PERFORMANCE DEFINITION AND STANDARDISATION OF ELECTRONIC NOSES

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SUMMARY

The performance of any electronic nose is ultimately determined by the properties of its constituent parts (e.g. the sensors, signal processing, and pattern recognition engine). Electronic noses currently exploit different sensor materials technologies (e.g. semiconducting oxide, conducting polymer, phthalocyanines and lipid coatings) as well as different pattern recognition paradigms (e.g. canonical analysis, back-propagation and learning vector quantification). This has led to the need to compare objectively the performance of an increasing number of both research and commercial electronic noses. This paper addresses this problem and suggest the need for odour standards to define both the range and resolving power of an electronic nose. We present a generic model from which we can define such parameters. The model can also be employed as diagnostic tool which can predict not only the relative performance of different electronic noses but also the effect of, for example, changing the number or type of odour sensor, temperature fluctuations or ageing. We believe that the definition of standard odour samples and standard performance parameters would be of great benefit in this field.

INTRODUCTION

A considerable amount of research has been directed towards the development of electronic nose instrumentation over the past decade. Research groups now exist in countries such as Australia, Denmark, France, Germany, Japan, Sweden, UK and USA. The general approach has been to develop an array of sensors based upon a single material or transducer in a *monotype* electronic nose. This approach has led to the arrival of three commercial instruments which dominate the world market, namely, the Fox 2,000 (Alpha MOS SA, France), Digital aroma analysis system (Aromascan Plc, UK) and the NOSE (Neotronics Scientific Ltd, UK) [1]. A number of other instruments are also under development and we may see 10 or more commercial instruments by the end of this decade.

The aim of this paper is to quantify the ability of an electronic nose to discriminate between different complex odours. Figure 1 shows a general representation of multidimensional odour space, Ω_3. The dotted lines demarcate the seven primary aromatic notes, i.e. camphoraceous, floral etc. An electronic nose may be designed to map out all of these regions or more realistically a subset of them relevant to the needs of a particular end-user. A set of primary odours or notes could be chosen (labelled A) to test the ability of an electronic nose across odour space and thus determine its range. Secondly, and more importantly, a second sample of a similar note could be chosen which is in close proximity in odour space (labelled B). The ability with which these samples (or a set of them) can be identified will determine the resolving or discriminating power of the electronic nose. This test is the more important one because users need to discriminate between similar smells arising from the same product, rather than, say, discriminating between a floral and musky perfume.

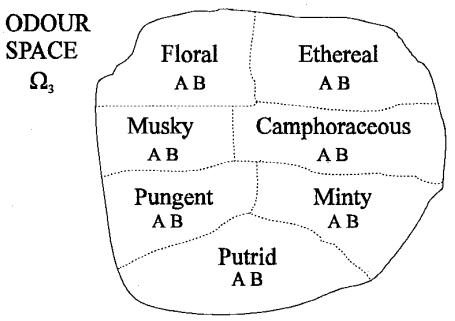

Figure 1. Defining standards in odour space for range and resolving power.

ELECTRONIC NOSE MODEL

Figure 2 shows the basic stages of signal processing in an electronic nose. Sample space Ω_1 is defined by either the chemical composition of the samples which may be a single compound (i.e. a simple odour), or more likely a number of compounds (e.g. a complex odour). The zero point represents odour-free air. The sensor array responds to the sample A and so maps one point in sample space onto sensor space Ω_2. This is a crucial stage in the process and broadly determines the resolving power of the electronic nose. In the human olfactory system, the front-end processing is elaborate and manages to boost the sensor sensitivity to the sub-ppb level yet at the same time suppress the signal noise. The integrity of the output from

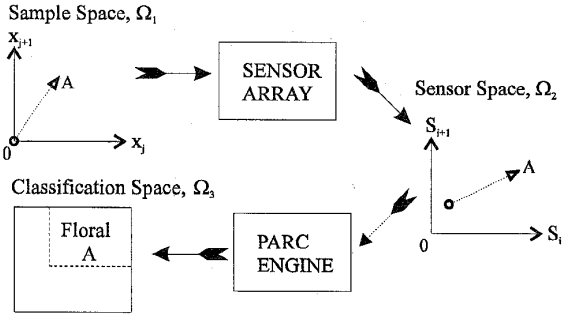

Figure 2. Signal processing in an electronic nose.

the sensor array thus largely determines the performance of an electronic nose. Key parameters are the number and type of sensors, the specificity of the sensors, their noise level, stability, thermal sensitivity and so on. In other words, if the samples are not distinct in sensor space, then the pattern recognition (PARC) engine cannot be expected to discriminate them. Any attempt to do so will be unproductive as the noise in sensor space will be mapped in proportion onto classification or odour space Ω_3. For example, it is possible to boost the ppm sensitivity of commercial tin oxide sensors to the ppb level through electronic circuitry [2] but the concurrent increase in noise and drift provides no benefit in resolving power. Therefore, we assume in this model that the performance of the sensor array dictates the overall performance of the nose and that any limitations due to the accuracy of the ADC [3] can be ignored. So provided the Euclidean distance between points in sensor space is adequate, then the PARC method can classify them using a range of methods (such as metric transformations, back-propagation or self-organising maps) appropriate to the nature of sensor space, i.e. linearity in concentration, sensor co-linearity, and dimensionality etc.

Model of Sensor Array

The exact relationship between the sample space and sensor space clearly depends upon the type of sensor used. In order to develop this analytical model we will assume an empirical power law dependency. In fact this is unphysical and in our computational model discussed later we have extended the choice to include a Langmuir adsorption isotherm which models a saturation process. So the output from a sensor i in an array of n sensors can be modelled as

$$S_i = a_{i0} + a_{i1}x_1^{k_i} + a_{i2}x_2^{k_i} + \ldots + a_{im}x_m^{k_i} \qquad (1)$$

where there is a regression coefficient a_{ij} or sensitivity factor for each of the m compounds present in the sample, and a_{i0} is the output of the sensor in odour-free air. x_j represents either the concentration of compound j or an odour note present in the sample. The exponent k_i would take a value of one for a linear sensor but is about 0.3-0.8 in semiconducting oxide conductance sensors. The model assumes that the compounds are independent which is realistic for polar organic molecules.

The general response $\boldsymbol{S}$ of the entire array can be written in matrix form as $\boldsymbol{AX+B}$ or explicitly:

$$\begin{pmatrix} S_1 \\ S_2 \\ . \\ S_n \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & . & a_{1m} \\ a_{21} & a_{22} & . & . \\ . & . & . & . \\ a_{n1} & . & . & a_{nm} \end{pmatrix} \begin{pmatrix} x_1^{k_i} \\ x_2^{k_i} \\ . \\ x_m^{k_i} \end{pmatrix} + \begin{pmatrix} a_{10} \\ a_{20} \\ . \\ a_{n0} \end{pmatrix} \qquad (2)$$

For an array of perfectly specific sensors, the regression matrix $\boldsymbol{A}$ reduces to the diagonal matrix as shown in equation (3). This sensor system can perform multicomponent analysis but clearly lacks the range of a nose as it could only identify n samples.

$$\boldsymbol{A} = \begin{pmatrix} a_{11} & 0 & 0 & 0 \\ 0 & a_{22} & 0 & . \\ 0 & 0 & . & . \\ 0 & . & . & a_{nm} \end{pmatrix} \qquad (3)$$

In practice, gas sensors are not orthogonal which means that some of the off-diagonal terms are non-zero and so increases the range of the system while decreasing the resolving power. Thus, in principle, hundreds of different odours could be discriminated with a small set of sensors.

The Role of Errors

In an ideal sensor system, for example a set of six orthogonal linear sensors, there are no errors and so in effect there exists an infinite number of response vectors. Vectors that are very close can be resolved by changing the distance metric (e.g. to Mahalanobis) and thus enhancing the gain. In practice, there a number of sources of error that will determine the number of odour samples that can be discriminated in sensor space and hence its capability. Errors arise from the variation of the concentrations of the components in the sample. These may be due to variation in the sampling method or due to natural variation in the sample itself. For example, Mackay-Sim has identified sources of experimental variability for piezoelectric odour sensors [4]. Clearly, a standard sample can be defined with a concentration variation below a specified limit of, say, 1% and so be used with a standard sampling procedure (e.g. standard temperature, pressure, a flow-rate of 100 ml/min, and a humidity of 50%) and to compare different electronic noses. Variations can also occur in the sensor coefficients which may be random in nature due to materials variability or systematic due to changes in, say, temperature or humidity. Indeed, in some cases deliberating changing the sensor's operating temperature can aid the resolving power of the array [5]. In addition, a variation in the base-line parameter a_{i0} could represent a systematic drift due to the ageing or poisoning of the sensor. In this case the sensor output will follow a drift

line and there is likely to be a correlation between the regression coefficients. All of these cases can be described within a sensor error model. For the general model given in equation (1)

$$S_i(1+\varepsilon_{S_i}) = a_{i0}(1+\varepsilon_{a_{i0}}) + \sum_{j=1}^{j=m} a_{ij}(1+\varepsilon_{a_{ij}})[x_j(1+\varepsilon_{x_j})]^{k_i} \quad (4)$$

where ε_a represents the fractional error on a sensor parameter.

Resolving Power of 'Stationary' Noses

Figure 3 illustrates the model of an electronic nose with a sample with error ε_x in sample space Ω_1 propagating through to a response vector with error ε_S in sensor space Ω_2. For randomly distributed errors, the response vector now falls into an ellipse (n=2) with the semi-major and semi-minor axis give by the standard deviation of the sensor output. The variance on the sensor can now be related to the variance on the sensor parameters and component concentrations using equation (1),

$$\sigma_{S_i}^2 = \sigma_{a_{i0}}^2 + k_i \sum_{j=1}^{j=m} a_{ij}^2 \sigma_{x_j}^2 + k_i \sum_{j=1}^{j=m} \sigma_{a_{ij}}^2 x_j^2 \quad (5)$$

where the first term contains the errors in the base-line signal, the second term contains the component concentration errors and the last term contains the errors in the sensitivity of sensor material to components.
The resolving power of a nose can now be defined for two samples (A and B) in type of a statistical t-test by,

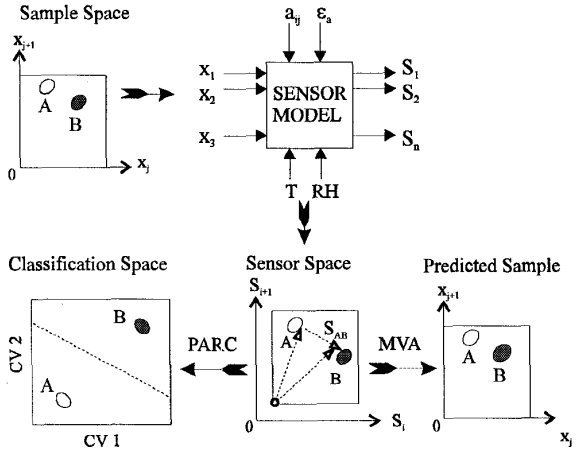

Figure 3. Modelling of errors in an electronic nose.

$$\text{Resolving power} = \frac{|S_{AB}|}{\sqrt{\sigma_A^2 + \sigma_B^2}} \quad (6)$$

where $|S_{AB}|$ is the distance between in the response vectors and σ_A and σ_B are the errors calculated along the direction of the distance metric. This parameter is essentially that referred to by Müller as the electronic selectivity [6].

The volume that the error on the response vector σ_S occupies in sensor space determines the discriminating power of the electronic nose and the total number of odours that can be recognised. The volume V_n of a hyperellipsoid comprising a set of n sensors with semiaxes defined by the standard error is:

$$V_n = \frac{2\pi^{n/2} \prod_{i=1}^{i=n} \sigma_{S_i}}{n\Gamma(n/2)} \quad (7)$$

The use of a hyperellipsoid model rather than a hypercuboid model is significant when considering a large sensor array as illustrated in Table 1. The ratio indicates the reduced volume that a hyperellipsoid occupies compared to a hypercuboid calculated from the prefactor in equation (7) and its hypercuboid equivalent.

Table 1. Effect of hypermodel on error volume.

n	Ellipsoid	Cuboid	Ratio
1	2 (line)	2 (line)	1.000
2	π (ellipse)	4 (square)	0.785
3	$4\pi/3$ (ellipsoid)	8 (cube)	0.523
6	$\pi^3/9$	64	0.081
n even	$\pi^{n/2}/(n/2)!$	2^n	-
n odd	$\pi^{n/2}/(n/2)!\Gamma(n/2)$	2^n	-

The number of response vectors that can be discriminated in sensor space (i.e. the range) is simply given by

$$N_n = \frac{\text{Volume of sensor space}}{\text{Volume of sensor error}} = \frac{\prod_{i=1}^{i=n} FSD(S_i)}{V_n} \quad (8)$$

where the FSD(S_i) is the full scale deflection of the output signal S_i from sensor i, and V_n is defined in terms of the model parameters and their errors by equations (5) and (7). For sensors that operate over a fixed range, the error volume determines the number of samples that can be discriminated.

An error on the regression coefficients or material sensitivity causes a concentration-dependent error volume, i.e. the error volume monotonically increases with increasing component concentration, see the third term in equation (5). To illustrate this, Figure 4 shows the concentration dependence of the number density (number of discriminated response vectors per unit range) due to a

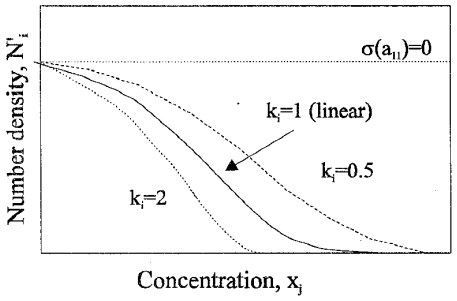

Figure 4. Effect of sensitivity errors upon the discrimination power of an electronic nose.

non-zero standard error on the regression coefficient a_{11}. The number density N'_i (using pre-factor for n=1) is given by,

$$N'_i = \frac{2}{\sqrt{\sigma^2_{a_{i0}} + k_i a^2_{ij}\sigma^2_{x_j} + k_i \sigma^2_{a_{ij}} x^2_j}} \qquad (9)$$

This is similar to the one dimensional parameter proposed by Müller [6]. In this case the number density of the nose falls with increasing concentrations. This is made worse when the exponent k_i is greater than one, and of course, for a Langmuir film the situation is worse as site saturation is approached.

In a similar manner it is now possible to define the performance of any electronic nose from the values of sensor model parameters, component concentrations and their errors.

COMPUTATIONAL NOSE

Although it is possible to obtain analytical expressions for an electronic nose with random errors, the situation is more complicated when modelling systematic errors such as temperature dependent parameters and ageing characteristics. Consequently, we have designed a computational model of an electronic nose with which to evaluate its performance. The sensor model now offers the choice of a Langmuir isotherm in which adsorption sites can be saturated as well as a conventional linear and power law. In addition, the exponent k_i can also have an error on it due to poisoning, ageing or temperature. Thus the sensor model of equation (4) is extended to become,

$$\begin{aligned} S_i(1+\varepsilon_{S_i}) &= a_{i0}(1+\varepsilon_{a_{i0}}) \\ &+ \sum_{j=1}^{j=m} a_{ij}(1+\varepsilon_{a_{ij}})[x_j(1+\varepsilon_{x_j})]^{k_i(1+\varepsilon_{k_i})} \qquad (10) \\ &+ \sum_{j=1}^{j=m} \frac{b_{ij}(1+\varepsilon_{b_{ij}})x_j(1+\varepsilon_{x_j})c_{ij}(1+\varepsilon_{c_{ij}})}{1+b_{ij}(1+\varepsilon_{b_{ij}})x_j(1+\varepsilon_{x_j})} \end{aligned}$$

Now the sensor parameters can be set for the appropriate choice of sensor (e.g. semiconducting oxides, conducting polymers). The effect of errors on the performance of the nose can be simulated by introducing errors such as a 10% increase in the base-line value, or a 5% decrease in the main sensitivity term, or the effect of interference through the off-diagonal regression coefficients. Alternatively, when it is not possible to distinguish between samples with an existing electronic nose, it is possible to simulate and identify the key parameters or alternatively to determine the effect of increasing the number of sensors or changing the type of sensor.

CONCLUSION

A model has been constructed which can be used to define the performance of an electronic nose based upon the errors present in the response vectors of a sensor array. Analytical expressions have been obtained for the resolving power and range of electronic noses with random distributed errors. In addition, a computational model has been set up which can describe linear, log-linear law, and Langmuir isotherm sensors. This computational model can be used to simulate the performance of current commercial electronic noses and predict the effect of adding sensors, changing sensors, noise, drift etc. The model predicts the ability of the electronic nose to resolve similar samples.

The definition of two odour standards is proposed. Firstly, a standard which determines the range of the electronic nose which comprises a set of primary odours Second, and more importantly, two similar odour samples which should be repeatably resolved by the electronic nose over a given period of time. These can be determined from a standard model of an electronic nose based upon reasonable values of the sampling error, materials variation and base-line error. It is assumed that when two samples are mapped onto two distinct regions in sensor space, then the pattern recognition system can classify them using a suitable metric as odours of differing type (or intensity). Should the user wish for a quantitative prediction of the original component concentrations then classical multivariate analysis (MVA) must be employed and further computational errors will occur.

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