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A NEURAL APPROACH FOR IMPROVING THE ODOUR RECOGNITION CAPABILITY OF AN ELECTRONIC NOSE

M. Chimenti, D. De Rossi, C. Di Francesco, C. Domenici, G. Pieri, G. Pioggia, O. Salvetti

Abstract

A hierarchical neural network was used to improve the ability of an electronic nose to recognize olive oil aroma components automatically. For this purpose an electronic nose based on eight conducting polymer sensors and an artificial neural network was developed and tested.

Introduction

In many industrial fields, such as food and beverage, cosmetics, car component manufacturing and others, the qualitative evaluation of products is strictly related to the human perception of odours. Traditional analytical techniques often fail to give an accurate representation of quality, since in most cases it is impossible or too expensive to determine the exact aroma composition and there is no way to recover synthetic human judgement from analytic outputs. Several of the larger companies are equipped with human panels, but this solution suffers many drawbacks (costs, low throughput, limited accuracy and reproducibility) so that the appearance of electronic noses has raised great expectations. In spite of the many applications of electronic noses in product evaluation which have been reported [1], these instruments are not as widespread as expected. Several causes for this, such as cost, inappropriate choice and treatment of samples, inappropriate use of instruments, instability and non-reproducibility of most sensors, can be identified. Some problems can be solved by developing instruments tailored to a specific application [2]. In this work, the preliminary testing of an electronic nose devoted to the detection of defects in olive oil is presented. The instrument was developed to monitor processing stages and for quality evaluation of olive oils. Conducting polymer sensors were exposed to several components of olive oil aroma and data were then analysed by a hierarchical neural network, based on both SOM (Self Organizing Maps) and Back-propagation components.

Materials and Methods

A block diagram describing the experimental set-up is shown in figure 1. Eight conducting polymer sensors (CPS) were prepared according to the procedures patented by *De Rossi* and *Serra* [3]; polymers, dopants and the molar ratios for each sensor are reported in table 1. An electronic card connected to a multimeter Keithley 2700 was used to measure their variation in resistance when exposed to odorants.

The sampling system, which conveyed the odour from the vials to the sensors, was composed of a bottle of ultra-pure nitrogen, a mass flow controller (MFC), a 4-way valve (mod. 0011522, Omnifit Ltd.) and a 16-way valve (mod. EMT4ST16MWE, Valco Instruments Co. Inc.) connected to sixteen 125 ml glass vials containing the samples. Inert PTFE tubing and fittings were used for the connections. Vials were kept at a constant temperature of 25 °C by means of a thermostatic bath.

The measurement protocol consisted of three phases: baseline acquisition, where sensors were flushed with nitrogen; exposure, during which sensors were exposed to the odours; desorption and cleaning, in which odours were flushed away by nitrogen to restore baseline conditions.

The 16-way valve was used to select the sample to be analysed, while the 4-way valve was used to switch the system between state 1 (sensors flushed with nitrogen, baseline acquisistion and cleaning, figure 2.a) and state 2 (exposure of sensors to odorant, figure 2.b). The whole system was controlled by a personal computer with a dedicated software. To ensure reproducibility in measurement data, the entire procedure was automatised.

Samples were composed of 10 ml of solutions (2.5 µl/ml) of different olive oil aroma components (table 2) in refined olive oil. The software procedure for odour recognition was based on a hierarchical neural network architecture [4], following a multi-step approach [5]. The procedure used a two-level architecture, each one composed of a specific kind of neural network that can be trained separately to perform a classification task. The classification task is based on selecting and processing pre-defined features extracted from the acquired sensor responses: in particular, at the first level, the classification of the single features is performed, while, at the highest level, the results of the first step are the input for the final recognition of odour.

The first level is composed of a set of different classifiers, each one being a SOM based neural network, trained in order to specialise in classification of a specific feature inside the global feature space selected. Each feature is input to only one single classifier of this specialisation level.

The highest level (*decisional level*) is composed of a single final classifier based on an *Error Back-Propagation* (EBP) algorithm, whose task is to combine the first level outputs and perform the final odour recognition.

In the SOM networks, the weights w_j of a generic neuron j at time t, for the input $F_k(I)$ are modified as follows:

$$w_j(t+1) = \begin{cases} w_j(t) + \alpha(t)[F_k(I) - w_i(t)] & \text{if } j \in N_i(t) \\ w_j(t) & \text{if } j \notin N_i(t) \end{cases}$$

where:

- w_i represents the weight at time t of the neuron i most excited by the input signal

- $\alpha(t) = \left(1 - \frac{t-1}{T}\right) \in]0 \ldots 1[$ is the learning coefficient; which depends on t and on the fixed maximum number of iterations, T

- $F_k(I)$ is the value of the feature k computed for the signal I (i.e. an odour)

- $N_i(t)$ is the set of neurons in a fixed neighbourhood of given radius and centred around i, influenced by the modification of $w_i(t)$.

The classifications performed by the specialisation level are the input to the top-level classifier, which is able to train the network by propagating the resulting error $\delta_l(I)$ backward. $\delta_l(I)$ is calculated as follows:

$$\delta_l(I) = \begin{cases} f_l'(net_l(I)) \cdot \left(C_{I,T} - O_l(I)\right) & \text{if } l \in \textit{output neurons} \\ f_l'(net_l(I)) \cdot \sum_{m \in \textit{output neurons}} \left(\delta_m(I) \cdot w_{l,m}\right) & \text{if } l \notin \textit{output neurons} \end{cases}$$

where:

- $O_l(I)$ is the output value of the neuron l for the input I

- $net_l(I)$ is the weighted sum of the inputs to the neuron l for the input I

- $f'(net_l(I))$ is the derivative of an activation function f used to compute the output

- $w_{l,m}$ is the weight of the connection between neurons l and m

- $C_{I,T}$ represents the correct classification value of the input I.

Results

Sensor responses are processed to extract a set of features that can be used to characterise the input data. The function $x_n(t)$, which defines the resistance of the sensor at time t, is normalised over the time interval $L = (t_1, t_2)$, during which the polymer is in contact with the gas; the result is a function $x_n'(t) = (x_n(t)/x_m - 1)$, where x_m represents the minimum value of $x_n(t)$ in the time interval L.

For each experiment, the behaviour of the normalised function $x_n'(t)$ is studied for extracting a number of statistical parameters (i.e. features) in such a way that a characteristic fingerprint can be obtained for each odour.

The features selected are the following:

- $E = \sum_{i \in L} x_n'(t)^2$, Energy
- $t_{\max}$, abscissa of the maximum value x_n
- S_c, angular coefficient of the line connecting $x_n'(t_1)$ and $x_n'(t_{\max})$
- D_c, angular coefficient of the line connecting $x_n'(t_{\max})$ and $x_n'(t_2)$
- N_z, number of *zeros* of the second derivative of $x_n'(t)$ with respect to t.

The set of features represents the output of the sensor array to the stimulus of a particular odour. The output is used as input to the SOM nets composing the first level of the hierarchical neural network.

Learning is preceded by an *initialisation* sub-phase obtained by inputting each SOM with a sub-set of values randomly selected from the features.

Subsequently, the SOMs generate a set of outputs that are the input to the decisional level of the network (EBP algorithm).

Once learning process is completed, the network is ready for odour recognition. It can then be evaluated for its accuracy, which can be assessed by presenting input samples (belonging to known classes) to the net and after that comparing the output classification obtained with the expected result. Owing to the characteristic of a SOM, the disposition of the nodes and the topological order introduced after the first level of classification can be checked. The experimental phase was undertaken at four different times. The first two sets of measurements were composed of 6 series while the two latter sets were of 3 series. Each series consisted of 15 measurements (3 for each of the 5 odours), thus the total number of measures was 270. The total number of measurements for each odour was 54. The data set was segmented to provide learning and test sets of 90 and 180 measurements, respectively.

The exposure time of the odours to the sensors took a time interval of 32 s; after this interval a desorption time occurred. Features were extracted considering different interval times of sensors desorption, where t_1 was always the starting exposure time while t_2 was chosen so that the network did learn correctly (20 s and 45 s, respectively). Results are shown in table 3.

The analysis of the topological maps resulting from the SOMs shows the existence of overlapping zones so that odour 1-4 and 2-3 are sometimes mistaken for one another. Grouping these odours together allows a remarkable increase of correct recognitions, as shown in table 4. The chemical structure of the compounds suggests a possible explanation for this fact. Odour 2, 3 and 5 belong to the same chemical class of alcohols and their structure differs only in the number of CH_2

groups (table 2). In particular, 1-pentanol and 1-hexanol are very similar, while ethanol has a shorter chain. Since the hydroxyl group of the odorant molecule is largely responsible for interaction with the sensitive layer, and to a lesser extent its chain length, these results are coherent. Similar considerations can be made for odour 1 and 4. Chemical similarity is less evident, but in both cases the interaction with the sensitive material occurs through the same carbonyl group C=O and molecules only differ by one carbon atom.

Conclusions

An odour recognition system has been presented using hierarchical neural networks. In particular, a SOM based network was used for its ability to recognise typical characteristics of the input data and to describe a topological order over the input stimulus space in an automated manner.

This latter feature proved to be effective in grouping different odours into categories which are in accordance with the chemical structure of the compounds. For this task, the recognition system obtained very good performance. The agreement between the chemistry of the molecules and the results of the data analysis is promising. Odour-sensor interaction mechanisms can be investigated by this kind of experiment if compounds are properly chosen on the basis of their chemical structure. On the other hand, it seems that our algorithm has been satisfactorily trained in spite of the limited number of measurements. This is important because the availability of large data sets is a key issue when dealing with neural networks, but the time required to obtain large data sets could highlight problems due to sensor drift.

Further experiments will enable us to verify whether more precise selectivity can be obtained with a larger number of measurements and to improve the network's capability in reducing the effects of drift on sensor response.

References

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Authors' affiliations:

G. Pieri, O. Salvetti (Istituto di Elaborazione dell'Informazione – Area della Ricerca CNR, Via G. Moruzzi 1, Pisa, Italy – pieri@iei.pi.cnr.it - salvetti@iei.pi.cnr.it)

F. Di Francesco, C. Domenici, (Istituto di Fisiologia Clinica – Area della Ricerca CNR, Via G. Moruzzi 1, Pisa, Italy)

D. De Rossi, G. Pioggia (Centro "E. Piaggio"- Facoltà di Ingegneria di Pisa, via Diotisalvi, 2, Pisa, Italy)

TABLES

Sensor	Polymer	Dopant salt	Molar Ratio
2DI2	3,3'-dipentoxy-2,2'bithiophene	Iodine	2
5TCR1	3,3''-dipentoxy-2,2':5',2''-terthiophene	Cupric chloride	5
3DPR2	3,3'-dipentoxy-2,2'bithiophene	Cupric perchlorate	3
3TPR3	3,3''-dipentoxy-2,2':5',2''-terthiophene	Cupric perchlorate	3
3DCF1	3,3'-dipentoxy-2,2'bithiophene	Iron chloride	3
3TI1	3,3''-dipentoxy-2,2':5',2''-terthiophene	Iodine	3
5DPR3	3,3'-dipentoxy-2,2'bithiophene	Cupric perchlorate	5
3DPF2	3,3'-dipentoxy-2,2'bithiophene	Iron perchlorate	3

Table 1

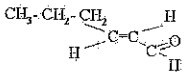
Odour number	Compound	Structural formula
1	Trans-2-Hexen-1-al	
2	1-Pentanol	$CH_3-CH_2-CH_2-CH_2-CH_2-OH$
3	1-Hexanol	$CH_3-CH_2-CH_2-CH_2-CH_2-CH_2-OH$
4	3-Pentanone	$CH_3-CH_2-C(=O)-CH_2-CH_3$
5	Ethanol	CH_3-CH_2-OH

Table 2

Odour	Success percentage Interval = 20 s	Success percentage Interval = 45 s
1	85.7	80.5
2	60.0	74.1
3	80.7	79.2
4	86.5	40.0
5	100	100
Average	82.2	79.3

Table 3

Odour Groups	Success percentage Interval = 20 s
A	91.2
B	95.6
C	100
Average	94.8

Table 4

FIGURES

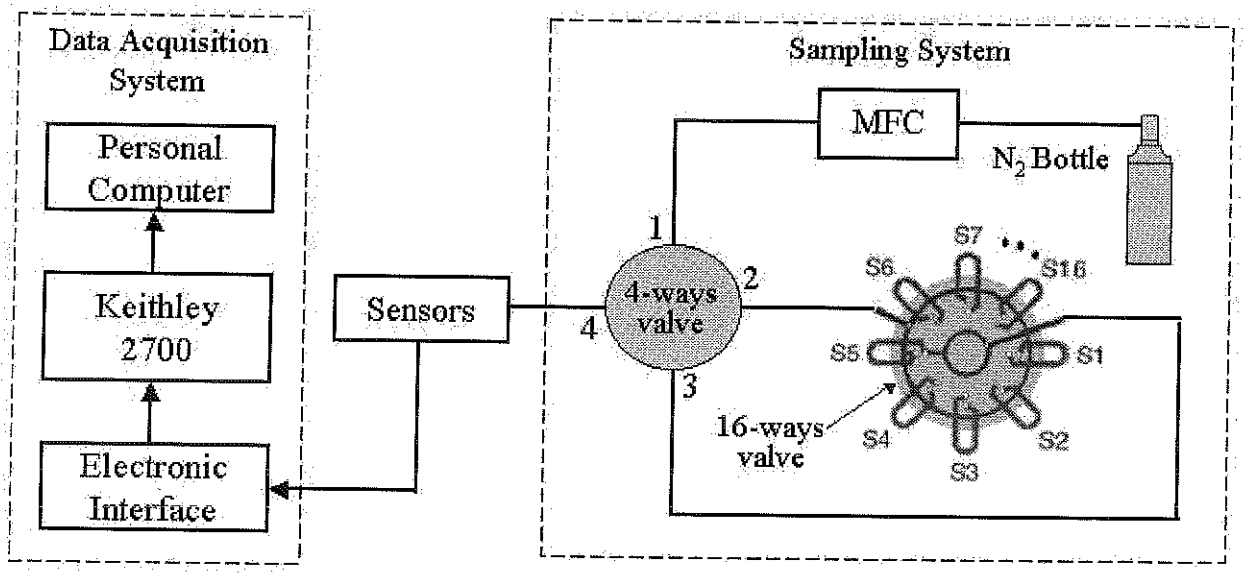


Figure 1

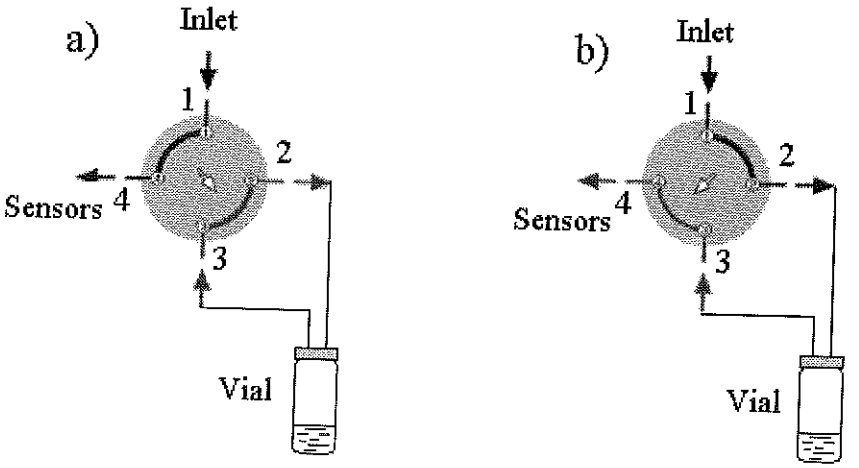


Figure 2

List of Figure Captions

Figure 1 – Scheme of the experimental set-up. MFC is the mass flow controller and S_1 ... S_{16} are the glass vials, connected to the 16-way valve, containing the samples.

Figure 2 – Positions of the 4-ways valve during a) baseline and desorption and b) exposure phases.

List of Table Captions

Table 1 – Polymers, dopants and the molar ratios used for each sensor.

Table 2 – Olive oil aroma components analysed.

Table 3 - Results of odours recognition at the different time intervals.

Table 4 - Results of grouped odours recognition at 20 s time interval.