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Using Artificial Neural Networks to Classify Unknown Volatile Chemicals from the Firings of Insect Olfactory Sensory Neurons

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Abstract— **The olfactory system detects volatile chemical compounds, known as odour molecules or odorants. Such odorants have a diverse chemical structure which in turn interact with the receptors of the olfactory system. The insect olfactory system provides a unique opportunity to directly measure the firing rates that are generated by the individual olfactory sensory neurons (OSNs) which have been stimulated by odorants in order to use this data to inform their classification.**

In this work, we demonstrate that it is possible to use the firing rates from an array of OSNs of the vinegar fly, *Drosophila melanogaster,* to train an Artificial Neural Network (ANN), as a series of a Multi-Layer Perceptrons (MLPs), to differentiate between eight distinct chemical classes.

We demonstrate that the MLPs when trained on 108 odorants, for both clean and 10% noise injected data, can reliably identify 87% of an unseen validation set of chemicals using noise injection. In addition, the noise injected MLPs provide a more accurate level of identification. This demonstrates that a 10% noise injected series of MLPs provides a robust method for classifying chemicals from the firing rates of OSNs and paves the way to a future realisation of an artificial olfactory biosensor.

I. Introduction

A chemical descriptor is a numerical representation of an odorant molecule's physio-chemical or pharmacological attributes that is based on its molecular structure or the results from a set of standardized experiments.

A biosensor emulating a biological olfactory system can be produced to detect and recognize various odours and flavours. Such a device has a broad range of applications such as: determining the ripeness of fruit; detecting contraband or explosives and for diagnosing illness in a patient. Recently, advances of such devices also recognize the direction from where the odorants emanate [1].

A. The Insect Olfactory System

The olfactory system of insects is capable of recognizing thousands of odours and tastants. The olfactory sensory neurons (OSNs) that detect odours are housed within specialised hairs known as sensilla that cover the antennae and maxillary palps of insects. In the vinegar fly, *Drosophila melanogaster*, sensilla contain one to four OSNs that respond to different odorants. There are multiple sensilla types that each contain a distinct set of OSNs.

Odours enter the sensilla through tiny wax-filled pores in the walls of the hairs. Inside is an aqueous lymph that contains high concentrations of odorant binding proteins that solubilise and transport odorants to receptors on the surface of the dendrites of OSNs that extend up into the lymph. Electrophysiological techniques have been established to record the firing rates of individual OSNs, revealing that each OSN has a characteristic spontaneous firing rate. Upon activation by a relevant odorant the firing rate changes, typically but not always increasing in response to the odour. Axons from each OSN extend to the antennal lobe where those expressing the same receptor converge within the glomerulus of the lobe. Signals within the lobe are then modulated by local interneurons and transduced to the higher brain via projection neurons.

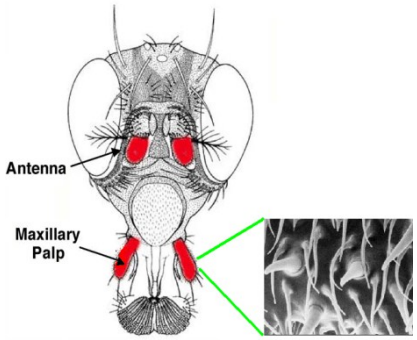

Fig. 1. The antennae and maxillary palps of the *Drosophila melanogaster* . A magnification of the maxillary palps highlights how their surface is covered with hair-like sensilla.

Insect odorant receptors are seven transmembrane receptors that were originally thought to be another subclass of G protein-coupled receptors. However, recent studies have shown they are orientated in the reverse orientation in membrane and can signal independent of the G protein signalling pathways [2-4]. There are two classes of receptor

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subunit; a ubiquitous subunit known as DmelOrco (previously Or83b) and a ligand binding olfactory receptor of which there are 61 in *Drosophila melanogaster*. Orco and ligand binding receptors form an active complex in the dendrites which when activated opens (or closes) as a cation channel. This activity then triggers a cascade of events resulting in depolarisation of the neuron and a change in the firing rate.

B. Creating an Artificial Olfactory System

Drosophila melanogaster are able to smell a diverse range of volatile compounds using their olfactory receptors. Hallem et al. [5] has characterised the majority of these receptors for their response to a standard set of odorants *in vivo*. Individual olfactory receptors were expressed in a mutant strain that provided an "empty" sensory neuron into which any receptor could be expressed. This allowed recordings of neuron firing rates for specific receptor responses to odorants.

Neuronal firing rates recorded from the empty neuron expressing each receptor are then analysed in order to interpret and thus classify the information to the user. Numerous techniques are available for classification: statistical methods such as regression analysis; clustering methods and multivariate data analysis [19]. In this work, we employ an 'Artificial Neural Network' (ANN) to classify the odorants. In the same conference proceedings we have investigated odorant classification using chemical descriptor values [20] rather than neuron firing rates.

The field of ANNs is based on the functionality of the biological neuron [6]. The wires and interconnections of an ANN model represent the axons and dendrites while the weighting functions of these connections represent resistances of the dendrites [6]**.** The activation function of an artificial neuron approximates the threshold level of the cell's membrane potential. The ANN is commonly used in a broad range of classification problems [7] and thus a viable method for recognising odorants.

II. Recognition of Odorants

A. Odorant Data Used & Pre-processing

The data used in this work was obtained from the report of Hallem et al. [5]. In this report, the firing rates from 24 OSNs of an adult fly to 104 different chemical volatile compounds or odorants was documented. The 104 chemical compounds fell into 8 distinct chemical classes (with number of chemicals listed in brackets): Lactones (5 chemical odorants); Acids (15); Terpenes (16); Aldehydes (8); Ketones (6); Aromatics (13); Alcohols (17) and Esters (24). This data was initially zero meaned and normalised [8] before use.

B. Neural Network Architecture and Training Procedure

The ANN employed is a feed forward multi-layered perceptron (MLP) network with binary sigmoid activation functions. The MLP used, depicted in figure 2, has three layers: an input layer with 24 neurons (x_1^0, x_2^0, x_2^0, ..., x_{24}^0) (corresponding to the firing rates of the 24 receptors), a single hidden layer with 48 neurons (n_1^1, n_2^1, n_2^1, ..., n_{48}^1) and an output layer with a single output neuron (y_1^2). With the input layer producing a 24×48 weight matrix (W_{ij}^0) and the hidden layer a 48×1 weight matrix (W_{ij}^1), shown schematically in figure 2.

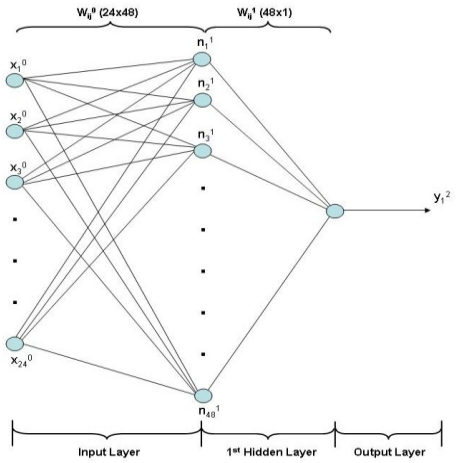

Fig. 2. The Multi-layer perceptron used to identify a single chemical class. Eight such networks were used to distinguish between the 8 separate chemical classes.

Eight separate MLP's of the above mentioned architecture were coded in Matlab software where each MLP's training was dedicated to predict one of the eight chemical classes.

Of the 104 chemicals available, 89 chemical compounds were randomly chosen to be used as the training and testing set for the MLPs and the remaining 15 chemical compounds were used as the MLPs' validation set. Since the number of chemicals in each chemical class was small, approximately 10% of the chemicals from each chemical class were removed from the training set and placed in validation set.

The number of chemicals in each chemical class of the validation set were: Lactones (1) chemical odorant); Acids (2); Terpenes (2); Aldehydes (1); Ketones (2); Aromatics (2); Alcohols (2) and Esters (3). Under supervised learning, each of the eight MLPs was trained on 200 shuffled epochs of the training set to produce an output of unity for their attributed chemical class and zero for all other classes. The MLP was trained with an added momentum function to enhance its convergence [9].

C. Improving Performance with Noise Injected Data

One very useful property and advantage of ANNs is their ability to generalize [10]. This is their ability to recognize and differentiate between different classes of objects. A technique known as noise injection [11-16] is well documented for improving the generalizing properties of an ANN. It was demonstrated in [12] that this leads to an improvement of performance of the ANN requiring the ANN to have more weights or hidden units. In [17] it was demonstrated that noise injection is independent from the type of noise used and that optimally ~10% of noise can be injected into the input space to improve the generalizing properties of the network. This technique was taken further in [18] where it was demonstrated how 25% of noise could be used to recognize patterns through obscuration. Thus, 10% of uniform additive noise was employed and applied to

a copy of the training and validating data sets and their performance compared.

III. Results

A. Predicting Chemical Class of 15 Unknown Odorants

A typical training regime is depicted in figure 4 for each of the 8 MLPs that were trained specifically on one chemical class. It highlights the improvement in the training of the MLP when employing a 10% noise injection versus training on the raw data.

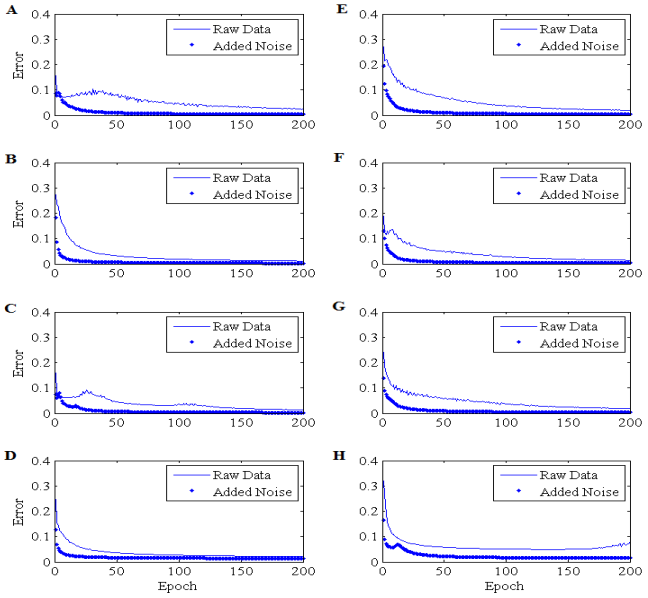

Fig. 4. Training for 200 epochs with raw and noise injected data for the 8 chemical classes A-H: A – Lactones, B- Acids, C-Terpenes, D-Aldehydes, E-Ketones, F-Aromatics, G-Alcohols and H-Esters. The thin blue line represents training on the raw data and the thick blue line depicts training on the noise injected data.

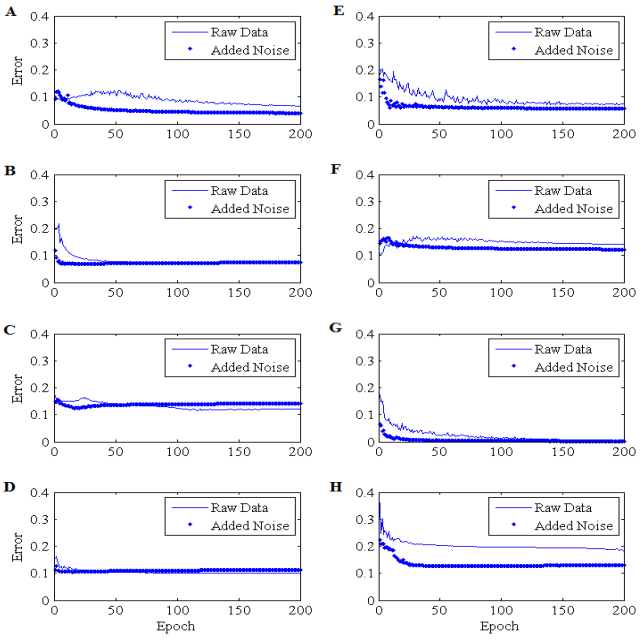

Fig. 5. Validation for 200 epochs with raw and noise injected data for the 8 chemical classes A-H: A – Lactones, B- Acids, C-Terpenes, D-Aldehydes, E-Ketones, F-Aromatics, G-Alcohols and H-Esters. The thin blue line represents training on the raw data and the thick blue line depicts training on the noise injected data.

Figure 5, shows how the recognition of the validating data set was clearly enhanced by introducing an optimal noise injection level of 10% onto the training set, as suggested in [17]. The accuracy of prediction of the validating vectors, from the unseen set, is shown in figure 6.

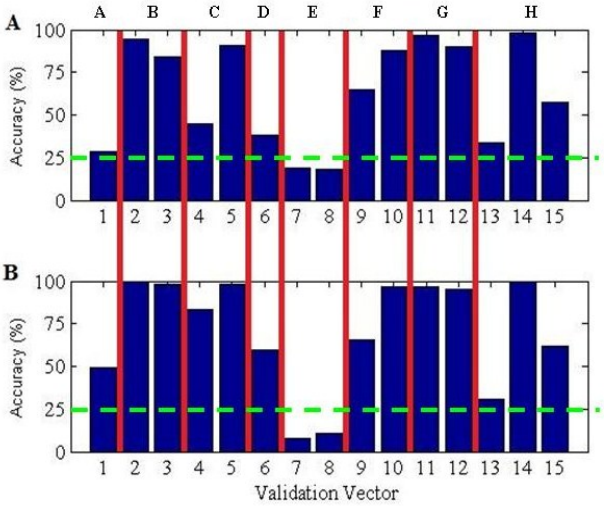

Fig. 6. Classification of the 15 unseen odourants of the validation set of the chemical classes A-H: A – Lactones, B- Acids, C-Terpenes, D-Aldehydes, E-Ketones, F-Aromatics, G-Alcohols and H-Esters. The upper plot (A) is MLP performance when trained on raw data and lower plot (B) is MLP performance when trained on noise injected data. The thick red lines separate the different chemical classes whilst the green broken lines represent a 25% detection threshold level that could be used to adequately identify the chemical classes.

The upper plot (A) depicts the accuracy in prediction of the 15 validating vectors of the 8 chemical classes when the MLP was trained on the raw data. The lower plot (B) depicts the accuracy in prediction when the MLP was trained on the training set which had received 10% noise injection. The largest chemical class was that of the Esters. Hence, this class had the most validating vectors, consisting of 3 chemicals. Therefore, out of the 15 validating vectors the probability of choosing an ester randomly was (3/15 = 20%). This value was used identify the minimum threshold level of accurate detection of the validating set. We introduced a margin of 5% to this value as an added safeguard. Thus, the threshold level of detection was set to 25%. It can be seen that by employing a 25% threshold level that the differently trained MLPs depicted in the plots of figure 6 correctly identified 87% of the chemicals (i.e 13 out of the 15 unseen chemicals). Although, the noise injected trained MLPs, depicted in plot (B) of figure 6 identified the same amount of chemicals than the MLPs trained on the raw data, it can be seen that their accuracy of identification outperformed the MLPs trained on the raw data by 7% accuracy on average with a standard deviation of 12.5%. This is evident as the bars of the plots are heightened in comparison to those of the MLPs trained on raw data implying more accurate identification.

IV. Conclusion

In this work, we demonstrate how it is possible to use the firing rates recorded from an array of insect olfactory sensory neurons (OSNs) in order to train a series of Multi-layer perceptrons (MLP) to differentiate between 8 distinct chemical classes.

We demonstrated how the MLPs, when trained on 108 chemicals, with both clean and 10% noise injected data can reliably identify 87% (i.e 13 out of the 15 unseen chemicals) of an unseen validation set using noise injection. It was found that the noise injected trained MLPs provided a more accurate level of identification than the MLPs trained on the raw data alone. Thus, we demonstrate that a 10% noise injected series of MLPs provides a robust method for classifying chemicals from the firing rates of insect olfactory receptors and paves the way towards artificially classifying odorants.

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