A Survey on Sensor's Drift Counteraction Using Dynamic Pattern Recognition System.

Tapsi Garg
Associate Professor (CS)
RKGIT, Ghaziabad

Dr. Rabins Porwal
Associate Professor (MCA)
ITS, Mohannagar, Ghaziabad

Abstract:

In past years, numerous electronic nose (e-nose) developments have been published describing analyses of solid-, liquid- or gaseous media in microbiological-environmental-, agricultural- or medical applications. However, little has been reported about complex methodological pitfalls that might be associated with commercially available e-nose technology.

As a novel bionic analytical technique, an electronic nose, inspired by the mechanism of the biological olfactory system and integrated with modern sensing technology, electronic technology and pattern recognition technology, has been widely used in many areas. Moreover, recent basic research findings in biological olfaction combined with computational neuroscience promote its development both in methodology and application

Our aim is to develop pattern recognition software that is responsible for interpreting the output from the gas sensors in the real environment where both the sensors and the environment are likely to drift.

Keywords: Electronic Nose, Pattern Recognition, Self Organizing Map, Headspace

Introduction:

For more than 20 years, so-called electronic noses (e-noses) have been widely applied for headspace- and trace gas analysis from solid-, liquid- and gaseous samples. During this time, different sensing methods have been developed but the e-nose principle remained the same [3-4]. Generally, e-noses consist of an odour delivery system, an array of sensors, a data acquisition- and a data analysis unit. In all types of e-nose, the sensor array exploits the conversion of changes in electrical-, thermal-, mass- or optical properties into an analysable signal. As for human noses, sensors show an overlapping specificity and therefore provide a non-quantitative sensor response, a so-called fingerprint, rather than a specific qualitative or quantitative answer. The lack of specificity is due to the fact that sensors react with functional groups and structures of analytes rather than specifically with the molecule itself. Sensor responses are then analysed using multivariate data analysis techniques in order to classify or discriminate a group of samples. But data analysis methods are complicated by the fact that there are multiple causes of variation –biological differences between samples or differences arising from the analysis itself (methodological variation). Methodological variation, including sensor drifts, may lead to unclear or contradictory results because the lack of repeatability or "disturbance" can be expressed as variation which may obscure biological variation. Hence the elimination of methodological variation is one of the biggest challenges associated with e-nose technology.

Gas chromatography-mass spectroscopy (GC-MS) is one of the most widely used techniques for the analysis of complex mixtures to be separated and the individual constituents identified and quantified. As the technique became widespread and more sophisticated, it was possible to separate and chemically identify the dozens or hundreds of individual substances present in food, flavour and fragrance products. However, this is a complex, expensive and time-consuming task which requires a well-equipped analytical laboratory and skilled staff. [8]

Electronic Nose:

According to Gardner (Gardner et al. 1999) "*An electronic nose is an instrument, which comprises an array of electronic chemical sensors with partial specificity and an appropriate pattern recognition system, capable of recognising simple or complex odours"[2]*

Two Main Components:

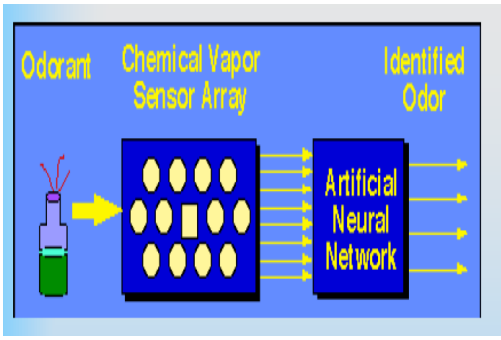

Fig 1.1: Block Diagram of E-Nose

Sensing System
(Array of chemical sensors, single sensing device)
Automated Pattern Recognition System
(Statistical, ANN approaches)

Since the mid 1980s there has been increasing interest in the development of so-called 'electronic noses', i.e., an electronic instrument that is capable of detecting and recognising complex odours. They are based around an array of sensors, each of which has a partial specificity. This array produces a finger print of the odour which is used by an appropriate pattern recognition system to identify the odour through comparison with a reference library of previously obtained measurements of known samples.

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).

A most important consideration for the successful operation of an odour sensor is its long-term stability. *Drift* is defined as *"a gradual change in any quantitative characteristic that is supposed to remain constant"*. Thus a drifting chemical sensor does not give exactly the same response even if it is exposed to exactly the same environment for a long time. [4]

The main aim of the research work is to investigate optimum pattern recognition approaches for electronic nose systems over long period – where both sensors and analytes may be drifting. 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.

Pattern Recognition Algorithms:

Pattern recognition is defined as the process of classification of data by comparison to known patterns. Patterns are typically described in terms of multidimensional data vectors, where each component is called a *feature*. The aim of a pattern recognition system is to associate each pattern with one of a number of possible *pattern classes* (or simply *classes*).[1] Obviously, different patterns should be associated with the same class or with different classes depending on whether they are characterised by similar or dissimilar features, respectively. In the case of the electronic nose, the patterns and the classes are, respectively, the responses of the sensor array to odorants and the odorants being considered. In order to develop a pattern recognition system, the sample data are split into two sets, namely, the *training set* and the *test set*. The training set is used to establish the design parameters of the pattern recognition system, whereas the test set contributes to evaluate the system performance. Typically, the performance of the pattern recognition system is measured by computing the percentage of correctly recognised patterns on all the patterns presented to the system. Of course, the performance of the pattern recognition system should be as independent as possible from how the sample data are split into training and test sets. Several different data processing and pattern recognition techniques have been used in the literature to

recognise signals produced by sensor arrays (Di Natale et al. 1995a). These include linear pattern recognition techniques, such as principal component analysis and cluster analysis (Gardner 1991) and non-linear pattern recognition techniques, such as classical multivariate analysis and artificial neural network (ANN) algorithms (Di Natale et al. 1995b). As the relationship between the signal produced by a sensor and an odorant concentration is usually non-linear, non-linear pattern recognition techniques are generally more successful than linear ones. However, the success of each technique heavily depends on the preliminary selection of the features, which are used in the recognition process.

The algorithmic part of an odour discrimination system consists of three steps:
(i) Signal conditioning and feature extraction
(ii) Dimensionality reduction and
(iii) Classification.

The role of the first step is to segment the pattern of interest from the sensor response, remove noise, normalise the pattern and any other operation that contributes in defining a compact representation of the pattern. Feature reduction should provide a small number of informative features in order to make the learning task simpler. Classification tasks address the problem of identifying an unknown sample as one from a set of recognisable gases.[6]

'Intelligent' Pattern Analysis Techniques

The nature of EN data is such that it is often desirable to use a more powerful PARC method that is able to cope with non-linear data, and has further advantages, over more conventional methods, such as learning capabilities, self-organizing, generalization and noise tolerance. An electronic nose must be capable of identifying low concentration (PPB-PPM) of chemical signals in an odorous environment with detection time of less then one second. Recent interest in learning from data has resulted in the development of biologically motivated methodologies such as Artificial Neural Networks (ANN). [7]

ANNs, sometimes called neurocomputers, consists of parallel interconnected and usually adaptive processing elements that are attractive as they, to a certain extent, mimic the neurobiological system. The processing elements represent the biological brain cells or neurons, and their interconnections, the synaptic links. The pattern recognition ability of the ANNs is potentially higher than the classical PARC paradigms described earlier, due to adaptability, noise tolerance, fault tolerance, distributed associated memory, inherent parallelism generating a high speed of operation subsequent to training, and additionally, ANNs are amenable to VLSI implementation. Disadvantages include the fact that the training time increases with the size of the network. The following section gives a comprehensive review of ANN-based EN systems and applications.

Radial Basis Function Network (RBF)

RBFs are attractive when other ANN methods fail to get a good classification due to a significant difference between classes in terms of shape, volume or density, of overlapping classes. RBF networks are supervised learning paradigms very similar to MLP except that they use radial basis transfer functions for the hidden layer rather than linear or sigmoid ones. Hence they classify data using hyper-spheres rather than hyper-planes. The purpose of RBF is to allow the screening of the input space with overlapping receptive fields. The non-adaptive RBF is a fast two-stage training procedure using a hybrid learning rule: [7]

Unsupervised learning in the input layer for the determination of the receptive field centres and widths.

Supervised learning of weights in the output layer simply using the delta learning rule via linear least squares.

Hence RBF implementations differ mainly in the choice of heuristics used for selecting basis function centres and widths. Although RBF networks do not provide error estimates, they have an intrinsic ability to indicate when they are extrapolating since the activation function of the receptive fields is directly related to the proximity of the test pattern to the training data. However, one of the main difficulties when using this type of system is the determination of the optimal architecture – the number of hidden nodes necessary to achieve a good classification. Although RBF networks classify bounded regions of sensor space, this can make them more sensitive to sensor drift and so less robust; this is a trade-off between model accuracy and robustness.

Kohonen Self-Organizing Maps (SOM)

Neural network learning is not restricted to supervised learning, wherein training pairs are provided. Another major type of learning is unsupervised learning, in which net seeks to find patterns or regularity in the input data. Self-Organizing Map, developed by Kohonen, groups the input data into clusters [3], a common use of unsupervised learning. It, also called topology preserving map, assumes a topological structure among the cluster units. There are m cluster units, arranged in a one or two dimensional array, the input signals are n-tuples.

The weight vector for the cluster unit serves as an exemplar of the input patterns associated with that cluster. During the self-organizing process, the cluster unit whose weight vector matches the input pattern most closely is chosen as the winner. The winning unit and its neighbouring units (in terms of the topology of the cluster units) update there weights.

Learning Vector Quantization (LVQ)

LVQ is a version of supervised SOM proposed by Kohonen. It is a pattern classification method in which each output unit represents a particular class or category. The weight vector for an output unit is often referred to as a reference (or codebook) vector for the class that the unit represents. It is a method based on a reward-punishment scheme in order to improve the quality of the decision surface. It is a useful method to refine clusters, and to reduce the area in between two or more cluster in which highest uncertainty is present. This area is also known as Bayesian borders. The designated categories of the training set are known in advance and are part of the training set.

After training, an LVQ net classifies an input vector by assigning to the same class as the output unit that has its weight vector closest to the input vector. The motivation for the algorithm for the LVQ net is to find the output unit that is closest to the input vector. Toward that end, if x and w_c belong to the same class, then we move the weights toward the new input vector; if x and w_c belong to different classes, then we move the weights away from this input vector. The training procedure is similar to SOM, but only the winning neuron is modified in LVQ.

Multilayer Neural Networks

The most commonly used ANN to analyse EN data is a multilayer network called the multilayer perceptron (MLP).[7] A multilayer perceptron is a three-layered network trained by Quasi Newton method, consists of three types of layers of units, namely: the input layer; the hidden layer; the output layer. Only the units in the hidden and output layers are neurons and so it has two layers of weights. The number of input nodes is typically determined to correspond to the number of sensors in the array. The number of neurons in the hidden layer is determined experimentally, and the number of odours analyzed generally determines the number of output neurons. A MLP has a supervised learning phase which employs a set of training vectors, followed by the prediction or recall of unknown input vectors.

In optimization, quasi Newton method is well known algorithm for finding the local maxima and minima of functions. It is based on Newtons Method to find the stationary point of the function, where the gradient is zero. Newton's Method assumes that the function can be locally approximated as a quadratic in the region around the optimum, and use the first and second derivative to find the stationary point. [6]

An Osmetech plc A32S electronic nose was used to generate large number of data sets over time. This instrument contained a conducting polymer sensor array with 20 elements. Data provided for testing the MLP was collected from the conducting polymer array over a period of 30 weeks. An auto sampler allowed repeated presentation of known concentrations of a set of volatile chemicals. Eight aqueous chemical solutions were made up in headspace vials and these were repeatedly measured. They consisted of 100ppm, 200ppm, 500ppm propanoic acid, ammonia. Numbers of repeat samples run on a carousel were 5 and numbers of water washes run on a carousel were 2 (3 repeats each time). We used ammonia and propanoic acid data with different concentrations as shown in table 5.1 to test the MLP performance.

Compound	Concentration	Nomenclature used
Propanoic Acid	100 ppm	100P
	200 ppm	200P
	500 ppm	500P
Ammonia	100 ppm	01N
	200 ppm	02N
	500 ppm	05N

Table 5.1: Chemical compounds, their concentrations and nomenclature used to test the mSom.

The *data-set* was prepared that contained the normalised patterns from original data with 17 features, which contains 407 patterns of Propanoic Acid and 409 patterns of Ammonia.

Table 5.2 shows the number of patterns available in data set.

Data-set	Features	Response	Compound	Patterrns
data-set	17	Steady-state	100P	407
			200P	
			500P	
			01N	409
			02N	
			05N	

Table 5.2: Data set used for MLP training / testing.

To test the MLP's discriminating capability, the system was trained with initial 100 pattern (containing temporal variation of the data) taken over a period of 15 weeks of the *data-set and* then it was tested to classify with remaining all patterns of these classes taken over 30 weeks.

Table 5.3 shows the number of training testing patterns used for the classification for the *data-set.*

	Ammonia	Propanoic Acid	Time
Training patterns	100	100	15 weeks
Testing patterns	309	307	30 weeks

Table 5.3: *data-set* for training / testing.

Figure 5.4 shows the classification of the data set of all available concentrations of ammonia, propanoic acid respectively, collected over 30 weeks.

01N	100P
283	26
11	296

01N 100P

Fig. 5.4: Confusion Matrix for the data set

In fig 5.4, Rows are showing the True Classes, which is the actual class of the pattern and Columns are showing the Predicted Classes, in which the pattern is being classified by the system.
The system is classifying the 283 pattern of 01N class correctly and 26 patterns are misclassified in 100P class. Similarly, 11 patterns of 100P are misclassified in 01N and 296 patterns are classified correctly.

Objectives of Research:

Gas-sensor array technology combined with various pattern recognition methods is widely used in the gas analysis field. The aim of the development of electronic nose technology is to provide cheap and small online instruments for fast discrimination, recognition and quantification of specific chemicals, odours, or toxic substances (Gopel 1998) with high spatial and time resolution. The pattern recognition system is trained on known patterns collected using the data acquisition electronics / software. These patterns form the knowledge base of the system. The mapping of each gas concentration or class identification is made using these trained patterns during the later measurements. But sensor drift will eventually destroy the initially trained pattern recognition capability, so that it is very difficult for the system to classify or predict the exact concentrations of the gas monitored. There are many factors such as poisoning, ageing or environmental changes that can cause the sensor drift.

The scope of the research is to develop a dynamic pattern recognition system to treat the generic drift problem of array based sensors. 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 over a long run.
In the design of electronic noses, as with other types of transducer, attention needs to be paid to the requirements of the user and in what areas the instrument is likely to be applied. For such an instrument to be useful in a variety of situations, it needs to be flexible enough to adapt to changing requirements of odour discrimination. In

view of the array nature of the human nose, it makes sense to design an instrument based on arrays of elements and to use classifier software that would be able to counteract the slow systematic drift problem of the sensors when used for a long period.

We will be using the different neural network and statistical techniques for Drift Countraction to classify electronic nose data collected in long run.

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