Computers learn to smell and taste

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Abstract: *They all stink: food and drink, perfumery, household products, soaps, shampoos, paints, manufacturing processes, printing processes, waste products, contaminated air, and automotive emissions and environmental testing. In every case, small is a criterion of quality.*
Automated techniques to 'smell' or 'taste' liquids using mass spectrometry and gas chromatography are time consuming, require skilled personnel and often do not give the information required for qualitative 'testing'. A new technique is now available due to the advances in neural computing technology and multi-sensor array technology. The combination of these two approaches tries to simulate the human olfactory system in a simplified form. This paper shows that the recognition ability of an odour sensor array will be significantly improved using a neural computing approach in order to discriminate between similar odours.

1. Introduction

The physical world is inundated with data, but existing technology is unable to transform it easily into usable information. Traditional approaches have not changed sufficiently in the past 5–10 years and are way behind in terms of our ability to interpret data (Ryman-Tubb 1994). To analyse complex sensory data other than by producing simple rules takes enormous effort and time. All these techniques suffer from the 'curse of dimensionality' (Eubank 1988): that is, they require enormous computing power for problems with more than a few input variables. Further, most approaches also fail to produce accurate results when there are a high number of complex nonlinear interactions among input variables (Stone 1985), which is the case for many new applications.

Sensors are typically designed only to sense what they are built for — the oxygen sensor tries to eliminate the effect of nitrogen oxide, the microphone removes background sounds. To remove these effects needs considerable skill and design knowledge, which takes time, costs money and produces a complex sensor. Rather than designing a single complex sensor to detect a known, why not design an array of simple sensors — where many sensors connected together and taken as a whole produce more information than looked at individually? This raises the question: are current computing techniques going to be able to cope with the task, given such a range of input sensory data? But perhaps more importantly, how long is it going to take to write the software required for such a system and, once written, how safe is it from bugs? No longer is there the luxury in development to calculate all the algorithms or identify all the rules in these increasingly complex sensory systems. In fact, data fusion between this many sensors is so chaotic that doing so would be futile and prone to failure — which is why sensors are designed as they are.

2. Chemometrics

Chemometrics may be defined as the use of mathematical techniques to extract valuable, but often hidden, information from data, thereby giving an increased understanding of the chemical systems from which the data were derived.

The traditional method of investigating the properties of a system as a function of a single variable becomes increasingly unreliable if it depends of a large number of variables, many of which interact. This problem becomes worse as the number of variables increases. Various methods of multivariate data analysis can be used, such as principal component analysis (PCA) and factor analysis, in order to extract useful chemical information and to optimise processes. An inherent assumption in these methods is that there is a linear relationship between a particular property and the data obtained. However, non-linear relationships are actually common in the chemical industry: the chemometric techniques currently available are unable to code adequately with such non-linearity (Muller & Horner 1986; Shurmer *et al.* 1989; Stretter *et al.* 1986).

Neural computers offer an alternative. The key task performed by a neural computer is pattern recognition (Hancock 1992) and this forms the basis for most current applications of the technology. Pattern recognition is an extremely difficult task for conventional computers to perform because it is hard to describe the solution for each possible input situation that can arise. Neural networks can discover complex relationships in any data automatically, finding hidden influences and non-linear relationships which conventional approaches miss. They can deal with incomplete, noisy or 'fuzzy' data as

The Advanced Modular Adaptive Network

Neural Technologies Limited has developed a proprietary neural network system known as the Advanced Modular Adaptive Network (AMAN). AMAN copies what has taken nature 100 million years of evolution to create — the olfactory cortex in the brain. This is where you learn new smells and recognise old ones. Mother Nature has overcome the problem of smells being very similar by creating a highly specialised structure which groups together similar smells in modules.

The hippocampus area of the brain was originally thought to control our sense of smell. However, dolphins have no sense of smell but do have a well-developed hippocampus. Research pointed to the hippocampus as instead being the area involved in the long-term memory storage of sensory input in the brain.

The development of AMAN looked into research on how long-term potentiation (LTP) operates in the hippocampus, and how odours are stored and recalled. The brain seemed to use a simple self-clustering algorithm to store different odours. When an odour is presented which does not match an existing cluster, the brain tries to re-partition its odour memory, to increase resolution. This process is repeated until either a similar odour is found or a new odour detected. This may even be why we have to sniff a few times before we can recognise the smell (you may need to sniff a glass a whisky several times before you recognise it!). The system is very simple yet extremely powerful: with only 100 000 cells, up to 50 000 000 different odour sequences can be stored.

A meta-neural network

AMAN is not a specific type of neural network in the way that a multi-layer perceptron or Kohonen neural network is, but rather it is a meta-neural network that combines the use of many types of specific neural networks. As such, it can be viewed as a general purpose learning system. By dividing a large, complex problem into many smaller, simpler sub-problems, the overall training time for an AMAN has been found to be significantly shorter than would be the case if a large single neural network was employed. This difference can be several orders of magnitude.

Many applications

Ongoing work is looking how AMAN can be used with other sensors, such as sound, vibration and SONAR to help solve complex industrial monitoring problems, ranging from listening to the sounds of lift cables, to the sounds a burglar makes when breaking into a bank.

AMAN is also being used in non-sensor type applications, such as:

- *UK High Street banks:* personal loan scoring, mortgage underwriting;
- *European Bank:* credit/debit card fraud detection system operating online transaction processing;
- *Marketing:* drinks market analysis.

well as with previously unspecified or unencountered situations. Neural computers can be kept up to date simply by continuing to train them with more recent data.

3. Sensory arrays

Thousands of odours can be identified by humans. An odour is identified from the output pattern of many biological receptors, in our olfactory system, each with slightly different characteristics ((Kurihara *et al.* 1987). Humans have a large number of 'simple' sensors in their nose, typically tens of thousands. From the biomimetic viewpoint it therefore seems obvious to create a similar array of simple sensors and then to analyse the output pattern from these sensors to identify kinds of odours. An odour sensor is desired in many fields such as the food, drink and cosmetic industries and in environmental and clinical testing fields; however, development of such a sensor applicable to all those fields is difficult.

There are a number of different single sensors available for gas and vapour analysis (Ikegami *et al.* 1983), including electrochemical sensors which are generally specific to one gas but cannot measure very low levels. The use of integrated sensor arrays to detect flammable and toxic vapours (Persaud & Dodd 1982; Zarcomb & Stretter 1984) can overcome problems associated with poor specificity and drift encountered by individual sensors. The majority of multisensor systems have employed metal oxides (Abe *et al.* 1987; Ikegami & Kaneyasu 1985; Kaneyasu *et al.* 1987) as the sensing material; others include:

- Phthalocyanines (Bott & Jones 1986);
- Langmuir-Blodgett films (Fard 1985);
- Piezoelectrics (Carey *et al.* 1987);
- Quartz resonators (Ema *et al.* 1989);
- SAW sensors (Ballantine *et al.* 1986);
- Electrochemical cells (Kurihara *et al.* 1987).

A new technique is now available due to the advances in neural technology (Hodgins 1993) and multisensor array technology. The combination of these two disciplines simulates the human olfactory system in a simplified form.

An electronic neural nose has been designed to do the same as a human nose but with considerably fewer sensors (typically 12). The sensor part of the neural nose uses special electrochemically-grown conducting polymers. Unlike many conventional sensors, the polymers used are very sensitive to certain vapours and odours but are not selective — therefore they can only be used in an array. These polymers are designed either to change their characteristics by absorbing the vapour directly, or to modify their structure due to the polarity of the vapour or the filling of chemical 'holes'.

4. New sensor materials

These new sensors have been developed and patented by UK-based Neotronics Ltd. Two polymer material types are used: polypyrrole and polyaniline. Variations between sensor materials are due to the use of different counter ions dissolved into solvents, which modify the polymer chain. The materials are electrochemically grown at a defined potential across an electrode gap.

The response from this material is unlike that of a conventional sensor. It is more like that of a biological olfactory sensor. When the vapour is first presented to the sensor there is an initial fast response, followed by a considerably slower long term effect which looks like drift. In some cases this latter effect can be over ten minutes whilst in others it can be over hours. An example of this is shown in Figure 1.

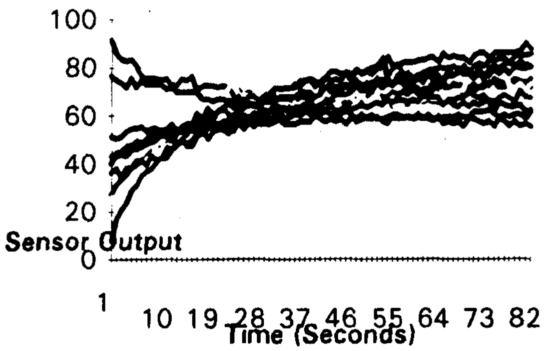

Figure 1: *Effect of presenting vapour to the sensor.*

When the polymer is exposed to a gas or vapour, this resistance changes. This change can be attributed to:

- direct absorption of the vapour into the polymer;
- modification of the polymer chain by the vapour due to the polarity of the vapour;
- the filling of 'holes' within the material by the gas or vapour.

There is limited agreement between theoretical predictions and experimental data, which suggests that the theoretical understanding is incomplete. However, there is sufficient evidence to suggest that all of these mechanisms occur, together with others that have not been mentioned.

The output from the sensor array is connected to the Advanced Modular Adaptive Network (AMAN). The AMAN is trained by example with various odour patterns and automatically creates whole new neural structures for each 'different' pattern. It can then be used to recognise similar patterns or can tell if the pattern has never been seen before (something 'new') and inform the user (Figure 2).

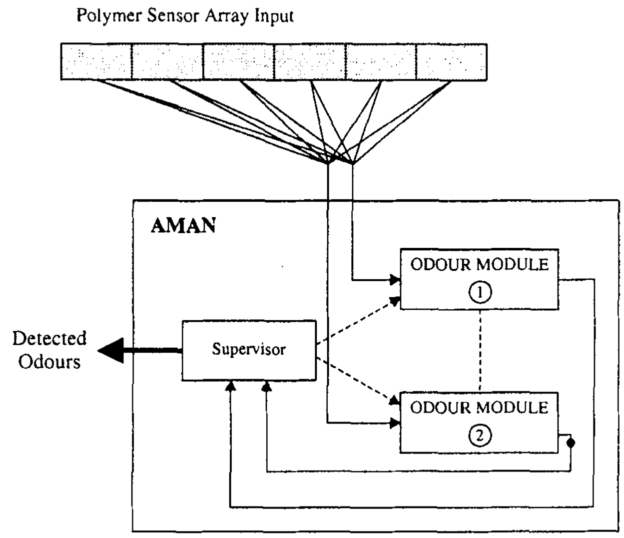

Figure 2: *Classification information as output.*

5. An application of the Neural Nose — spirit testing

Human nosing panels are currently used to determine the quality of distilled spirits (such as vodka, gin, etc.) to ensure that product consistency is maintained. These panels are costly to conduct, labour intensive and are naturally subjective. An automated method of supplementing the conclusions of the panel would increase the rate at which spirit samples could be analysed and reduce the often erroneous conclusions drawn by the subjective effects of the panel.

Spectroscopic analysis techniques such as infrared spectroscopy, nuclear magnetic resonance spectroscopy, mass spectrometry and gas chromatography are already used to provide a trained analyst with a vast amount of data relating to the chemical and physical properties of a spirit sample. Unfortunately, the task of extracting all the useful information from the data often proves difficult due to the complexity and the large volumes of data involved. Traditional methods for the quantitative interpretation of this data require the presence of an independent, non-overlapped band relating to a component or property of interest. Frequently this condition is not met, making these methods unsuitable. Improvements to chemometric methods of analysis are therefore needed. The development of methods that can cope with non-linear relationships would greatly increase the information that could be successfully extracted from spectroscopic data.

The output from the sensor array is an 'odour fingerprint' or smell that is unique to a particular odour. However, the fingerprint is contained within noisy signals that make it very difficult to identify the specific characteristics associated with a particular odour.

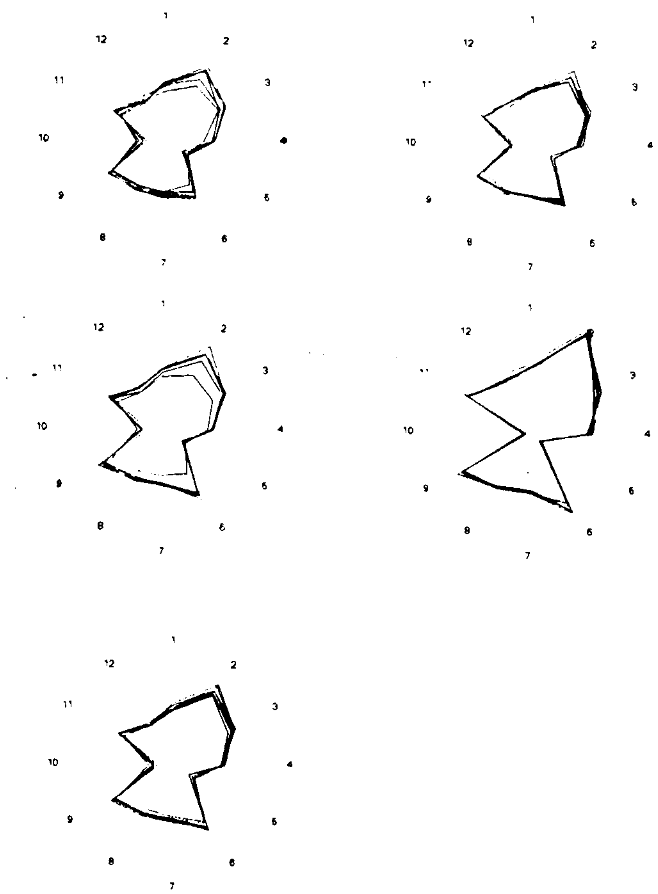

Figure 3: *Odour fingerprints for the five spirit types. There is very little obvious difference between each of the types but the neural computer is able to differentiate between them.*

Exposure to examples of many spirit odour fingerprints enables the neural computer to build up a profile of the specific characteristics unique to each spirit. The sensor characteristics vary slightly due to temperature drift and ageing, so a cyclic process of data sampling and training was used to ensure that the system was adaptive to environmental changes. Once trained, this profile can then be used to identify different specimens of the same spirit to which the neural computer has not been exposed (Figure 3).

Specimens of each spirit type are presented to the sensor array and analysed by the neural computer. The changes to the sensors in the 'nose', caused by the spirit odour, are converted into electrical signals that are then used to train the neural computer.

Applying a neural computer comprises two distinct phases:

(1) Training;
(2) Testing (or validation).

Table 1: *Confusion matrix using test samples.*

Actual ⇓ Predicted ←	Type A	Type B	Type C	Type D	Type E
Type A	100%				
Type B		100%			
Type C			100%		
Type D				100%	
Type E					100%

Different data is used for each phase so that the ability of the trained neural computer to react correctly to new (previously 'unseen') data can be measured. A number of spirit odour fingerprints are collected and then split into two data sets, one to train the neural computer and the remainder reserved for testing (validating) the performance of the trained neural computer.

Using these techniques, the training of the neural computer was successful. The neural computer was able to map the complex multi-dimensional input signals into the output classification spirit types.

The ability of the neural computer to distinguish between each of the training odour fingerprints was entirely successful.

The ability of the AMAN system to react to the test fingerprints was perfect, with each 'unseen' odour being correctly identified, as can be seen in Table 1.

By showing the neural computer many specimens of each type of spirit, it will be able to build up more knowledge about each type. Each specimen of the same type of spirit has some variations in odour. The neural computer must learn to distinguish between this natural variation in type, so that it can then distinguish between different types of spirit in a more general manner.

The ability of AMAN to identify various spirit specimens from noisy sensor signals has been shown. This application clearly shows that combining the two technologies has great benefit. The Neural Nose could make an ideal tool with which to monitor the quality of spirits (or other food and drink products). It does not tire, it is not subjective, it is not affected by ailments (such as the common cold) and it can be used anywhere in the production line.

6. Conclusions

Using analysis such as Principal Components Analysis or a standard neural network, it is often impossible to separate very similar signals, especially as the data is buried in noisy and clutter-rich non-linear signals. However, when these signals are connected to the Advanced Modular Adaptive Network (AMAN) it is able to separate such signals.

The concept of mimicking what nature has taken 100 million years to create seems natural. Combining neural processing and new types of sensors gives a step function in performance — making new and interesting applications possible.

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