Forming Odour Categories using an Electronic Nose

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Abstract. The ability to use linguistic concepts to describe perceptions of measured data is an emerging feature for artificial sensing systems. In this work, we address the problem of symbolically representing odour categories using the data from an electronic nose. One objective is to facilitate human and computer interaction and therefore, the names given to the odours are coorelated with a human user. Perceptual differences that arise between the human perception of odours and the electronic one, represent a challenge to the system. Therefore, to cope with these differences, the system maintains the freedom to evaluate how appropriately the linguistic concepts represent the sensory perceptions. Finally, some experimental results are shown where the odour categories are formed and new odours are described using these categories.

1 Introduction

Electronic noses are rapidly increasing in popularity in both industry and research. In the industry, electronic noses can be used to detect poisonous or obnoxious odours, tract an odour source, and provide quality control for different foodstuff. In research, a diversity of gas sensors are continuously being developed from the traditional metal oxide sensors to other emerging technologies such as infrared and optical sensors. Also, in the data processing aspect, different pattern recognition techniques have been applied. The technological advances in mimicking human olfactory senses, make it more feasible to quantify odours, but this recent progression has also highlighted some conceptual problems about olfaction that need to be considered. These problems are of particular concern in applications where human and machine need to communicate about perceptions.

Unlike vision which has pre-determined scales to decompose different colours such as hue, saturation and value, or even audition where frequencies using the decibel scale can describe the volume of a particular sound, olfaction lacks similar quantifiable transformations [4]. Furthermore, the few attempts that have been made to standardize odour classification such as Amoore's odour tables [1] have only considered a small selection of possible odours and are not generally used in real situations. The consequence in electronic olfaction is twofold. The first is that most works on e-noses consider experiments with a restricted amount of odours in a specific context. Secondly, often a human expert is needed to understand the results from the e-nose data and then provide the mappings from data clusters of similar odour patterns to the correct odour name.

In this work, we consider how to automatically create a correspondence between symbols, in this case linguistic names, and categories of e-nose data. To accomplish this task, we create a system that first creates categories using unsupervised clustering and then generalizes from these categories by evaluating how well an odour name applies to its own sensor representations. Since part of the objective is to facilitate human and machine interaction, the names outputted from the system are correlated and with those of a human user. This may mean that in the context of an unsupervised categorization, perceptual differences between the human and the electronic nose may arise. However, these differences can be considered an asset especially when dealing with olfaction, for example when the electronic nose detects carbon monoxide that is normally perceived as odourless for a human. Therefore, to cope with the perceptual differences, the system is tuned to provide as explicit information about the categorization of odours as possible. We accomplish this task by adapting existing fuzzy-based algorithms to generate informative odour descriptions.

This paper begins with a presentation of related work in Section 2. In Section 3, the data from the electronic nose and the necessary pre-processing steps are described. Section 4 details the process of creating odour categories using an existing fuzzy-based clustering algorithm and also explains how odour names are mapped to the sensor data. Also, relative issues such as the identification of unknown odours and performance evaluation are discussed. Finally, in section 5, experimental results are presented that illustrate the function of our method under different situations in odour classification.

2 Related Work

The relevant work can be approached from two angles. On one hand, there is the work that has been accomplished in electronic olfaction and the different kinds of classification techniques that have been used on e-nose data. On the other hand, there is a handful of related works that pertain to the more general problem of how to bind language, concepts, and sensor data in autonomous sensing systems.

Considering first electronic olfaction, the general definition proposed by [6] of an e-nose includes both an array of gas sensors of partial selectivity and a respective pattern recognition process to detect simple or complex odours. Both a variety of sensing technologies (metal oxide semiconductors, conducting polymers, acoustic wave devices and fiber-optic sensors) as well as pattern recognition techniques have been applied in research, industrial and recently, even commercial domains. The most commonly used technique to analyse e-nose data has been the artificial neural network. Although, ANN's have provided good results in applications with limited odour categories as shown in [9], using black-box classification fails to address the problems of representing the knowledge of odour categories in order to classify a larger spectrum of odours. Also a well-trained network requires a large number of samples, which can be an elaborate process considering the long sampling times required for e-noses (2-5 minutes), sensitivities to environmental conditions, and hard-to-model long term drift of the sensor results. There are also other relevant issues considering odour classification, such as the inherent uncertainty present in the human models of evaluation and as

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described by Dubois [4] the psycho-schematic difficulties to associate an odours' chemical composition to its name (e.g, the smell of rose consists of more than 400 different components). Thus in recent years, there has been a movement to capture the vagueness and/or uncertainty in the e-nose data and treat the data in a more human-like manner. Both systems that rely on expert knowledge have been considered [2], as well as the use of fuzzy-based logic and hierarchical clustering techniques as presented in [10].

In other sensor systems that have attempted to use symbolic representations to represent artificial perceptions, works done in vision tend to dominate the literature. These works can be divided into two different approaches. The first approach is works which try to explicitly represent perceptual knowledge. Contributions include Gardenfors' [5] conceptual spaces where a geometrical modeling of concepts is used. For example, in vision, the different primary colours are mapped onto a conceptual space where similar colours are located closer to each other. The problem with using explicit representations in olfaction are again the lack of accepted classification standards and also the range of odours would make the geometrical modeling a tedious and complicated task.

Another approach is to use non-explicit representation of concepts but instead apply different learning techniques to coordinate the perceptions between artificial sensor system and a human user. This is usually accomplished by using language dependent learning where words are bootstrapped. This approach is successful in vision based sensors, mainly because the capacity of the sensing mechanisms is known. For example in [12] an Sony Aibo robot is trained to associate the word "ball" with the visual perception of the object. Since the human has access to the images produced from the camera and since these images are somewhat similar to own our perception of objects, the algorithms are tuned to determine how to decompose images. The problem with olfaction is that there is little if no correspondence between how we perceive odours and how an electronic nose perceives them. The advantages from the differences in sensing mechanism is the possibility for the e-nose to outperform the human senses, for example in quantifying concentrations and in the detection of some odourless gases like carbon monoxide. Therefore, the risk of using supervised algorithms is that these unique sensing features are compromised.

In this work we consider a hybrid approach and consider a semi-explicit representation of odours. This is accomplished by first representing the knowledge of odours based only on the sensory data from an electronic nose. Then a symbolic interpretation of that knowledge is achieved by coordinating a human vocabulary of odour names to the sensory perceptions. In cases where the perceptions disagree, this information is explicitly highlighted in order to provide a human user with more information about the sensing abilities of the e-nose.

3 Electronic Nose Data

In this work, the odours were sampled using a commercially available electronic nose, Cyranose 320. This e-nose consisted of 32 thin-film carbon-black conducting polymer sensors of variable selectivity. The array of sensors are contained in a portable unit also consisting of pumps, valves and filters that are required to expose the sensor array to a vapor gas.

The sampling of an odour occurs in 3 different phases. The first phase is a baseline purge, where the sensors are exposed to a steady state condition, for example the air in the room. The duration of the purge is 30 seconds. The second phase is a sampling cycle where a valve is switched to allow vapors from a sampling inlet to come into contact with the sensing array. The duration of this cycle is 20 seconds. Finally, a sequence of purging cycles is used to remove the sampled odour from the unit and restore the sensor response to the baseline values. Figure 1, illustrates a typical response from one sensor.

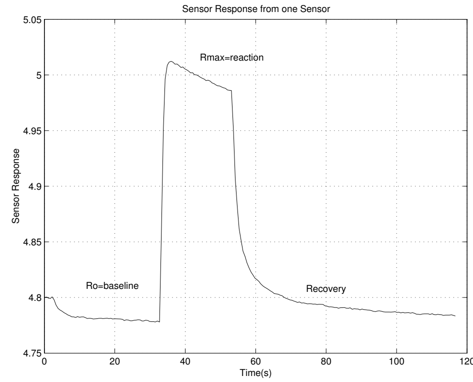

Figure 1. Example of sensor data throughout the three phases of sampling an odour with one of the 32 gas sensors.

The signals are gathered in a response vector where each sensor's reaction is represented by $\Delta R/R_o = (R_{max} - R_o)/R_o$ as shown in Figure 1. The response vectors are then normalized using a simple weighting method and auto-scaled. As each odour is sampled, the name of the odour is provided. Therefore, every sample is represented by a linguistic name, O_n (for n different odours) and a 32x1 response vector.

4 Category Acquisition

The process to obtain the odour categories that represent the perceptions from the electronic nose data is summarised in Figure 2.

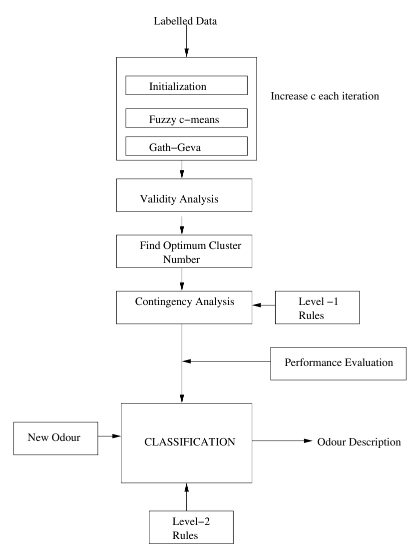

Figure 2. Overview of the system that forms odour categories using electronic nose data

4.1 Clustering

The sensor data is organized into clusters by applying different fuzzy-based clustering techniques. The process is iterative and consists of first implementing a fuzzy c-means algorithm (FCM) with a known number of clusters. To do this, a partition matrix is initialized with random variables and an objective function is minimized resulting in a new classification vector. This classification vector is then used as an initial condition for the subsequent Gath-Geva algorithm (GG) presented in [7]. The Gath-Geva presents some advantages over the FCM in that it allows for clusters of different shape and size. The FCM, however, is still needed to provide a good initialization to reduce the risk of the Gath-Geva converging in local minima/maxima. Through each iteration, the known number of clusters is increased. In order to determine the optimum number of clusters, a set of validity measures are used throughout each evaluation. In this work, optimum criteria for cluster partitioning is defined as clusters with good separation, minimal volume and maximal number of points located in the vicinity of the cluster center. Three different global validity measures are applied namely Compactness and Separation [13], Partition Coefficient and Partition Entropy [8], to satisfy this criteria. A voting vector is created which combines the results from the different validity measures giving more weight to the separation criterion. The results from the validity measures are then used to determine which number of clusters generates optimum partitioning. More about the validity measures and the clustering algorithms can be found in their respective references.

Once the clusters are formed, they are made into categories by associating the appropriate odour names to each cluster. This is done by creating a contingency table. The contingency table is a statistical technique that allows us to examine the relationship between subjects' scores on two categorical variables [11]. Typically, in a contingency table, the rows of the table represent the categories in variable i, and the columns represent the categories of variable j (where i and j are nominal). Each entry of the table is then a non-negative integer giving the number of observed events for each combination of row and column. In our contingency table, the rows are the different odour names n assigned by the human at sampling time, and the columns are the c, unlabeled clusters found by the clustering algorithm. Since fuzzy-based analysis was used, each point on our data space belongs to every cluster with a degree membership between 0 and 1 (although it should be noted that the GG tends to provide slightly crisper clusters). Therefore, each entry of the table is represented by the number of *prototypical* points having label O_n in cluster C_c. Prototypical points are points whose membership degree to a cluster is equal to 1.

4.2 Level-1 rules

Level-1 rules are used to manage the results from the contingency table. They are fuzzy-based rules which examine every column of the contingency table and map the appropriate odour name to each of the clusters. Since there is no guarantee that clusters will not overlap, or that the e-nose data is able to differentiate between two different odours, we create rules that allow for the possibility of using compound category names (e.g sweet and fragrant). The rules can also be used to differentiate between two clusters that may have the same name. This is used in cases where the e-nose may be more sensitive and splits the same odour into two or more clusters. The fuzzy rules therefore allow the user to either better coordinate the names between human and electronic perception or to emphasize cases where the number of clusters exceeds the number of available odours.

4.3 Identification of New Odours

Unknown points or new odours can be classified by evaluating the degree of fulfillment $\beta(x)$ where x is the unknown odour. The expression for the degree of fulfillment is given by,

$$\beta(x) = \mu_{x,C_1}(C_1) \wedge \mu_{x,C_2}(C_2) \wedge \ldots \wedge \mu_{x,C_3}(C_c). \qquad (1)$$

where the membership degree of x is computed for each cluster C_c for c clusters found in the unsupervised algorithm. If the categorical name for each cluster $\mathcal{L}_c$ replaces C_c, Equation 1 can be rewritten as,

$$\beta(x) = \mu_{x,C_1}(\mathcal{L}_1) \wedge \mu_{x,C_2}(\mathcal{L}_2) \wedge \ldots \wedge \mu_{x,C_3}(\mathcal{L}_c). \qquad (2)$$

The next step is to transform this expression into a fully symbolic description by applying a secondary set of rules called Level-2 rules.

4.4 Level-2 rules

The level-2 rules are applied to the degree of fulfillment to better describe unknown odours by mapping an odour's relation to the different clusters into symbolic adjectives. At this stage of the work, the rules are used to interpret the membership relations μ_{x,C_c}, into meaningful symbols. In the experiments described in this paper, this is acheived using the following:

$$\mathbf{M} = \left\{ \begin{array}{ccc} \mathcal{M}_k & : & 0 \leq \mu_{A_{i,j}} < 0.3 \\ \mathcal{M}_{k+1} & : & 0.3 \leq \mu_{A_{i,j}} < 0.7 \\ \mathcal{M}_{k+2} & : & 0.7 \leq \mu_{A_{i,j}} \leq 1 \end{array} \right\} \qquad (3)$$

$\mathbf{M}$ is now the set of linguistic descriptions and Equation 2 can be re-written as,

$$\beta(x) = \mathcal{M}_{k,1}(\mathcal{L}_1) \wedge \mathcal{M}_{k,2}(\mathcal{L}_2) \wedge \ldots \wedge \mathcal{M}_{k,c}(\mathcal{L}_c). \qquad (4)$$

The result from the classification is a odour description that contains explicit information on how an unknown odour relates to the known odours. This can be interpreted as a more natural method of providing classifications since it is not unlike the human model of interpreting odours (e.g. Smells a lot like...) [4]. A potential problem, however, is that the larger the repository of odours sampled by the electronic nose, the larger the descriptions may be. In this case, some form of trimming the description is implemented, where the terms with the highest degree of similarity are preserved.

4.5 Performance Evaluation

Evaluating the performance of a system that preserves its own representation of odours is difficult since misclassified points cannot necessarily be interpreted as erroneous. In, supervised algorithms, the category boundaries are determined by linguistic concepts, however, in non-supervised algorithms, the sensor data dictates how the categories represented and thus a more individualistic learning approach is used. Therefore, in this work our performance measure is not based on the number of correctly classified odours. Instead, we develop a measure that reflects how well the electronic perception of odours matches the human perception. To obtain this measure we examine the properties of the contingency analysis. From the contingency table, one can obtain a measure of dependency of the clusters to the human labels. This is obtained by calculating the entropy of the table also known as the coefficient of uncertainty U.

$$U(C|O) = \frac{H(C) - H(C|O)}{H(C)}, \tag{5}$$

$$H(C|0) = -\sum_{o,c} p_{oc} \ln \frac{p_{oc}}{p_{o\bullet}}, \tag{6}$$

$$H(C) = -\sum_{o} p_{o\bullet} \ln p_{o\bullet}, \tag{7}$$

where $p_{\bullet o} = \sum_c p_{co}$, $p_{c\bullet} = \sum_o p_{co}$, and p_{co} is the probability that the prototype is in c and the human label is o. The coefficient of uncertainty can range between 0 and 1. A value of $U = 1$ implies that there is a strong association between the human odour names and the clusters of sensor data. A value of $U = 0$ implies that there is no association between these two variables.

5 Experiments

5.1 Case 1

Experiments are performed on a number of different odours extracted from an ASTM atlas of odour character profiles by Dravnieks[3]. The odour profiles were designed to develop odour character information of 168 chemical compounds. Dravnieks' tables are useful for the purpose of our experiments since they contain a statistical analysis using a human panel. Of the total profiles listed in Dravniek's tables, 6 profiles were chosen to be used as subjects, shown in Table 1. These particular profiles were chosen in an attempt to represent as large as a spectrum of odour descriptions as possible.

Table 1. The substances and their respective descriptions taken from [3]

Odourant	Descriptors
Hexanal	woody,resinous,herbal,green
Hexanoic Acid	sour, vinegar, pungent, acid
3-Hexanol	alcoholic, etherish,anaesthetic
Octanol	oily, fatty
Linalool	fragrant, perfumery, light
Vanillin	sweet, chocolate, vanilla

Using these subtances, the experiments performed consist of the following steps:

- Examine how well the electronic nose can differentiate between the six profiles and recognize unseen samples of the same odours.
- Determine how well the electronic nose can use the six profiles as descriptions for unseen samples of five additional complex odours that are not in the profiles list.

For the first step, 50 samples of each odours in the profile list were taken, for a total of 300 samples. These samples were inputted into the clustering algorithm and the total number of optimum clusters were found to be 5.

The contingency table in Table 2, shows the labels of each of the cluster prototypes. Recall that prototypical points are points with a membership value equal to 1. Making allowances for compound cluster names, the 5 clusters obtain the odour names according to Table 3.

From this table, it can be seen that the electronic nose can distinguish only 5 of the profile odours whereas a human can distinguish all six. This lack of sensitivity of the nose is explicitly shown from Table 3, by the fact that Cluster 4 contains a compound description of alcoholic and sour. The consequence is that these adjectives that the e-nose uses to describe "alcoholic" odours are the same adjectives used to describe "sour" odours. By evaluating the entropy of the Table 2, the coefficient of uncertainty $U(C|O)$ is approximately 0.74 which reflects some degree of matching between the perceptions of the nose and the human.

Table 2. Prototypical points found in each cluster with a given name

Odourant	C_1	C_2	C_3	C_4	C_5
Vanillin	42	0	0	0	0
Octanol	3	37	0	0	0
Hexanal	0	0	23	0	0
Hexanoic Acid	0	0	0	23	0
3-Hexanol	0	0	0	21	2
Linalool	0	0	0	1	31

Table 3. The final names assigned to each cluster

Odourant	Descriptors
C1	sweet, chocolate vanilla
C2	oily, fatty
C3	woody,resinous,herbal,green
C4	alcoholic,etherish,anaesthetic $\wedge$ sour, vinegar, pungent, acid
C5	fragrant, perfumery, light

The next step is to test a series of complex odours. The choice of the odours are targetted towards the existing descriptions contained in the profile list. For each unknown odour, 10 samples were taken. Table 4 summarizes which substances were used for testing, their perceptions from a human user, and the descriptions given by the nose. From these results, it can be seen that the electronic nose and the human panel agree on some of the substances (e.g both describe chocolate as sweet substance). The level-2 rules have been used to better illustrate the relation between these points and the known categories, through the use of adjectives such as, very or moderate. For example, the Corn oil was only considered moderately woody and moderately oily, which may indicate that the point resides between these two categories. Therefore, from this information, it can also be deduced how the known concepts relate to each other.

5.2 Case 2

The second experiment examines a situation where the e-nose is more sensitive than a human user. We consider a situation where 12 containers contain 4 different substances. Each of these containers is given a number and the actual chemical contents of the container is shown in Table 5. A blindfolded human is allowed to sample (by smelling) the contents of each container only once. The task of the human is twofold. The first task is to discriminate among the odours, that is to say, determine which among the 12 samples are similar to each other. This is a process of categorisation. Once the odour categories are formed, the second task is to give each of the categories a name, Table 5.

The experiment is then repeated but using an electronic nose to sample the odours. Unlike the human user, the electronic nose is capable of making a distinction between the 20% ethanol and the 30% ethanol. 4 cluster prototypes are found using the unsupervised algo-

Table 4. The identification of new odours with respect to the trained concepts

Odourant	Human Descriptors	E-nose Descriptors
Melted Chocolate	chocolate, sweet	very sweet
Corn Oil	oily, fatty	moderately woody,herbal $\wedge$ moderately oily
White Wine Vinegar	vinegar, pungent	very alcoholic, sour
Ethanol	alcoholic, strong	little woody,herbal $\wedge$ moderately acoholic,sour

Table 5. Contents of the odour containers and the respective names assigned by the human user according to his/her perception. Note that two different ethanol contents are given the same name.

Container	Actual Contents	Human Assigned Name
1-3	100 % Ethanol	OdourA
4-6	30% Ethanol	OdourB
7-9	20% Ethanol	OdourB
10-12	5% Ethanol	OdourC

rithm each corresponding to the different concentrations of ethanol. This is an obvious advantage to using an electronic nose that is particularly sensitive to concentrations of certain gases such as ethanol.

To handle the fact that the e-nose can detect more odour categories, three solutions are possible. The first solution is to acquire the category names according to the human perception, making no explicit emphasis on the extra cluster formation. The symbolic classification would be co-ordinated with the results from the human user. When the testing data is categorized, even though a single point may belong to any one of four different categories, only one of three different category names would be outputted. The classification result is comparable to that from a supervised algorithm such as the ANN (multi-layer feed-forward network, MLFF)as shown in Table 6. If the intention of the application is to match perceptions between the artificial nose and the human, then this approach would be sufficient.

Table 6. Correct classification results on the testing data on 20 new samples of each odour

Method	OdourA	OdourB	OdourC
MLFF	98%	100%	98%
GG	92%	99%	91%

A secondary approach can be taken in order to enhance the classification and attempt to communicate the fact that there exists a discrepancy between the two categories which were merged in the human perceptual context. This is accomplished by using the parameters found from the fuzzy clustering process in order to better describe the unlabelled data not only in terms of the categories to which they belong but also in terms of the categories to which they possess a similarity as shown in Equation 2.

Finally, a third alternative would be to differentiate between two categories that have the same name using the level-1 rules. This would occur when the category names are being determined. For example, if two categories in the contingency table C_2 and C_3 both have a dominating association to OdourB, they could be differentiated from one another by the addition of a suffix to the name such as $OdourB1$ and $OdourB2$. This method explicitly tells the user that another category has been created, however, generating a more descriptive classification would be beneficial in order to understand the relationship between these different odour categories.

6 Conclusion

In this work, we have discussed the implementation of using unsupervised techniques to represent the perception of odours from an electronic nose. Although unsupervised algorithms create a greater chance for perceptual conflicts than supervised techniques, we argue that perceptual differences can be highlighted and used as a means to inform the user. Futhermore, in sensing system such as olfaction which are continuously evolving, this information can be used to make actual hardware implementations, such as the addition of a new sensor designed for special selectivity. Ultimately, the understanding of where and how perceptual differences may occur, allow us to better handle the sensing systems.In this work, linguistic concepts were used as a means to better promote this understanding, provided that the concepts adequately represent the sensor data to which they refer. In sensing systems, such as olfaction which currently, is absent of any quantifiable metric to classify odours, it is believed that this kind of representation can be equally appreciated from a human user interacting with the system.

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