OPTIMUM PATTERN RECOGNITION METHOD FOR THE ELECTRONIC NOSE SYSTEM

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Abstract

An electronic nose (EN) is an artificial olfactory system that tries to perform the same task as human olfactory system and widely used in the gas analysis field. EN consists of an array of chemical sensors possessing broad specificity, coupled to electronics and software that allow feature extraction – extraction of salient data for further analysis, together with pattern recognition – identification of sample odour.

Here, we present a neural architecture based on several self-organizing maps that counteract the parameter drift problem for an array of chemical gas sensors. The neural architecture named mSom, since m is the number of odours to be recognized and is mainly constituted of m maps, each one of them approximate the statistical distribution of a given odour. Competition occurs both in each single map and between maps for the selection of the minimum map distance in the Euclidean/Mahalanobis distance space. Fuzzy-C-means has been used to find three optimum centres for the training data and then initializing SOM weights (system was called mSomFuzzy) with these centres instead of random weights. The system is called mSomFuzzyMaha, while the Mahalanobis distance is being used as a distance metric.

The main aim of the research work is to investigate the optimum pattern recognition method for the electronic nose system under normal conditions subjected to drift, no matter how different the concentrations. Although chemical patterns from the sensor array should be the same for a particular sample, the actual responses are affected by many factors such as temperature, humidity, and sensor drift.

Index Terms: Electronic Nose, Self Organizing Map, mSom, PCA.

1. INTRODUCTION:

The human nose is widely used as analytical tool in industry today. The human sense of smell is influenced by many factors such as age, gender, state of health and mood. The response of subjects to different odours and odour concentrations is highly subjective as the human sense of smell can vary dramatically from person to person. An artificial sensing system that emulates the human sense of smell is desired in a range of fields, such as food and drink production, tobacco and cosmetic industries, and for environmental monitoring in chemical plants. An instrument that can perform simple odour discrimination and provide measurement of odour intensity, without subjective influences, would be very useful in modern industry. These systems have been given the terminology ‘electronic nose’ (EN) and consists of an array of chemical sensors [1] possessing broad specificity, coupled to electronics and software that allow feature extraction – extraction of salient data for further analysis, together with pattern recognition – identification of sample odour. EN is capable of detecting and recognizing a wide spectrum of odour patterns[2, 3]. Its performances mimic some aspects of the biological olfactory system[4].

Since many sensors (variables) are used to characterize a chemical environment, pattern recognition methods are used to help interpret the signals, e.g. principle component analysis, K-nearest neighbour and artificial neural network (ANN). The pattern recognition system is being trained with the help of known patterns. The mapping of each gas concentration or class identification is made using these trained patterns during the later measurements. But the sensor drift will destroy the initially trained pattern recognition capability after a certain period, so that it is very difficult for the initial trained pattern to classify or get the exact concentration value of the monitoring gas.
However, it has been impossible to fabricate chemical sensors without drift up to now. The sensor drift has to be treated in some way in order to achieve reliable measurement data from the sensor array. Methods based on self-organising neural networks [5, 6] and adaptive resonance theory [7, 8] have been proposed, for their ability of processing non-stationary sources of data such as sensor outputs subjected to drift effects.

2. ELECTRONIC NOSE

An electronic nose incorporates an array of chemical sensors, whose response constitutes an odour pattern. A single sensor in the array should not be highly specific in its responses but it should respond to a broad range of compounds, such that different patterns are expected to be related to different odours.

A chemical sensor consists of a chemical sensitive layer and a transducer. The chemical sensitive material captures the interaction with the analyte molecules present in the environment and generates a physical change which is sensed by the transducer that converts the signal into an analogue electrical output. The transduction mechanism makes available several physical signals where it has been widely used the approach of electrical measurements (current, resistance, voltage, and capacitance), mass changes, heat generation, and measurements of optical changes (absorption, fluorescence, and reflectivity).

In an array of chemical sensors a pattern can be acquired and processed as shown in Fig. 2.1. Let us consider a simple odour (pure gas) or a complex one represented as a concentration vector of the jth odour class \( c_j(t) = (c_{1j}, c_{2j}, \ldots, c_{pj}) \), where \( p \geq 1 \) is the number of odorant components.

![Fig. 2.1 An intelligent artificial olfactory system](image)

The first stage of the description of the system is the impact of the odour with the sensor surfaces. The most likely effect of the transduction process is the measurement of the electrical resistance, but in other cases could be a change in mass (for BAW sensors) or electrical potential (for Pd-gate Mosfet).

The signal generated by the sensor material is then converted into an electrical signal and then conditioned. The output signal, for example the resistance \( R_{ij}(t) \) (i.e. the signal of sensor i for class j at time t) readout by the electronics is then digitized as a result of the Analog to Digital conversion in order to have a ready to be recognised signal. The converted signal is given by the vector

\[
y_j(t) = \begin{bmatrix}
y_{1j} \\
y_{2j} \\
\vdots \\
y_{nj}
\end{bmatrix}
\]
The array response may be pre-processed for noise and complexity reduction in order to accomplish the odour recognition task and visualization purpose. A typical gas sensor response is shown in Fig. 2.2 (ideal case), where the sensor is exposed to a certain odorant \( j \) with a certain concentration \( c_j(t) \). The value \( R_0 \), called baseline, is referred to the value of the referring gas injected into the vial before injecting the sample odorant for which the response changes until reaching the saturation value \( R_s \). Usually the rise time \( \tau_r \) and the decay time \( \tau_d \) are different. However, the output signal \( R_j(t) \) is subjected to divergence from the ideal case by interfering signals.

There are several interfering inputs, the most common being changes in temperature and relative humidity of odours. Usually the heater of a chemo resistor is maintained at constant voltage but in reality the operating temperature varies due to any changes in ambient temperature. Humidity also has a strong effect on most sensors. The baseline resistance usually decreases as the humidity increases, although the exact slope depends on the operating temperature of sensors.

![Sensor Response](image1.png)

(a)

![Sensor Response (drifted)](image2.png)

(b)

3. DRIFT COUNTERACTION

Ideally, a chemical sensor will always give the same response when exposed to an identical gas mixture [9]. This will, however, not be true when the sensors are operated over a long period of time. There will be a change in the size of the sensor response for a certain amount of a given gas; the selectivity of a sensor may change, i.e. the response changes differently for different gases (fig. 2.3). (a) shows the response as it appears without drift; (b) shows the response to the same gases when the response of the sensor has decreased by the same amount for each gas. Note that the pattern is preserved, even though the absolute value changes; (c) shows the response to the same gases when the response has changed differently for the different gases. This is referred to as a change in the selectivity of the sensor. These changes in the sensor behaviour together give rise to drift in the sensor responses.
4. METHODS

The main aim of the research work is to investigate the optimum pattern recognition method for the electronic nose system under normal conditions subjected to drift, no matter how different the concentrations. Although chemical patterns from the sensor array should be the same for a particular sample, the actual responses are affected by many factors such as temperature, humidity, and sensor drift. If no drift correction of the sensor signals is made, the model will have a continuous need for re-calibration. Hence, a new architecture that we call mSom (where m is the number of independent maps), has been developed on the basis of the self-organizing map (SOM) theory developed by Kohenen. Unlike other neural techniques where the input-output learned mapping is static, the architecture here presented reduces the drift problem (thus increasing the time of re-calibration) by addressing the dynamic input-output mapping.

4.1 SOM:

The principal goal of the self-organising map (SOM) is to transform an incoming signal pattern of arbitrary dimension into a two-dimensional discrete map, and to perform this transformation adaptively in a topological ordered manner. The embedded competition paradigm for data clustering is done by imposing neighbourhood constraint on the output units, such that a certain topological property in the input data is reflected in the output’s unit weights.

4.2 mSOM:

mSom preserves the self-organization paradigm by considering as many maps as the various odour classes which are taken into consideration to accomplish the classification task. The novelty in this architecture is the possibility of adjustment of the individual maps overtime to be able to predict gas measurements which have suffered from drift.

4.3 Discrete Wavelet Transform:

The filtering algorithm associated with the discrete wavelet transform is an effective tool for smoothing out the high-frequency content without losing the important features in the process signal. The wavelet transform decomposes signals over dilated and translated wavelets. It maps the input signal into a new space, the basic functions that are quite localized in space and provides a multi resolution signal decomposition. This signal analysis technique analyses the signal at different frequency bands with different resolutions by successively projecting it down onto two basis functions, which are obtained by applying shift and scaling operations to two prototype functions called the scaling function $\varphi(t)$ and the wavelet function $\psi(t)$, respectively:

$$\varphi_{a,b}(t) = \frac{1}{\sqrt{a}} \varphi \left(\frac{t - b}{a}\right)$$  \hspace{1cm} (3.6)

$$\psi_{a,b}(t) = \frac{1}{\sqrt{a}} \psi \left(\frac{t - b}{a}\right)$$  \hspace{1cm} (3.7)

where $a$ is the scaling parameter and $b$ the shift parameter, and $a,b \in R, a \neq 0$. $R$ is a real continuous number system. It should be pointed out that only those functions that have a zero net area can be used as a mother wavelet and must have a non-zero response for a finite interval of time. This suggests that the transformation kernel of a wavelet transform is a compactly supported function (localized in time).

4.4 Fuzzy-C-means:

Fuzzy-C-means algorithm (FCMA) was initially attempted to find the optimum centres where a single centre was assigned for each class. In real applications, however, a class could not always be represented by a single centre, especially when a large number of data sets or each class did not form a tight cluster.

The original Fuzzy-C-means algorithm was introduced by Bezdek[13]. FCMA method was based on a classical “crisp” clustering method, which was modified and extended by fuzzy set theory. Generally, the classical “crisp” clustering algorithm

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(c) Sensor response

1 2 3 4 5 6 7 8 9 10
0 10 20 30 40 50 60 70 80 90 100

Fig. 2.3 Examples of the sensor response shown as bar charts for one sensor when exposed to ten different gases.
generates partitions such that each pattern is assigned to exactly one cluster. However, it is not always possible to adequately assign patterns strictly to one cluster when patterns are located between clusters. FCMA resolves these problems by solving the necessary conditions of the cluster centres and membership grade of pattern through an iterative process.

4.5 K-Nearest Neighbour:
The K-nearest neighbour (KNN) technique is a simple non-parametric pattern recognition algorithm, based on the Euclidean distance metric, which can handle complex data spaces. In this method unknown is classified according to the majority vote of its K-nearest neighbours in the training set in n-dimensional space. Should there be a tie; the closer neighbours are given greater weight. The Euclidean distance is given by equation:

\[ d_{ij} = \sqrt{\sum_{k=1}^{n} (x_{ik} - x_{jk})^2} \]  

(3.17)

where \( d \) is the Euclidean distance between patterns \( i \) and \( j \), each with \( n \) variables (sensors). Euclidean distance can sometimes produce unexpected results unless normalization or scaling of pattern vector is performed. Instead of the Euclidean distance Mahalanobis distance (eqn. 3.17) is being used to find the nearest neighbour.

4.6 Mahalanobis distance:
Mahalanobis distance metric is a measure of how far the observation is from the centre of all values. A mean vector for each class and the pooled covariance matrix in order to define the class boundaries are computed. To classify a new pattern \( (x_j) \), the Mahalanobis distance to the mean vector \( (\bar{x}_m) \) for each class is computed as:

\[ d_{jm} = \sqrt{(x_j - \bar{x}_m) C^{-1} (x_j - \bar{x}_m)} \]  

(3.18)

where \( d \) is the distance between pattern vector \( j \) and the mean pattern vector for class \( m \) and \( C^{-1} \) is the inverse of the pooled covariance matrix (estimate of the common covariance of the class).

4.7 Principal Component Analysis (PCA):
PCA is a linear, unsupervised pattern analysis technique that has been used by many researchers to project the response of an electronic nose to simple and complex odours, in reduced dimensional space. PCA seeks to reduce the number of variables that need to be considered (i.e. \( n \) sensors) to a smaller number of indices, called principal components \( X_p \), that are a linear combination of the original variables (i.e. sensor responses):

\[ X_p = a_{1p}x_{1j} + a_{2p}x_{2j} + \ldots + a_{np}x_{nj} \]  

(3.19)

The principal components (sometimes referred to as scores) are calculated from the scalar product of the set of orthogonal (principal) vectors with the response vectors themselves. Each principal vector accounts for a certain amount of variance in the data with a decreasing degree of importance. The indices or principal components \( X_p \) are ordered so that \( X_1 \) displays the greatest amount of variance, followed by the next greatest \( X_2 \), and so on. The first principal component \( X_1 \) is calculated such that its variance is as large as possible, whilst the sum of the coefficients \( a_{ij} \) of the orthogonal (eigen) vector is set to unity. The second principal component is calculated in a similar way with the additional constraint that it is uncorrelated with \( X_1 \), and so on. The corresponding eigenvalues give an indication of the amount of information the respective principal component represent.

5. OBJECTIVES OF RESEARCH:
Our aim is to improve the performance of the pattern recognition system based on multiple self-organising maps with four clustering methods Fuzzy-C-means, PCA, KNN, and the Mahalanobis distance and develop software responsible for interpreting the output from the gas sensors in the drifted environment. The software required must be fast and reliable at distinguishing gases and/or odours of interest as well as be able to compensate for the drift in the sensor array data in the long run.

6. FURTHER WORK:
The next step is to test the limitations of mSom in presence of different types of drift and check how far it is able to track the drift in the data. This requires testing mSom with drifted data collected in real environment. Another aspect is to integrate mSom software with data acquisition software.

Independent Component Analysis (ICA) is a novel method in the analysis of gas-sensor array measurement data and seemingly indicates potential to improve the performance of the instrument. For a data set following a Gaussian distribution, PCA provides directions for data projection that allow an adequate decomposition. However, assuming that gas-sensor array measurement data have a Gaussian joint distribution is not realistic due to various reasons. Underlying sources, like the mechanism of a sampling system or sensor drift, are unlikely to follow a Gaussian distribution. In fact, the joint distribution of gas-sensor array measurement data often appears to be non-Gaussian. Therefore, PCA is not the optimal
analysis tool for gas-sensor array measurement data, since other types of distributions have to be assumed for the data.

We would like to use ICA to track the sensor drift embedded in the real time data collected in real environment.

REFERENCES


