A Bio-inspired Data Processing Method for Classification of Chinese Liquors Using Electronic Nose

Ya-Qi Jing, Qing-Hao Meng, Pei-Feng Qi, Xue-Mei Jia, and Shu-Gen Ma

Abstract—We proposed a bio-inspired neural network to perform data processing in an electronic nose (e-nose) system. The structure of the proposed neural network is similar to mammals’ olfactory system which contains olfactory sensing neurons, mitral cells and granule cells. This neural network largely simplifies traditional data processing steps in e-noses. It uses the original data collected from gas sensors without data preprocessing and feature reduction. We innovatively use recurrence quantification analysis to perform feature selection. Recurrence rate and determinism are calculated according to the network’s output curves and these values are used as features extracted from the proposed olfactory neural network. Linear discrimination analysis and support vector machine are used as classification methods. The performance of the proposed neural network was tested by “leave-one-out” cross-validation. The classification rates were 93.75% and 96.25% using these two methods, respectively, which were higher than traditional data processing methods (85% and 91.25%).

I. INTRODUCTION

Olfactory system plays an important role in animals’ life. For example, animals can use their olfactory system to seek food, find mates and avoid danger. Through tens of years’ study, researchers have obtained great achievements on exploring the basic structure and mechanism of mammals’ olfactory system [1]. It is generally acknowledged that the olfactory system is mainly composed of odor receptors, olfactory bulb and piriform cortex [2]. Odor receptors can change the chemical signals into electric signals and then pass these signals to olfactory bulb. Olfactory bulb further analyzes these signals and piriform cortex makes final decisions.

Research findings in biological olfaction have promoted the appearance of new instruments that can mimic the ability of olfactory systems. These instruments are called electronic noses (e-noses) [3]. They often contain an array of gas sensors which can change the chemical signals into electric signals, and data processing system that can derive useful information from sensors’ response curves and pattern recognition methods.

E-noses can characterize a wide range of odors due to the broad and partially overlapping selectivity of gas sensors as well as proper data processing methods. In recent years, several e-noses have been invented and used to assess the smell of various products such as fish [4], fruits [5], tea [6], and milk [7]. These e-noses have different data processing methods because every method has its own characteristics and is suitable for specific situations. Data processing methods in e-noses often consist of data preprocessing, feature selection and reduction. Data preprocessing can eliminate the influence of noise and sensor drift. Feature selection methods help to obtain useful information through sensors’ response curves. Feature reduction methods can make sure that most of the redundant features are eliminated and this is helpful for pattern recognition. Each step discussed above has many methods to choose from and these steps strongly influence the performance of an e-nose [8]. In order to obtain a satisfying result, one has to choose the appropriate methods according to the type of sensors and applications e-noses are used for. However, as far as we know, there is no guideline on how to choose these methods for people to comply with. So people may have to try many data processing methods and then choose the most suitable ones. This procedure often takes enormous time and effort [9].

As mentioned above, e-noses are instruments inspired from olfactory system. So e-noses combined with olfactory models have certain advantages such as higher sensitivity, better ability of noise reduction and sensor-drift compensation. Plenty of olfactory models have been proposed. Some models mimic the whole olfactory system [10] and some mimic the structure of olfactory bulb [11]. However, most of these researches focused on the structure or mechanism of olfactory system. There are only a few literatures discussing the utilization of the olfactory models [12]. As far as we know, there is no research on e-noses using the original data collected from gas sensors without data preprocessing. In this paper we proposed an olfactory neural network and combined it with an e-nose system. This olfactory neural network is inspired from the structure of olfactory system which contains olfactory sensing neurons, mitral cells and granule cells. It uses the original data collected from gas sensors without any preprocessing such as filtering or denoising. Feature reduction is also omitted because we only selected twenty features according to the network’s outputs. Using the proposed olfactory neural network as a data processing method, we don’t need to try a large number of data preprocessing, feature selection and reduction methods and then find out the most suitable ones. This largely simplifies.
traditional data processing steps in e-noses.

The remainder of this paper is organized as follows: Section II presents the basic structure of the proposed olfactory neural network. Section III discusses the experimental implementation using our designed e-nose as well as the data processing method using the proposed olfactory neural network. Section IV shows the classification results. Finally, conclusions are given in Section IV.

II. THE PROPOSED OLFACTORY NEURAL NETWORK

The basic structure of the proposed olfactory neural network is shown in Fig. 1. This network contains 100 olfactory sensing neurons, 10 mitral cells and 10 granule cells. Each mitral cell represents the activity of a single glomerulus olfactory sensing neurons, 10 mitral cells and 10 granule cells. Each granule cell connects with one mitral cell as shown in Fig. 1. Every single neuron was modeled using (HR) neuron model [13]. The HR neuron model is described as follows:

$$\dot{x} = y - ax^3 + bx^2 - z + I$$
$$\dot{y} = 1 - 5x^2 - y$$
$$\dot{z} = r(4(x - x_{rest}) - z)$$

where $x$ means the membrane potential of the neuron, $y$ indicates the recovery variable associated with inner current (sodium ion or potassium ion), $z$ is the slow variable current, $a$ represents the qualitative behavior of the model, $b$ allows one to switch between bursting and spiking behaviors and to control the spiking frequency, $I$ is the external stimulation and $r$ controls the speed of variable $z$. As shown in Fig. 1, olfactory sensing neurons connect with different mitral cells and have different connection weights and parameter values. This mimics the selectivity in olfactory sensing neurons. That is to say, even under the same stimulation, olfactory sensing neurons connecting with different mitral cells may have different outputs. Granule cells are inhibitory cells and mitral cells are excitatory cells.

![Fig. 1. The basic structure of the proposed olfactory neural network. This olfactory neural network has 100 olfactory sensing neurons, 10 mitral cells and 10 granule cells.](image1)

The connection weights between olfactory sensing neurons and mitral cells are settled using Hebbian learning rule [14]. Neurons with larger oscillation intensities are given larger connection weights. Connection weights between mitral cells and granule cells are the same.

Mitral cells are considered as the outputs of the olfactory neural network. There are 10 mitral cells in this olfactory neural network so we derive features from these 10 mitral cells during data processing.

III. EXPERIMENTS AND DATA PROCESSING METHODS

A. Experimental Implementation

In this study 7 kinds of Chinese liquors of the same aroma style were used. Their name and characteristics are shown in Table I. Ethanol solution with the concentration of 38%Vol was also used as a control group.

![Image 2](image2)

**TABLE 1: THE DETAILS OF 7 KINDS OF CHINESE LIQUORS.**

<table>
<thead>
<tr>
<th>Name</th>
<th>Abbreviation</th>
<th>Alcohol content</th>
<th>Raw material</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bainianwanjiu</td>
<td>BNJW</td>
<td>38%Vol</td>
<td>Sorghum, wheat, barley, pea</td>
</tr>
<tr>
<td>Daohuaxiang</td>
<td>DHX</td>
<td>42%Vol</td>
<td>Sorghum, wheat, rice, polished glutinous rice, corn</td>
</tr>
<tr>
<td>Jinjiu</td>
<td>JJ</td>
<td>45%Vol</td>
<td>Sorghum, wheat, barley, pea</td>
</tr>
<tr>
<td>Jinjiu (Bianfenghu)</td>
<td>LJ</td>
<td>48%Vol</td>
<td>Sorghum, wheat, barley, pea</td>
</tr>
<tr>
<td>Luzhoulaojiao</td>
<td>LZLJ</td>
<td>38%Vol</td>
<td>Sorghum, rice, wheat,</td>
</tr>
<tr>
<td>Niulanshan</td>
<td>NLS</td>
<td>42%Vol</td>
<td>Wheat, sorghum, rice,</td>
</tr>
<tr>
<td>Qingjiu</td>
<td>QJ</td>
<td>38%Vol</td>
<td>Sorghum, wheat, nuogu, corn</td>
</tr>
</tbody>
</table>

The basic structure of the e-nose used in this study is shown in Fig. 2. Ten metal oxide gas sensors from two companies which have partially overlapping selectivity are used in this e-nose system. They are TGS822, TGS880, TGS2610, TGS2611, TGS2620 from Figaro and MICS5121, MICS5135, MICS5521, MICS5524, MICS5526 from E2V. All of these sensors are sensitive to volatile organic
compounds (VOCs), which make them suitable for detecting Chinese liquors.

Sampling method used here is dynamic headspace sampling. 1μL for each kind of Chinese liquors and ethanol solution were kept in an Erlenmeyer flask being maintained at a constant temperature of 70°C for 10 min. After evaporation of Chinese liquor samples, the carrier gas’s flow was set at 200sccm to carry the volatile compounds in headspace into the sensor chamber to allow the sensors react with volatile compounds. This procedure lasted for 1 min and then cleaning step began. During cleaning step the mass flow controller was set at 5L/min to allow the sensors recover the baseline. We must make sure that before each measurement the pipes and sensor chamber were clean and no volatile compounds from Chinese liquor samples were attached to the sensors and pipes. So the cleaning step lasted for 30 min and the pipes and sensor chamber were cleaned using clean dry air.

B. Data Processing Methods

Firstly, we discuss data processing method using the proposed olfactory neural network.

Ten gas sensors’ response curves were sent to the proposed olfactory neural network without any data preprocessing. Then we obtained ten mitral cells’ outputs as the neural network’s outputs. The outputs of the olfactory neural network for NLS are shown in Fig. 3. From Fig. 3, we can see that different mitral cells have different outputs.

In order to observe the network’s outputs more clearly, we also show the first three mitral cells’ outputs in Fig. 4. We can see that different kinds of Chinese liquors have different outputs. In order to distinguish between different kinds of Chinese liquors, we derived useful features from these output curves. The output curves were nonlinear time series so we used recurrence quantification analysis to further explore the essence of the output curves.

Fig. 2. The basic structure of the e-nose.

Fig. 3. Ten mitral cells’ outputs of the olfactory neural network for NLS.

Fig. 4. The first three mitral cells’ outputs for 3 kinds of Chinese liquors. From top to bottom are NLS, LJ, and DHX, respectively.
The cross recurrence plot of mitral cell 1 for NLS is shown in Fig. 5. According to the characteristics of the cross recurrence plot, two most common quantification approaches namely recurrence rate and determinism [15] were applied. The details are as follows:

1) Recurrence rate

\[ RR = \frac{1}{N^2} \sum_{i,j=1}^{N} R_{i,j}^{m,e} \]  

where

\[ R_{i,j}^{m,e} = \Theta(\varepsilon - \| \tilde{x}_i - \tilde{x}_j \|) \]  

\( \varepsilon \) is a predefined threshold and \( \tilde{x}_i, \tilde{x}_j \) are phase space trajectories in an \( m \)-dimension phase space.

2) Determinism

\[ DET = \frac{\sum_{i=1}^{N} \sum_{l=i}^{N} lP^r(l)}{\sum_{i,j}^{N} R_{i,j}^{m,e}} \]  

where \( P^r(l) = \{ l_i; i = 1, 2, \ldots, N_i \} \) is the frequency distribution of the lengths \( l \) of diagonal structures and \( N_i \) is the absolute number of diagonal lines. \( N \) is the length of a data series and \( l_{\text{min}} \) is an integer that predefines the minimal length of a diagonal line.

We calculated these two values from each mitral cell’s output and this meant the total number of calculated values was 20. Then we used these 20 values as features derived from the proposed olfactory neural network. In order to better test the performance of the olfactory neural network, we used two classification methods: linear discrimination analysis (LDA) and support vector machine (SVM) [16].

Secondly, traditional data processing methods are also used as a comparison.

Traditional data processing in e-noses often contains data preprocessing, feature selection and reduction. Four data preprocessing methods were used to eliminate the influence of noise and compensate the drift. Then we selected ten features from each sensor’s response curve, the derivative, integration, curvature and radius of curvature of the response curve. After that we employed 8 algorithms based on information theory to perform feature selection. Kernel entropy component analysis (KECA) was then used as a feature reduction method. Details of the traditional data processing methods could refer to [17]. Classification methods were also LDA and SVM.

Figure 6 shows data processing steps using the proposed olfactory neural network and traditional methods. From Fig. 6 we can see that the proposed olfactory neural network largely simplifies data processing steps for e-noses.
IV. RESULTS

We use the “leave-one-out” cross-validation to analyze the performance of the proposed olfactory neural network and traditional data processing methods. Figure 7 shows the 3-dimensional LDA plots using both data processing methods. It is clearly seen that the result using our proposed olfactory neural network is better than traditional data processing methods. Different kinds of Chinese liquors are more separable using the proposed olfactory neural network as a data processing method. The classification rates of the proposed olfactory neural network and traditional method are 93.75% and 85%, respectively. SVM was also used as a classification method. Table II summarizes the results. It shows a prediction ability of 96.25% and 91.25% for the 7 kinds of Chinese liquors and ethanol solution using the proposed neural network and traditional method, respectively.

![LDA plots](image)

Fig. 7. 3-dimensional LDA plots using the proposed olfactory neural network and traditional methods. The top figure is the result using traditional methods and the bottom figure is the result using proposed olfactory neural network.

<table>
<thead>
<tr>
<th>Classification method</th>
<th>Classification rate using different data processing methods</th>
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<tbody>
<tr>
<td></td>
<td>Olfactory neural network</td>
</tr>
<tr>
<td>LDA</td>
<td>93.75%</td>
</tr>
<tr>
<td>SVM</td>
<td>96.25%</td>
</tr>
</tbody>
</table>

The proposed method makes data processing steps in e-noses much easier. E-nose using the proposed olfactory neural network also has a higher classification rate.

V. CONCLUSIONS

In this paper we proposed a bio-inspired olfactory neural network and successfully introduced it to an e-nose system as a data processing method. It is widely acknowledged that original data collected from gas sensors often contain noises which are useless and have disadvantages for classification. So these original data cannot be used directly in e-noses. However, the proposed olfactory neural network can use the original data collected from gas sensors without any data preprocessing. This largely simplifies traditional data processing steps in e-noses. The proposed network has ten output neurons and can change the sensors’ response curves into new curves which contain intrinsic information of the tested odors. In order to extract the useful information, we performed recurrence quantification analysis and obtained 20 features. This is the first time to introduce recurrence quantification analysis into an e-nose system as a feature selection method. We also used both linear (LDA) and nonlinear (SVM) classification methods to validate the performance of the proposed method. The classification rates were 93.75% and 96.25%, respectively, which were higher than traditional methods.

In the future, we’d like to further optimize the function of the olfactory neural network, for instance, adding a piriform cortex layer which enables the neural network to have a feedback mechanism. We may also try to use other methods that can obtain useful information from the network’s outputs. We’d also like to combine this olfactory neural network with other e-nose systems and we hope that this method can be a universal method for data processing in e-noses.

REFERENCES


