Polish Journal of Environmental Studies Vol. 14, No 4 (2005), 477-481

Original Research

An Artificial Neural Network Is Capable of Predicting Odour Intensity

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Received: August 4, 2004
Accepted: December 21, 2004

Abstract

For the first time, an artificial neural network (ANN) has been employed for predicting the intensity of gas mixtures comprising different odour components. Sensory assessments are necessary but they are time-consuming, harmful, and expensive. Therefore, an instrumental quantification of subjective sensory assessments is highly desired. Because of nonlinearities arising in sensory-instrumental relationships, we decided for an ANN that was trained by gas chromatographic signals of gas mixtures. The ANN could be demonstrated to classify odour intensity fairly well.

Keywords: intensity of odour, artificial neural network

Introduction

The intensity of the composite odour, together with hedonic evaluations, is most characteristic in medicine, food production, and in environmental protection. In order to predict the influence of all components on odour intensity, equations were determined empirically relating the intensity of a composite odour to concentrations of individual compounds. However, these equations have only been validated for two (exceptionally three) odourants [1, 2], the ranges of concentrations and component rations are limited [3, 4] and therefore lack general applicability.

Consequently, instrumental quantifications of composite odours are problematic and sensory assessments are necessary [5-10]. Such assessments are time-consuming, harmful, and expensive. Thus, there is a necessity for developing devices that mimic the human nose. Therefore, we decided to train artificial neural networks (ANN) with gas chromatographic (GC) data and the corresponding sensory assessments.

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ANNs are useful in many applications. In environmental protection, ANNs have been successfully used in monitoring of water and air quality, e.g., classifications of waste material and sewage have been performed by means of an ANN [11]. Classification of volatile compounds has been published by Keller et al. [12].

In the food industry, ANNs are increasingly used for quality inspection of raw materials and products or monitoring of manufacturing processes. The successful classification of aromatic compounds produced by different species of bacteria in poultry processing are exemplary [13]. Products like crystalline sugar were classified by ANNs based on GC data [14]. Results of GC analyses and ANNs were also used successfully in the flavor intensity prediction of blackcurrant extracts from different geographical areas and processes [15].

The obvious appeal of ANNs for modeling sensory-instrumental relationships lies in their ability to describe complex nonlinear relationships. However, there is neither a systematic way to set up the topology of a neural network nor a way to determine its various learning parameters. Thus, we used a recently developed neural network soft-

ware tool called ACMD (Approximation and Classification of Medical Data) that provides far-reaching automatic learning. Moreover, referring to several benchmarks, ACMD has been shown even to classify more accurately than comparable fine-tuned networks [16].

Experimental Procedures

Sample Preparation

132 static samples of air were prepared in foil bags using clean atmospheric air, lemon oil for aromatherapy, and admixtures (odourants): acetone, ethanol, isopropanol, or isoamyl acetate. The procedure was:

— preparation of basic sample with lemon oil (matrix),
— addition of admixtures,
— sample dilution with clean air.

The matrix sample was made using 2 cm^3 of lemon oil in Rychter scrubber and afterwards blowing the scrubber with a stream of air (100 cm^3/min. reciprocating pump). The matrix sample (12 dm^3) was split into four parts in smaller bags. Precise and various volumes of odourants were led with syringe (Hamilton 700 Series Syringe) into the bags. Chromatographic and sensory analysis of the samples were made in a 35-minute course.

Odour Intensity Assessments

Sensory assessments of odour intensity were performed by panels of twelve assessors (8 women, 4 men, all of them students with previous experience) in a ventilated laboratory. One-day sensory assessments series were made during two four-hour sessions, with two-hour break in between. Odour intensity of 6-7 samples was determined in each session. When the odour intensity of all 132 samples was determined, 1,578 individual intensity assessments were collected.

Odour intensities were compared with those of standard aqueous solutions of *n*-butanol prepared by diluting the basic solution in 50 cm^3 conic flasks. Standard dilutions were provided by a geometrical series of n-butanol concentrations. In headspace phase in equilibrium, *n*-butanol concentrations ranged from 20 g/m^3 (Standard 1 — very intensive odour) up to 1.5 mg/m^3 (Standard 10). Since scale was linear the Weber-Fechner law was kept.

For assessing each sample the protocol used by the assessors was:

— determination of the individual odour detection threshold
— nasal assessment of the air stream of one of the samples
— comparison with the *n*-butanol scale of standards

To determine the individual odour detection threshold, an assessor starts from standard 10. When the threshold is defined, the assessor compares the odour intensity of the sample and the *n*-butanol standards starting from his individual threshold detection standard. When he perceives both intensities as similar (crosses in Table 1), the final odour intensity value *I* can be calculated as the difference between the number of the indicated standard and the odour detection threshold.

Table 1. Examples of individual odour intensity assessments. In cases of difficulties of an assessor's decision on two adjacent answers, the mean value is assigned.

n-butanol	Odour detection threshold	Sample 1	Sample 2	...	Sample 132
< 1					
1 – 2					
2 – 3		x			
3 – 4		x			x
4 – 5					x
5 – 6					
6 – 7					
7 – 8			xx		
8 – 9	x				
9 – 10					
> 10					

Moreover, for purposes of simplification three rough classes of odour intensity were defined: weak ($I < 2.5$), distinct ($2.5 \leq I \leq 4.0$), and strong ($I > 4.0$).

Gas Chromatographic Analysis

GC analysis was performed on Carbowax 20M (2 m · 4.00 mm i. d.); 60-80 mesh Chromosorb W NAW using Chromatron GCHF 18.3 gas chromatograph with FID detector. The conditions of analysis were: column linear flow of nitrogen: 1.2 atm; initial column temperature: 90°C (3 min); increase: 6°C/min; final column temperature: 210°C (3 min); detector temperature: 120°C. We used Loop-injection with regular heating. Every analysis was performed three times. Figure 1 demonstrates a chromatogram of one of the samples comprising five peaks: acetone ($t_{3,8\,min}$), ethanol ($t_{5,3\,min}$), first matrix peak and isopropanol ($t_{8,4\,min}$), second matrix peak and isoamyl acetate ($t_{11,8\,min}$), and third peak of matrix ($t_{15,5\,min}$). The corresponding peak areas were used as input variables for the subsequent ANN analysis.

Neural Network Analysis

ANNs are computer-based techniques using nonlinear mathematical equations to successively develop

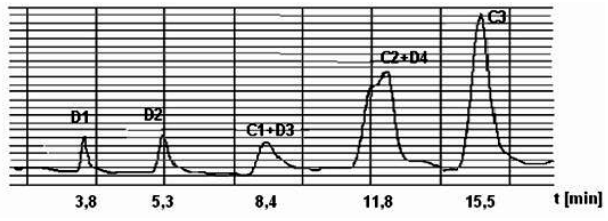

Fig. 1.A typical chromatogram of industry gas mixture model comprising the peaks D1 (acetone), D2 (ethanol), C1+D3 (first peak of matrix, i. e. lemon oil, and isopropanol, C2+D4 (second peak of matrix and isoamyl acetate), and C3 (third matrix peak).

meaningful relationships between input and output variables through a learning process. They have a "training phase" and a "recall phase." In the training phase, the relationships between the different input and output variables are established by adaptations of the weight factors assigned to the connections between the layers of artificial neurons. This adaptation is based on rules that are set in the learning algorithm. At the end of the learning process, the weight factors are fixed. In the recall phase, data from cases not previously interpreted by the network are entered, and output is calculated based on the abovementioned, and now fixed, weight factors.

Fig. 2 presents a diagrammatic representation of a standard feedforward network. Data are entered at the input neurons and further processed in the hidden layer and output layer. The output neurons produce a number between 1 and 0, the so-called activity of the output neuron. Tackling multiclass classification problems, the output neuron with the highest number represents assignment to the corresponding class ("Winner takes all" rule). The activities of the output neurons are dependent on the inputs and the weights at the connections between the layers. Therefore, the key feature of ANNs is that the weights at the connections are 'learned' by training the network. "Experience" in the trained network is stored in these interconnection weights [17].

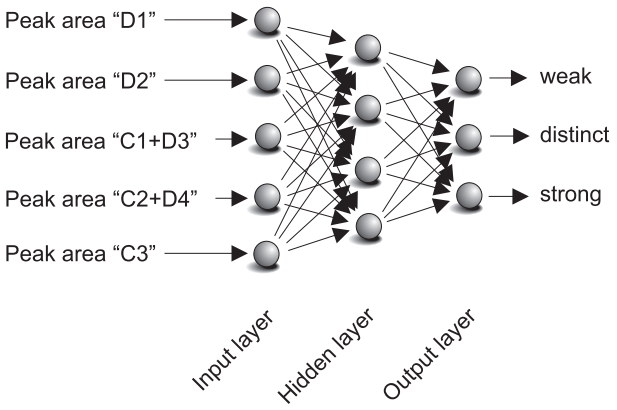

Fig. 2. Structure of a standard feedforward network that could serve for the assignment of different classes of odour intensity.

Before an ANN is trained, the system begins with random weights at the connections between the neurons. A training data set with known outcome is entered at the input neurons. The ANN compares its own output value with the known outcome and calculates an error value. The error will change as the weights at the connections change. The ANN attempts to minimize the error by adjusting the weights according to a learning algorithm. This process is repeated for a pre-defined number of times. The ANN can then be tested on test data with known outcome values.

a. **Classification**. Considering the three-class classification problem (weak, distinct, strong odour), the five input variables (peak areas) were fed into a feedforward network implemented as a prototype called ACMD, standing for "Approximation and Classification of Medical Data." This approach mainly relies on an expanded version of a multi-neural-network architecture by Anand et al. [18], in connection with *adaptive propagation* [19], a new development of the backpropagation algorithm [20]. The multi-neural-network architecture is a modular approach, where each module represents a single output network, which determines whether or not a certain sample belongs to a certain class (e. g. weak, distinct, strong smell), thereby reducing a *k*-class problem to a set of *k* 2-class problems. Each 5 modules were arranged as an ensemble, which makes them more robust than single networks and more suitable for training with only a small amount of data [21]. To make the training less susceptible to so-called overfitting [22], a strategy known as "Early Stopping" was used [23]. ACMD comprises a number of further strategies improving both the generalization performance and accelerating the convergence speed. In addition, further multi-neural-networks were trained to distinguish between two classes each, e. g. "weak odour" vs. "distinct odour." Therefore, testing an unknown sample was done not only by using one multi-neural-network and afterwards classifying the sample using the "winner takes all" strategy, but the two classes with the highest output activities were further examined by following a multi-neural-network that was specialized for these two classes in question. Several benchmarks give evidence that ACMD provides an excellent tool for training feedforward networks [16].

b. **Regression**. When conducting quantitative analysis, ACMD was used to predict the continuous odour intensity value *I* within the quasi-linear section of the sigmoid activation function of the only output neuron (i. e., within the interval 0.4-0.6). In order to validate both approaches — classification and regression — 5-fold cross-validation was used. This method requires deriving ANN calculations using 80% of the samples and evaluating the remaining samples, repeating this procedure 5 times. Evaluating regression results, values estimated by ACMD ($I_{estimated}$) were assumed to be correct when differing not more then 0.5 (1.0) from median assessments by the panel ($I_{median\ assessment}$).

Results

As a result of sensory analysis 132 panel assessments were carried out (Fig. 3). Self-learning ANN can detect and model complex nonlinear relationships between different GC signals as well as nonlinear interactions between the signals and corresponding odour intensity. Classifying odour intensities into three classes, the ANN correctly assigned 81.82% of the records (Table 2).

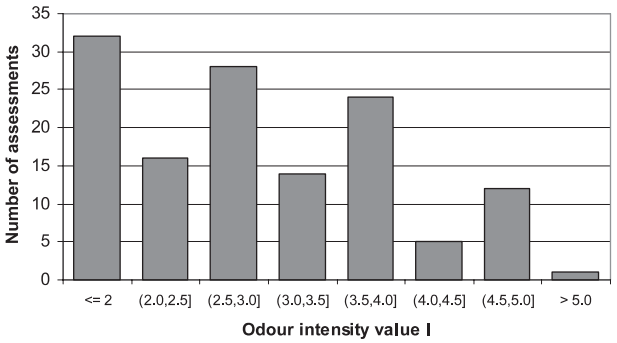

Fig. 3. Distribution of the odour intensity values *I*.

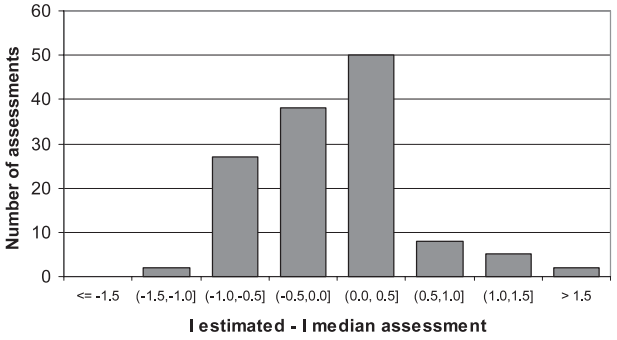

Fig. 4. Distribution of the differences between the estimated and the actual odour intensity values *I*.

Therefore, they are assumed to be advantageous to classical statistics like regression methods or the linear discriminant analysis requiring a linear relationship between input and output variables [24]. In order to prove that there were actually nonlinear relationships within our data, we predicted odour intensity by linear regression (using again 5-fold crossvalidation). As a result, the Root-Mean-Square-Error (RMSE) achieved was 0.647 and thus evidently worse than the RMSE achieved by the ANN. Estimating odour intensity at value I, the RMSE was 0.554. Fig. 4 indicates the distribution of the errors.

In 66.7% (93.2%) of the samples $|I_{estimated} - I_{median\ assessment}|$ was lower than 0.5 (1.0).

Table 2. Contingency table

		$I_{estimated}$		
		weak	distinct	strong
$I_{median\ assessment}$	weak	29	3	0
	distinct	7	65	10
	strong	0	4	14

Discussion

To our knowledge, it is not possible to determine the odour intensitity for complex mixtures comprising odorants in different ratios and concentrations. Because of the presumed nonlinear relationships between the components and the entire odour intensity, we decided to investigate the usefulness of an ANN trained by gas chromatografic data. Therefore, we created an industrial gas model using lemon oil as a matrix. Four admixtures were added in order to vary the shape of the GC signals as well as to change the odour intensity. Two of them were already part of the matrix signals. Two further admixtures (acetone, ethanol) were raw materials for the production of lemon oil.

When comparing the predictions of the ANN with panel assessments, in 81.8% of the samples the ANN correctly differentiated between weak, distinct, and strong odour intensity. Employing the ANN for a direct prediction of the degree of intensity scale, in 93.2% of the samples $|I_{estimated} - I_{median\ assessment}|$ was lower than 1.0 degree. Considering a range in invidual assessments of about 3.5 degrees for most samples, the ANN predictions were reasonably good.

Although ANN are used for estimating flavor intensity, they have not been employed for predicting odour intensity. However, nonlinear relationships are assumed to be more important when predicting odour intensity. So the usage of ANN technology may be even more promising. At first glance both objectives seem to be quite similar — flavor detection uses a *threshold flavour number*, TFN [25], and odour detection uses a *threshold odour number*, TON [26-31]. TFN as well as TON directly correlate with the concentrations of the involved components. Estimating odour intensity is something completely different, because it means a subjective olfactory impression. The panel assessment relates to the complex interaction mechanism between specific odourants on various ratios and concentration levels.

As an alternative to the time-consuming, harmful, and expensive panel assessment, a decision support system like that presented in this article would be capable of 24 hours a day monitoring. Because signals are derived from popular chromatographs, there is no need for sophisticated, expensive equipment.

In the past, ANNs were advocated as intelligent systems which, whatever the problem, would find the solution and so take over much of the hard work from the modeler. This article indicates that the same should be true in modeling sensory-instrumental relationships for predicting odour intensity. However, further analyses are necessary for a final evaluation.

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