Comparison of different feature reduction methods in the improvement of gas diagnosis of a temperature modulated resistive gas sensor

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Abstract. The present study aims to analyze dynamic responses of a temperature modulated resistive gas sensor with the emphasis on the comparison of different feature reduction methods. For this purpose, four selected feature reduction methods consist of Linear Discriminant Analysis (LDA), Principal Component Analysis (PCA), Generalized-LDA (GDA) and Kernel-PCA (KPCA) are applied and compared. The sensor selected for the experiment is a tin oxide based sensor, FIS commercial type. A staircase voltage with the step length of 40 s and voltage range of 1-5 V constitutes the input of the sensor. Sensor system was modeled by ARMAX linear model. The effects of induced gases were recorded as parameter vectors in the data obtained by the model. After applying the methods of feature reductions, the performance of gas separation was compared. It was found out that LDA and GDA yielded the best data classification.

1. Introduction

In the last few decades, scientists in the machine olfaction field have developed a tool called electronic nose which its name was taken from arranging a number of sensors in an array along with a sophisticated pattern recognition engine [1]. Today, development of an electronic nose, similar to human nose is highly important. Already commercial systems from several companies are targeting applications, present and potential, that range from quality assurance of food and drugs to medical diagnosis, environmental monitoring, safety and security, and military use.

If the sensors are able to detect aromas in an environment contaminated with different gases, one of the most important goals of the development of a machine olfaction systems is to increase the quality of gas detection by a certain sensor or a set of sensors. The question whether it’s better to use more sensors or to develop a more sophisticated sensor has brought debates among researchers who study on the machine olfaction. Although it’s possible to increase the quality of analysis by adding more sensors or additional properties, it’s not easy to answer the above question [3-6]. On the other hand, it’s necessary to use combined sensors for the pattern of an electronic nose. A combined sensor possesses more selectivity and the power of analysis than a single sensor. Additional sensors are useful for decreasing detection error and increasing the sensitivity of array. However, it increases dimensions of pre-processing, the complexity of calculations and also causes a high level of noise [7]. Attempts
have been made to create selectivity in a single sensor [8]. One of the techniques that’s commonly used for creating the capability of selectivity in single sensors is the modulation of sensor temperature [9-10]. Various studies have shown that gas sensors with modulated working temperature yield more discriminant features. This method allows one to feed sensor’s heater with variable voltages instead of using sensors at fixed temperature, which is produced by applying fixed voltage on the sensor’s heater. This leads to a change in the planned temperature of sensors during the measurement stage [11]. The stage of feature identification includes a vector of inputs which is produced by different methods of linear and non-linear feature reduction either with or without supervision for the next stage (i.e. gas classification). Babaei and Hosseini-Golgoo applied temperature modulation to the micro-heater of an RGS (as input) and recording temporal responses of a sensor (as output), and modelled the system by a linear system identification technique. Then, they used linear discriminant analysis (LDA) for decreasing dimensions of feature vector of the model [10]. In this work, output model could classify four target gases: Methanol, Ethanol, 2-Propanol and 1-Butanol. In another work by Babaei and Amini, they applied temperature modulation in the form of different voltage waves and used principal component analysis (PCA) method to reduce dimensions of feature vector. By doing so, they managed to reduce the dimensions of feature vectors to three dimensions and identify four Butanol isomers [12].

The present article is organized as follows. In the first section, the stages of sensor response recording in the presence of 7 target gases are discussed. Different stages of study on recorded response and the identification of a feature vector for the classification of target gases are considered in sec. 3. Then, feature extraction and the four methods of dimension reduction – LDA, PCA, GDA and KPCA – are explained and compared for the classification of gases. Lastly, results from above mentioned methods are analyzed and compared.

2. Experimental studies

Seven target gases including methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, acetone and hydrogen were imposed on the sensor in 11 concentration levels from 250 to 2000 ppm. A commercial sensor from FIS family (SP3-AQ2) based on tin oxide is selected for the present study. Stages used for the classification of data from a single sensor are the same used in electronic nose. Resistive gas sensors are the most common gas sensors which their basic performance principle is based on conductivity changes of the sensitive layer in the presence of target gas. Sensor input is a staircase temperature modulation as shown in figure 1. The modulation is imposed on sensors microheater. Then, the changes which occur in sensor’s resistance are recorded by the circuit shown in the figure 1. If the applied voltage on the sensor’s micro-heater, $V_s$, and the value of the series conductance, $G_o$, are constant, then the changes of sensors conductance, $G_s$, will precisely calculated by measuring output voltage, $y(t)$, as:

$$G_s(t) = G_o \left( \frac{V_s}{y(t)} - 1 \right)$$

(1)

Using the above expression, the changes of responses in different gas concentrations were computed by recording $y(t)$. For instance, figure 2 shows the recorded response of FIS sensor in the presence of 11 concentration levels of methanol. The staircase heater voltage of the sensor in the gas atmosphere is shown in figure 2, as well. Sensors responses are converted into digital signals by an analog to digital convertor and are transferred into a computer. These responses are in transient state. Sensor’s recorded responses to 11 concentration levels of seven target gases are, then, sent to pre-processing unit in order to be processed, identified and separated.
Figure 1. Measurement system paradigm in a controlled atmosphere chamber for measuring sensor’s response to a target gas.

Figure 2. Temporal response of a temperature modulated FIS gas sensor subjected to 11 concentration levels of methanol.

After recording sensors responses by the circuit shown in the figure 1, the responses are filtered and normalized in order to prevent effects such as environmental changes like temperature changes and moisture in atmosphere as well as the effects of high frequency. The noise from high frequency is reduced for all gases by a digital moving low pass filter with 28 sample window length. Then filtered responses, $y_n$, were normalized as the following expression:

$$y_n(t) = \frac{y(t) - y_{\text{min}}}{y_{\text{max}} - y_{\text{min}}}$$

in which $y_{\text{max}}$ and $y_{\text{min}}$ are maximum and minimum values of sensor response, respectively. In order to enter sensor’s non-linear responses into a linear modelling system, we used 5 segment of sensor responses and 5 corresponding input heater voltage as 5 systems. Figure 3(a) and (b) show total normalized sensor response and its second segment for methanol, respectively. As can be seen in this figure, sensor responses are limited between 0 and 1 after normalization and the length of each output step will be equal to its input modulation, i.e., 40s.
3. Modelling and feature extraction

A single input- single output (SISO) system was selected for modelling. We used n-order, nk delay dynamic linear ARMAX (n,n,n,nk) in our research. In this model, the relation between input, u(t), output, y(t), and noise transfer function e(t) are expressed in the following:

\[ y(t) = \frac{B(q^{-1})}{A(q^{-1})} u(t - n_k) + \frac{C(q^{-1})}{A(q^{-1})} e(t) \]  

in which

\[ A(q^{-1}) = 1 + a_1 q^{-1} + a_2 q^{-2} + \ldots + a_{na} q^{-na} \]
\[ B(q^{-1}) = b_1 + b_2 q^{-1} + b_3 q^{-2} + \ldots + b_{nb} q^{-nb} \]
\[ C(q^{-1}) = 1 + c_1 q^{-1} + c_2 q^{-2} + \ldots + c_{nc} q^{-nc} \]  

where coefficients of \( a_i \), \( b_i \), and \( c_i \) are arranged in a feature vector

\[ \theta = (a_1, \ldots, a_{na}, b_1, \ldots, b_{nb}, c_1, \ldots, c_{nc})^T \]  

In order to compare measured output and the output of a trained network, fitness criterion is computed for each segment [9]. Based on the results of fitness computations, the smallest and best model order for each five defined systems is selected. The values for \( n \) are one or two. According to the relation (4), for \( n=2 \), the number of features is 6 and for \( n=1 \), the number of features is 3. In this way, segment-I, II and V are modelled by the 2nd order model, while segment-III and IV are modelled by the 1st order model. Thus, we'll have 24 features in total. Parameter vector from each recorded response is used as a feature vector for encoding operations in feature reduction methods like PCA, which is the representative of linear unsupervised training methods and LDA, which is the representative of linear supervised training methods. Utilization of kernel functions let us use linear feature extraction methods such as LDA and PCA for non-linear systems. Kernel PCA and generalized discriminate...
analysis (GDA) methods are two examples of feature extraction methods which have been generalized from LDA and PCA methods by kernel function. In the present study, we used a kernel function as the following expression:

$$\phi(x) = \begin{bmatrix} x_1, & x_2, & \ldots, & x_n, \\
x_1x_1, & x_1x_2, & \ldots, & x_1x_n, \\
x_2x_1, & x_2x_2, & \ldots, & x_2x_n, \\
\vdots & \vdots & \ddots & \vdots \\
x_nx_1, & x_nx_2, & \ldots, & x_nx_n \end{bmatrix}^T$$

Thus, dimension of feature vector, first increases and then reduce in a new feature space (3-dimensions). As a matter of fact, the system must be able to separate new concentrations (test data), as well. Therefore, three randomly selected test data are also introduced into the system. Training and test data after LDA, PCA, GDA and KPCA methods are given in the figure 8(a)-(d), respectively. In these figure, test data shown by filled markers, could join their class in LDA and GDA methods. It should be noted that LDA linear method could perform better than non-linear GDA method in terms of data separation and dispersion. This means that LDA is a more suitable method for separating classes of both training and test data.

Figure 4: feature extraction, parameter dimension reduction and the separation data for each class by encodings (a) LDA, (b) PCA, (c) GDA, (d) KPCA after selecting two different concentrations of 450 ppm and 1700 ppm.
4. Conclusion

In this paper, staircase temperature modulations with 5 voltage steps and plateau length of 40s were imposed on sensor's micro heaters as the inputs of the sensor. Then sensor's output responses were recorded. Then, each input and output increment was imposed on a model called ARMAX, a feature vector with 24 dimensions was obtained. Using four selected feature reduction methods, 24 dimensions were reduced to 3 dimensions. We tried to compare linear and non-linear feature reduction methods for extracting features from responses of a resistive sensor. Also we evaluated the separation of gases in test and training concentrations. Although linear LDA methods performed better than non-linear GDA methods, results suggested that LDA could separate both test and training data better than other methods.

5. References

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