21].

The third approach, which is employed in this work for classification of the response patterns of a thermally modulated gas sensor, is to train the individual classifiers with data that consist of different feature subsets, or so-called ensemble feature selection [22]. While traditional feature selection algorithms seek to find an optimal subset of features, the goal of ensemble feature selection is to find different feature subsets to generate accurate and diverse classifiers. In the random subspace method [6], the ensemble system is built by randomly choosing the feature subsets. These feature subsets are generated by randomly selecting m features from the n -dimensional feature space ($m < n$). Then, each feature subset is fed into an individual classifier. Finally, all classifiers are aggregated by an appropriate combination rule. While common classification systems suffer from the high-dimension data, the ensemble feature selection approach takes advantage of large number of features [6].

Regardless of the base classification algorithm used, the diverse classifiers are then fused by a combination technique such as voting methods, fuzzy integral, Markov chains, Dempster-Shafer rule, and behavior knowledge space [18].

3. Experimental

Experiments were carried out to establish a database of response patterns recorded in air contaminated with three different volatile organic compounds each at different concentrations. The sensor used is a generic tin oxide-based general sensitivity gas sensor (SP3-AQ2, FIS Inc., Japan), which is operating temperature-modulated

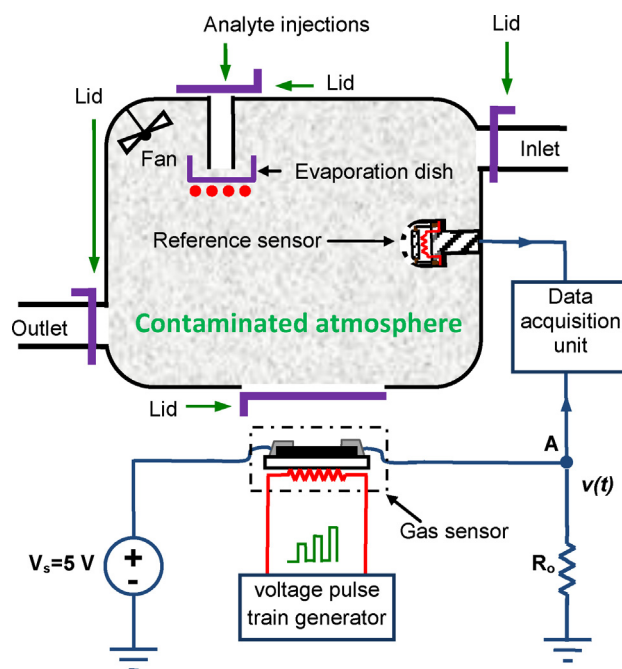


Fig. 2. The schematics of the experimental setup.

with different voltage waveforms applied to its microheater. The microheater of the sensor is a ruthenium oxide-based thick film with a room temperature resistance of $\sim 57 \Omega$. The experimental setup is schematically shown in Fig. 2.

An atmosphere-controlled chamber of 8-l volume (Fig. 2) is utilized for response recordings. The background gas is clean air, and the analytes examined are methanol, ethanol, and 1-butanol vapors at concentration levels ranging from 100 to 2000 ppm. The clean air in the chamber is contaminated by injecting predetermined volumes of the liquid chemicals with a sampler, which are evaporated in the closed chamber. The chamber air is mixed with a small electric fan for homogenization. The contamination level is continuously monitored using a reference sensor. Data obtained from the reference sensor is used only for the purpose of comparison of the experimental conditions; analyte concentrations given in relation to the response patterns are calculated based on the amount of the liquid analyte injected to the chamber. No specific control was imposed, and no compensation measure was taken [23], on the temperature and humidity level of the chamber atmosphere. Throughout all the experiments; the respective ranges of temperature and relative humidity were 22–27 °C and 30–50%. The chamber has a gas impermeable lid which opens to allow the insertion of the temperature-modulated gas sensor. The sensor is mounted on a ceramic probe through which the heating and response signal carrying wires are connected to the related peripheral electronic units.

Voltage pulses of different temporal profiles are generated using a computer programmable “multifunction card” (PCI-1711L, Advantech Co., USA) connected to the microheater of the gas sensor via a custom-designed buffer circuit which prevents overloading of the card. The circuit used for obtaining the responses, shown in Fig. 2, converts the variations of the resistance of the sensor pallet to a voltage signal. This includes a $2.2 \text{ k}\Omega$ resistor (R_0) connected in series to the gas sensor and a DC voltage source. The voltage drop on R_0 is approximately proportional to the conductance of the gas sensor. Regardless of this approximate relationship, the temporal signal, $v(t)$, measured at point A, is considered as the response pattern related to the prevailing contaminated atmosphere. $v(t)$ is sampled at a rate of 100 s^{-1} , digitized and recorded.

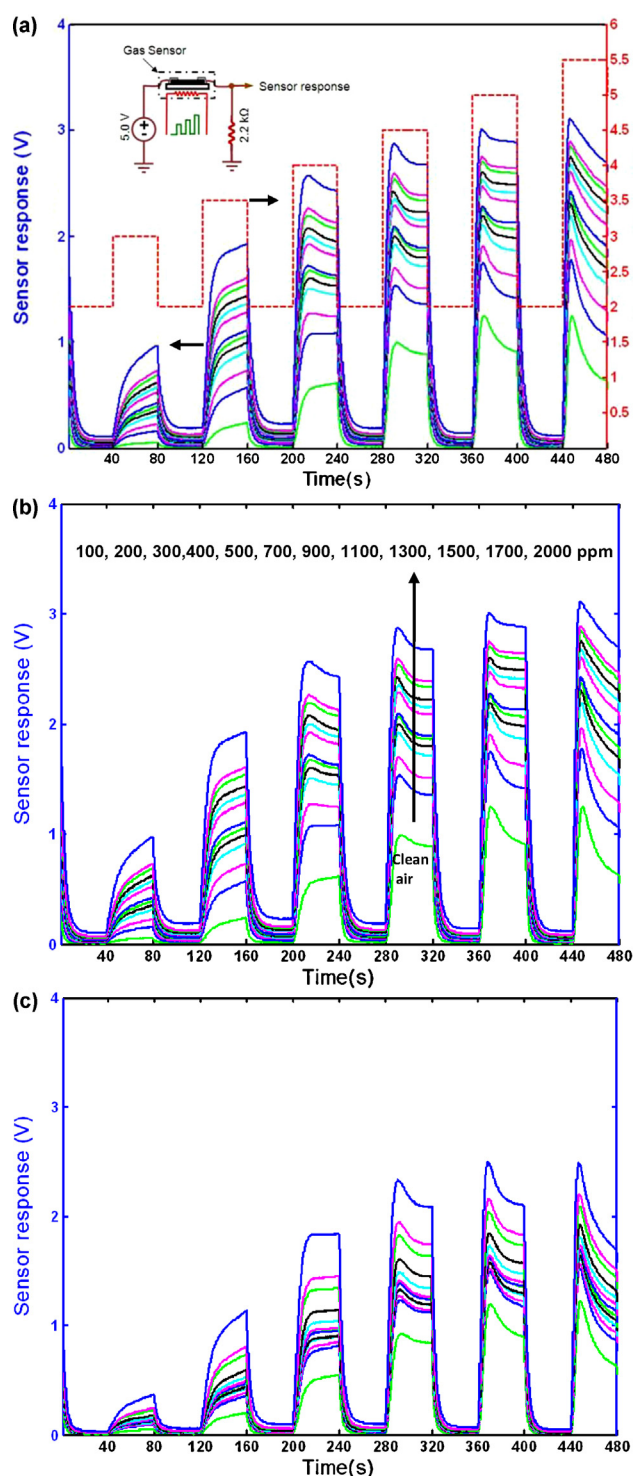


Fig. 3. (a) Six rectangular voltage pulses (dotted line) used for the thermal modulation of the gas sensor along with the responses recorded for methanol at different concentrations in the 100–2000 ppm range in air. The inset shows the response recording circuit; (b) and (c) similar responses recorded for ethanol and 1-butanol, respectively.

Prior to each experiment, the device is constantly at its nominal operating temperature in clean air, at least for 15 min. The nominal temperature on the sensitive oxide layer is achieved by applying the nominal heating voltage of the device (5 V DC, according to the sensor's data sheet) to its microheater. This is to clean up the pallet surface from the probable residues of the previous measurements and to bring the device to thermal equilibrium. The probe was, then,

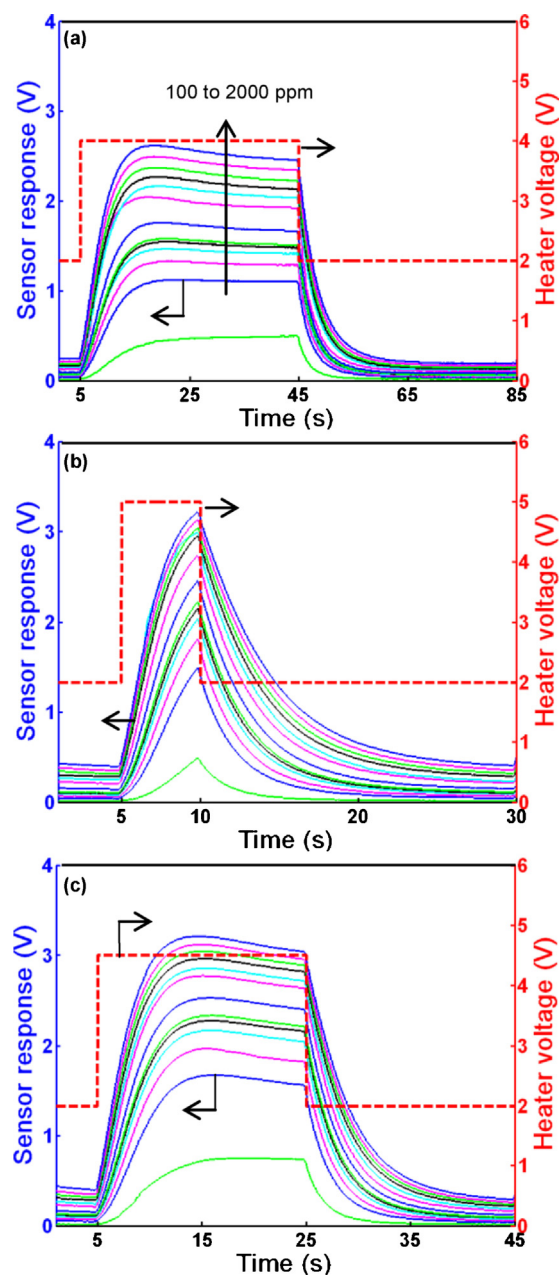


Fig. 4. (a–c) Three example microheater voltage waveforms are given along with their respective responses. All the responses shown are related to methanol at different concentrations in the 100–2000 ppm range in air.

inserted into the above described gas chamber containing air contaminated with a predetermined concentration of a known target gas. The heating voltage remains at 5.0 V for another 3 min. During this period, the sensor reaches its steady-state response level related to the contaminated atmosphere of the chamber.

Starting at $t = 0$, defined to coincide the end of the 3 min soaking time, the temperature modulating voltage waveform is applied to the sensor microheater. All the waveforms examined start with a step fall from 5 to 2 V. The different waveforms used for thermal modulation, presented in Fig. 3, finally bring the heating voltage level back to its nominal level, when another measurement sequence can be started. The voltage waveforms are simple rectangular pulses with different amplitudes and/or durations. The responses recorded for methanol, ethanol, and 1-butanol at different concentration levels using 6 different amplitude heating voltage pulses of constant duration (40 s) are given in Fig. 3a–c.

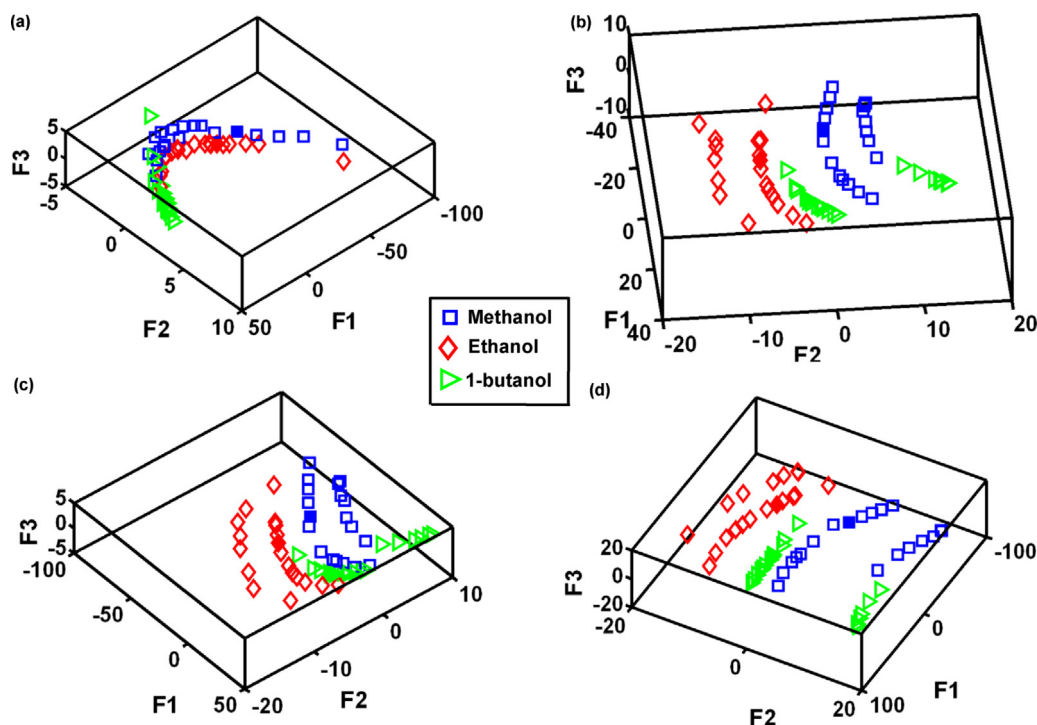


Fig. 5. Results of PCA mapping of the feature vectors of the three target gases, each at various concentrations in the range of 100–2000 ppm, to a 3-D feature space using the feature subsets extracted from three couples of different rectangular heating voltage pulses (a–c). (d) Feature space segregation of the different target gases achieved by fusing all the information related to the six different pulses used for obtaining (a)–(c).

Responses were generated for three different pulse durations of similar general configurations. As a result a collection of 18 different pulsed responses were available for each target analyte at any concentration; examples are given in Fig. 4a–c.

4. Results and discussion

The voltage waveforms used for the temperature modulation of the sensor consist of 18 different rectangular voltage pulses which result in 18 temporal responses for each atmospheric condition examined. Only six out of these responses were selected for subsequent processing. The reason was to make the case challenging for the different classification techniques being compared. Each recorded single pulse response, similar to the examples presented in Fig. 4, is transformed by db2 wavelet [24] for feature extraction. The obtained wavelet coefficients are defined as the feature vector of the response. The three different contaminants each examined at 19 different concentrations with six different temperature modulating pulses applied, produced a total of 57×6 feature vectors. These vectors were utilized for the classification of the analytes with the different techniques described below.

Principal component analysis (PCA) was used for mapping the feature vectors to separate 3-D feature spaces. The PCA results obtained are given in Fig. 5a–d indicating somehow overlapping of the clusters in the feature space. In these calculations 18 out of the 19 feature vectors related to each class are considered as the training vectors. The remaining vector is assumed as the test data and is utilized for examining the success rate of the classification process (see Fig. 5). The classification results were cross-validated by reshuffling of the test vector position among all vectors available. The overall classification success rates are given in Table 1.

In a different attempt, the data processing described in the flowchart given in Fig. 6 was utilized for the classification of the produced feature vectors. The process consists of defining six

feature subsets based on the db2 transformed responses related to the different heating voltage waveforms, training of six similar structure support vector machines (SVMs) as the base learners with the Gaussian kernel on these training subsets, and forming an ensemble of classifiers for the classification of the input data. Six different temporal responses are recorded for an unknown analyte. Each response consists of 2.5–8 kB of data which is db2-transformed to 0.3–1 kB to form the feature subset related. These were fed to their respective expert SVMs for classification. Six votes were cast by the six SVMs each relating the unknown analyte to one of target classes. The classification verdict was determined by the majority voting among these classifiers. In Table 2 the classification results of the individual SVM classifiers and those obtained from fusing the classifiers output by majority voting are presented.

A comparison of the results presented in Table 2 to those given in Table 1 indicates the superiority of utilizing an ensemble of expert classifiers to a single generally trained one. The method is general and can be utilized on the target gas-related data obtained via different selective gas sensors [25–28]. In a similar process all the SVMs were replaced with the same number of multi layer perceptrons (MLPs). The obtained classification results are also given in Tables 1 and 2 indicating a classification enhancement level close to those obtained by utilization of SVMs.

In the suggested ensemble technique, the computation involves matrices of lower dimensions: in the traditional method, the dimension reduction calculations are performed on a $342 \times n$, where n is the selected number of wavelet coefficients, feature matrix formed by wavelet transformation of all recorded responses. In the multi-classifier case, however, the feature matrix is divided into six $57 \times n$ subset matrices. In this case, calculations on the $342 \times n$ matrix are omitted and classifications by the ensemble members are carried out directly on the $57 \times n$ feature subsets.

Although the observed gas recognition accuracy enhancement is around 10% (Tables 1 and 2), it clearly indicates that an ensemble of

Table 1

The classification success rates obtained using the traditional classification method using only one SVM/MLP classifier along with the utilization of PCA dimension reduction technique.

Dimension Reduction Classifier	PCA SVM				PCA MLP			
	a	b	c	a, b, c	a	b	c	a, b, c
Pulse train								
Example of related sensor responses	Fig. 4a	Fig. 4b	Fig. 4c	–	Fig. 4a	Fig. 4b	Fig. 4c	–
Related feature space	Fig. 5a	Fig. 5b	Fig. 5c	Fig. 5d	Fig. 5a	Fig. 5b	Fig. 5c	Fig. 5d
Success rate of cross validation %	69.2	85.7	80.9	82.2	61.8	82.3	78.4	80.0

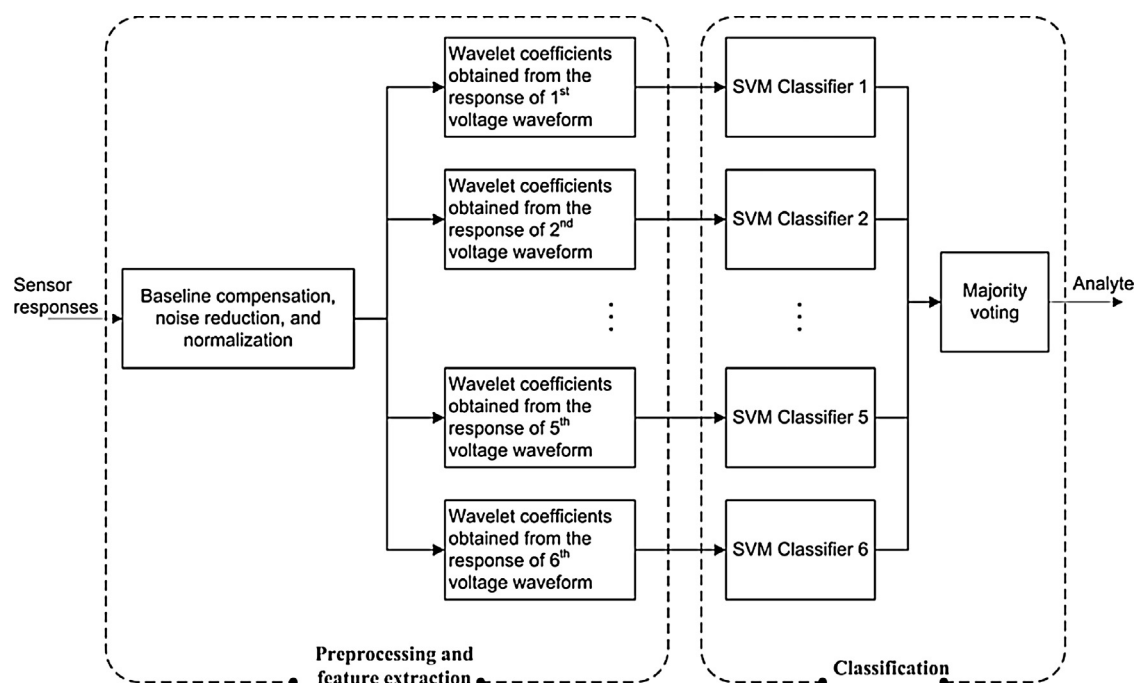


Fig. 6. The flowchart of the data processing carried out on the recorded responses of a sensor temperature modulated with six different microheater voltage pulses. The goal is to discriminate between methanol, ethanol and 1-butanol.

Table 2

The classification results of six different base classifiers, all SVMs or all MLPs, each operating individually on the feature subsets extracted from the responses related to a specific microheater pulse, and the result of their fusion by ensemble forming and majority voting.

Classifier code	Base classifiers						Ensemble
	1	2	3	4	5	6	Fusion
Accuracy obtained with SVM %	82.8	63.8	84.5	89.6	87.9	89.6	92.0
Accuracy obtained with MLP %	81.1	68.6	85.2	88.1	87.9	88.3	92.4

expert classifiers results in better classification. It has been shown that this enhancement level may depend on the type of the dataset, as well [18]. Hence, similar approaches on differently collected gas sensor responses may result in even higher levels of classification enhancement. Further work in this respect is recommended.

5. Conclusion

Using a generic gas sensor, operating temperature modulated with six different heating voltage pulses, six different temporal response patterns were generated for each analyte. The features of these responses were subsequently extracted by wavelet transformation. For the purpose of comparison, two different approaches were utilized for analyte classification: the first approach comprised feature dimension reduction followed by classification with a support vector machine trained based on all the training feature database. In the second approach, an ensemble of six structurally similar support vector machines, each trained based on a

predetermined feature subset related to a specific heating voltage pulse, were directly applied to the respective feature subset. The fusion of the information contents of these feature subsets was, then, carried out by majority voting among these expert classifiers.

The classification success rate achieved by the ensemble of expert classifiers is higher than that of the generally trained classifier. Further work is required for clarification of the source(s) and maximization of this classification enhancement. At this stage it can be attributed to variety of procedure specifications such as the amount of analyte-related information lost in the dimension reduction process or the higher efficacy in expert classifier training. The findings reported are useful for the researchers in the field of artificial olfaction as the majority of the work reported in the related literature have utilized a single classifier. The technique is computation cost effective, significantly reduces the dimensions of the feature matrices involved, and is of general applicability to various array- and quasi-array-based gas analysis systems.

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