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Research Article

Identification of Vinegar Flavor using Electronic Nose☆

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Abstract: As one of the most popular condiments, vinegar's quality has been widely concerned. Discrimination of vinegar which is composed of a complex mixture of very similar compositions by chemical analysis means is a remaining challenge. In order to explore possibility of identification of vinegar's quality by electrochemical methods, we have developed an electronic nose with gas sensor array of different selectivity composed of eight sensors (TGS813, TGS822, TGS826, TGS2600, TGS2602, TGS2610, TGS2611 and TGS2620). The experiment process is automatically measured by a virtual testing application platform with LabVIEW, which can realize data acquisition, data storage, data processing and so on. The odor's fingerprint of five different flavor vinegar, including white vinegar, mature vinegar, rice vinegar, balsamic vinegar and apple vinegar, are collected using the electronic nose. Multivariate statistical analyses, such as Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA), are employed to analyze all of these samples. Meanwhile, the multilayer perceptron (MLP) recognition model is established. The results show that both PCA and LDA can distinguish different flavor samples and the MLP has achieved higher recognition accuracy. It's a feasible way to discriminate different flavor vinegar with the self-developed electronic nose.

Keywords: Electronic nose, linear discriminant analysis, multilayer perceptron, principal component analysis, vinegar

INTRODUCTION

Vinegar is one of the most widespread and common acetic acid diluted solution products. Its quality directly affects people's health because vinegar is a popular seasoning (Li *et al*., 2015; Zeng *et al*., 2015). Methods of measuring odors can be divided into three main types: sensory analysis, chemical analysis and electronic nose (Zhang *et al*., 2008). And these methods of analysis are highly accurate and suitable for assessment of vinegar's quality (Jiang *et al*., 2015; Li *et al*., 2012). The aroma or flavor is certainly one of the most important determinants of vinegar's quality (Jo *et al*., 2013). So the electronic nose device is designed as a simple simulation of human olfaction (Peris and Escuder-Gilabert, 2009; Wilson, 2012). Generally, the electronic nose system associated with pattern recognition algorithms is attractive for a number of significant features (Montuschi *et al*., 2012; Falasconi *et al*., 2012), such as non-invasive detection (Hartyáni *et al*., 2013), a qualitative identification (e.g., cluster analysis (Trirongjitmoah *et al*., 2015)) or quantitative calculation (e.g., linear fitting regression (Hong *et al*., 2015), partial least squares regression (Yan *et al*., 2015) of a gas or Quadratic Discriminant Analysis (QDA) (Oliveros *et al*., 2002), Support Vector Machines (SVM) (Brudzewski *et al*., 2004).

With developments in sensor technology in recent years, electronic nose techniques have become valuable tools in application areas (Jiang *et al*., 2015). Neural network architecture has been successfully applied to many applications, ranging from adaptive signal processing to system control. These neural network models were proposed, including Feedforward Neural Networks (FNN) and Recurrent Neural Networks (RNN). They were applied successfully to various real world problems (Han *et al*., 2011; Bao and Zeng, 2012). As one of the feedforward neural network, Multilayer Perceptron (MLP) is by far the most popular network with a relatively simple construct, significant capabilities and so on. The ability of classification and approaching makes MLP applicable to the application areas such as quality evaluation and adulteration recognition in food detection (Zhang *et al*., 2014; Abbasi *et al*., 2015).

The electronic nose device crudely mimics human smell that interacts with odor molecules (Baldwin *et al*., 2011). In this study, a homemade electronic nose system is developed to classify five flavor vinegars. Classifications of the electronic nose dataset by the MLP and Cluster-then-Label approach based on PCA and LDA are compared.

Table 1: Basic information of the vinegar samples

Sample names	Raw material	HAC/(g·L^{-1})	Fermentation	Origin	Number
White vinegar	Water, rice, sugar	≥50.0	Liquid	Zhenjiang	1-10
Mature vinegar	Water, glutinous rice, wheat bran	≥54.9	Solid	Zhenjiang	11-20
Rice vinegar	Water, rice	≥90.0	Liquid	Zhenjiang	21-30
Balsamic vinegar	Water, glutinous rice, wheat bran	≥54.9	Solid	Zhenjiang	31-40
Apple vinegar	Apple juice, drinking water	/	Liquid	Yantai	41-50

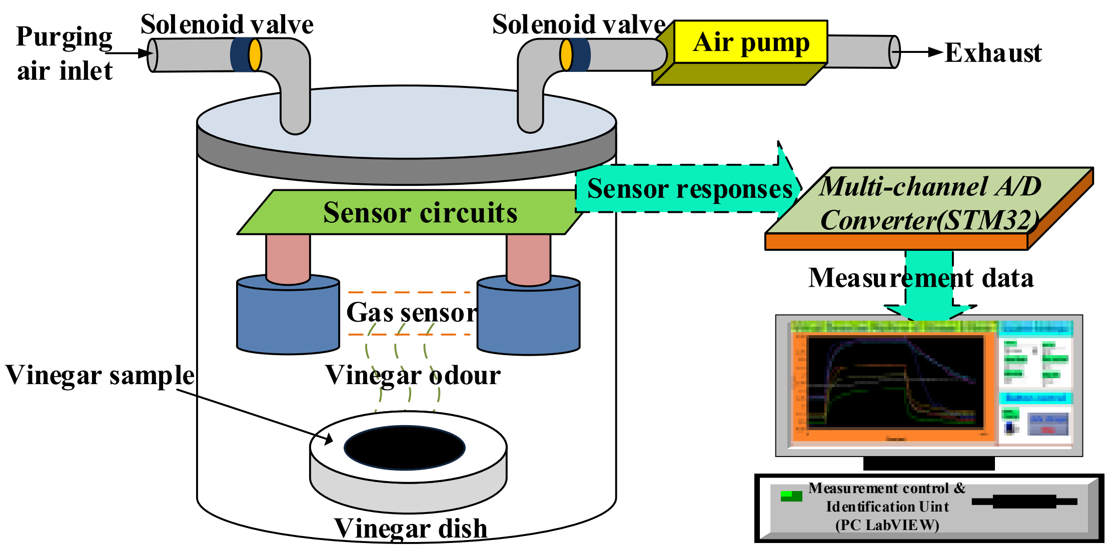

Fig. 1a: Schematic of the electronic nose system

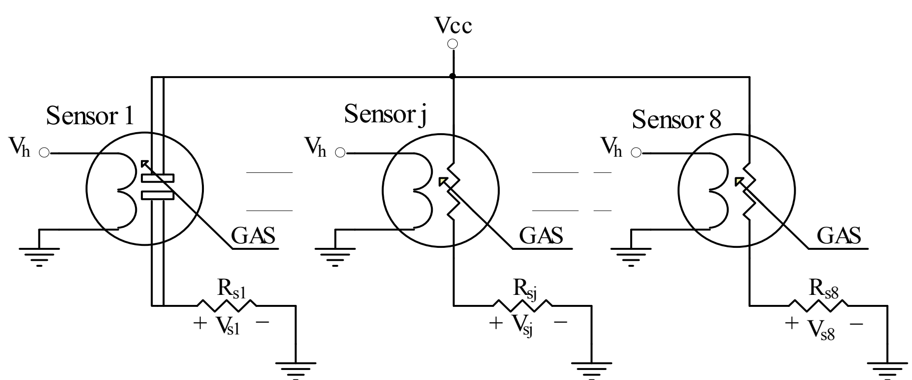

Fig. 1b: Sensor array circuit

MATERIALS AND METHODS

Vinegar samples: A total of five different flavor of vinegar were purchased from a local big supermarket, namely: White Vinegar (WV), Mature Vinegar (MV), Rice Vinegar (RV), Balsamic Vinegar (BV) and Apple Vinegar (AV). Each of these vinegar samples are about 500 mL. The basic information of the samples can be easily measured. And it is shown in Table 1, including sample names, raw material, acetic acid concentration, fermentation model, origin place and serial number.

Electronic nose system: Professional sensory panelists can identify a significant difference in sample odors, but the human nose has a fatigue symptom (Desrochers *et al*., 2002). In this study, the electronic nose system is developed independently for measuring and classifying vinegar odors. Because the characteristic flavor of vinegar is the result of representing a fingerprint of the sample (Ubeda *et al*., 2011). The structure of the electronic nose is presented schematically in Fig. 1a. It consists of three components: pump and solenoid valves unit; sensor array and chamber unit; measurement control and identification unit. Eight gas sensors with different selectivities are arranged in the lid of a 2.5 L air chamber to form the sensor array, namely: TGS813, TGS822, TGS826, TGS2600, TGS2602, TGS2610, TGS2611 and TGS2620 (Figaro

Table 2: Mean and standard deviation of measured voltage from each sensor at 180 s (mean±S.D. N = 10)

	Sample values (V)				
Sensor	white vinegar	mature vinegar	rice vinegar	balsamic vinegar	Apple vinegar
TGS813	0.53±0.16	0.43±0.09	0.60±0.18	0.14±0.09	0.08±0.07
TGS822	1.56±0.07	1.97±0.07	1.80±0.05	1.90±0.05	0.86±0.05
TGS826	1.25±0.17	0.86±0.09	1.44±0.09	0.70±0.06	0.29±0.02
TGS2600	1.92±0.17	1.80±0.08	1.98±0.14	1.85±0.05	1.00±0.05
TGS2602	1.51±0.15	1.19±0.10	1.75±0.06	1.05±0.07	0.44±0.03
TGS2610	1.86±0.24	1.81±0.06	1.97±0.04	1.74±0.06	0.93±0.04
TGS2611	1.60±0.20	1.20±0.11	1.84±0.08	1.05±0.10	0.40±0.03
TGS2620	2.58±0.14	2.85±0.03	2.73±0.07	2.69±0.09	1.88±0.07

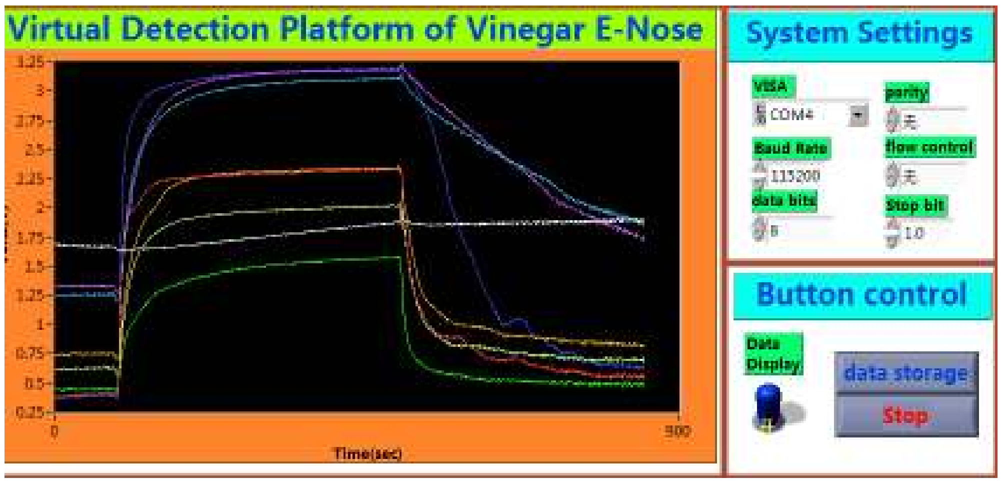

Fig. 2: Virtual testing platform

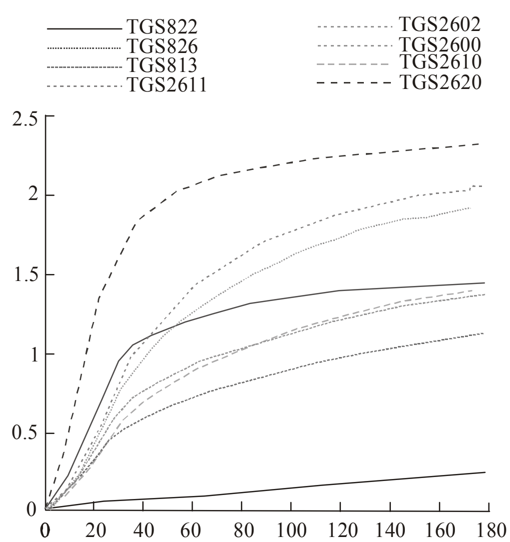

Fig. 3: Responses of the gas sensors

Engineering, Osaka, Japan). The measuring circuit of each sensor is also shown in Fig. 1b. Series with each sensor are connected to the load resistor with selected resistance in order to achieve appropriate sensor response.

The odor from the vinegar sample is collected by the sensor array for 800 s, the data from the sensor array being acquired five data points a second. The output voltages of the sensors were converted into digital signals with a Multi-channel A/D Converter (STM32) and sent to PC LabVIEW for processing (Trirongjitmoah *et al*., 2015). The measurement process is automatically controlled by a virtual testing platform which developed with LabVIEW (National Instrument) as shown in Fig. 2.

Data acquisition: Sensors collect the data and convert it into a more suitable electrical signal pattern (Scott *et al*., 2007). Changes in the vinegar odor concentrations are responsible for changes in the gas sensor output voltages. In Fig. 3, the sensor response signals 180 s after the start of the measurement are selected as being representative and are used to classify the different flavor vinegars.

Table 2 shows the means and the standard deviations of the measured response signal of each sensor at 180 s. As is shown in Table 2, these response signals can be measured with high repeatability based on this developed system. Figure 4 shows the normalized response signals for the eight sensors during the last second of a measurement with a radar graph.

METHODS

Principal Component Analysis (PCA): PCA used for reducing the dimensionality of data is a one of the well-known multivariate statistics methods (Trirongjitmoah

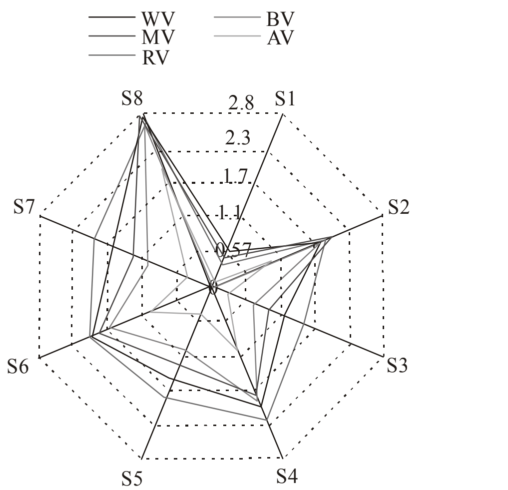

Fig. 4: Radar graph of the 8 sensors. S1 = TGS813, S2 = TGS822, S3 = TGS826, S4 = TGS2600, S5 = TGS2602, S6 = TGS2610, S7 = TGS2611, S8 = TGS2620

et al., 2015). And it is a feature extraction way to explore underlying data structure (Hong *et al*., 2015). In this study, the data set of different flavor vinegar samples will be transformed into two-dimensional (2D) and three-dimensional (3D) coordinates, by employing two and three main components of PCA, respectively.

Linear Discriminant Analysis (LDA): LDA is supervised approach that constructs discriminant function through linear combination of data (Hong *et al*., 2015). The purpose of LDA is to find a linear transformation to achieve maximum class discrimination (Guan *et al*., 2014). LDA has been widely used to build classification model with electronic nose and it provides a feasible method for quantitative analysis (Trirongjitmoah *et al*., 2015). In this study, the data set of different flavor vinegar samples will be transformed into 2D and 3D coordinates, by employing two and three main normal variables of LDA, respectively.

Multilayer Perceptron (MLP): MLP is a modified standard linear perceptron and distinguish non-linearly separable data (Cybenko *et al*., 1989). MLP has been used to solve some difficult and diverse problems successfully, for which error back-propagation is the most popular training algorithm. To illustrate the classification method fully, the MLP model with Multi-Input Multi-Out (MIMO) is chosen (Abbasi *et al*., 2015). The architectural graph of MLP model with one hidden layer is shown in Fig. 5. Without loss of generality, there are M nodes in the input layer, N nodes in the hidden layer and Q nodes in the output layer.

The input-output and activation function of each layer are described in the following:

Input layer: There are M nodes in input layer. By these nodes, the input variables which represent all attributes of data are inputted to the MLP. The output values of input nodes can be expressed as:

$$u_i = x_i, \quad i = 1, 2, \cdots, M, \tag{1}$$

where, u_i is the ith output value and the input vector is given by

$$X = [x_1, x_2, \cdots x_M] \tag{2}$$

Hidden layer: There are N nodes in this layer. By each hidden node, the MLP's input nodes connect with output nodes. The output values of hidden nodes are:

$$\varphi_j = f(\sum_{i=1}^{M} w_{ij} u_i), \quad i = 1, 2, \cdots, M, j = 1, 2, \cdots N, \tag{3}$$

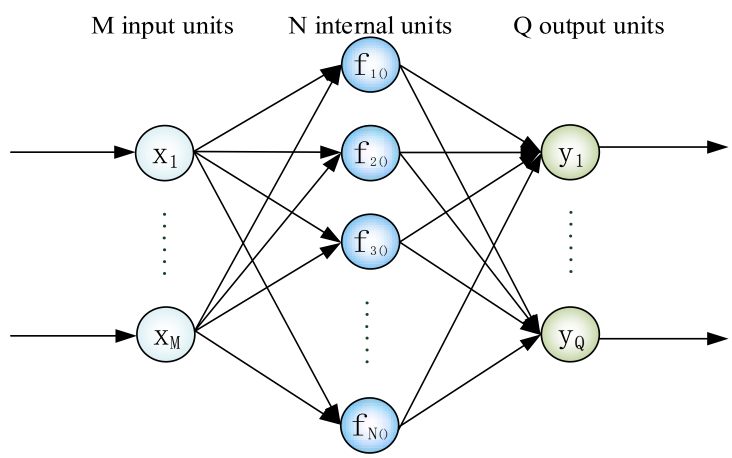

Fig. 5: The multilayer perceptron (MLP) structure

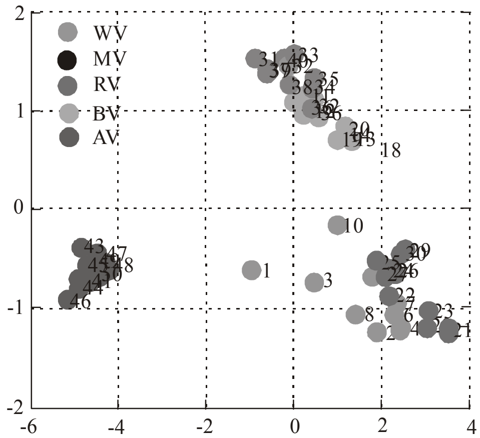

Fig. 6a: 2D

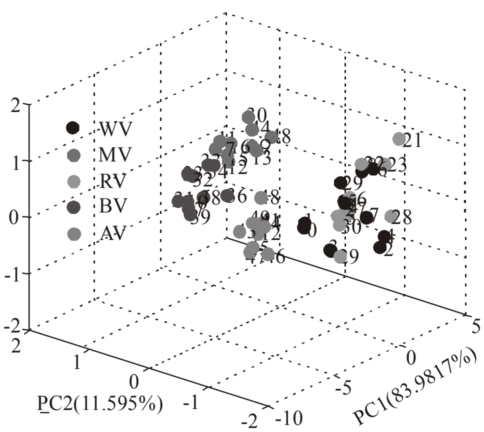

Fig. 6b: 3D PCA score scatter plots

where, $f(x) = (1 + e^{-x})^{-1}$, ϕ_j is the output value of jth node, $\boldsymbol{\phi} = [\phi_1, \phi_2, \cdots \phi_N]^{\mathrm{T}}$ are the output vector of the hidden layer whose dimension is $N \times 1$ and w_{ij} is the weight value connecting the ith input node with the jth in the hidden layer, $W = [w_{g1}, w_{g2}, L, w_{gN}]$ whose dimension is $M \times N$ and $W_{gj} = [w_{1j}, w_{2j}, w_{Mj}]^T$.

Output layer: There are Q nodes in this layer. The output value of each output node is given by:

$$y_q = \sum_{j=1}^{N} v_{jq} \varphi_j, \quad j = 1, 2, \cdots N, q = 1, 2, \cdots Q, \tag{4}$$

where, y_q is the output value of the qth node in the output layer, $y = [y_1, y_2, y_Q]$ are the MLP model's output vector, v_{jq} is the weight connecting the jth node in the hidden layer with the qth output node, $V = [v_{g1}, v_{g2}, v_{gQ}]$ whose dimension is $N \times Q$ and $v_q = [v_{1q}, v_{2q}, v_{Nq}]^T$.

In order to estimate and train the MLP model, the MSE for the output nodes is defined as:

$$E(t) = \frac{1}{T} \sum_{t=1}^{T} \sum_{q=1}^{Q} (y_q(t) - d_q(t))^2, \tag{5}$$

where, $y_q(t)$ and $d_q(t)$ are the output and desired output of the qth node in the output layer calculated at time t, respectively and T is the total number of samples.

RESULTS AND DISCUSSION

Statistical analysis: Figure 6 depicts the PCA score scatter plot for vinegar of five flavors. In the 2D Fig. 6a, the contribution rats of the first Principal Component (PC1) and the second principal component (PC2) are 83.98% and 11.60%, respectively. Several errors in classification are observed between white vinegar and rice vinegar, also between mature vinegar and balsamic vinegar. In the 3D Fig. 6b, the contribution rat of the first three PCs reaches 98.87% and all of the samples are clustered into their respective groups except between white vinegar and rice vinegar (there are some crossing points).

Figure 7 demonstrates the LDA score scatter plot for five flavor vinegars. As is shown in the 2D figure (Fig. 7a), the contribution rats of the first normal variable (LD1) and the second normal variable (LD2) are 34.20% and 33.75%, respectively. No confusions or errors in classification are observed among the three flavors vinegar (i.e., white vinegar, rice vinegar and apple vinegar) except between mature vinegar and balsamic vinegar. As is shown in the 3D figure (Fig. 7b), the contribution rat of the first three LDs exceeds 85% and all of the samples are successfully clustered into their respective groups.

Classification using MLP: Before establishing MLP recognition model, each sample in the feature data set is attached a tag, which white vinegar is defined as 10000, mature vinegar as 01000, rice vinegar as 00100, balsamic vinegar as 00010, apple vinegar as 00001. To reduce errors caused by too little sample data, 10 times ten-fold cross-validation are used in experiments. The 50 samples of data set are divided into 10 parts that every part includes 5 samples. In a ten-fold cross-validation, every part is selected as a test set in turn and the remaining 9 parts as the training set. Finally, all samples are sent into the recognition model for testing. After using 10 times ten-fold cross-validation, the training and testing set numbers reach 4500 and 500, respectively.

The test results are shown in Table 3. As can be seen from the table, for each 100 test samples of vinegar, the numbers of vinegar samples which are identified correctly are 87, 99, 100 and 100 and the total accuracy reaches 97.20%. From the perspective of specificity, no other specimen is identified mistakenly as white vinegar and apple cider vinegar, while, 10, 3, 1 samples are classified mistakenly as mature vinegar, rice vinegar, balsamic vinegar, respectively and the total specificity reaches 97.39%. Therefore, the MLP

Table 3: Results of MLP

Sample	Recognition results					Average accuracy%
	WV	MV	RV	BV	AV	
WV	87	10	3	0	0	87
MV	0	99	0	1	0	99
RV	0	0	100	0	0	100
BV	0	0	0	100	0	100
AV	0	0	0	0	100	100
Specificity%	100	90.83	97.09	99.01	100	97.39/97.20

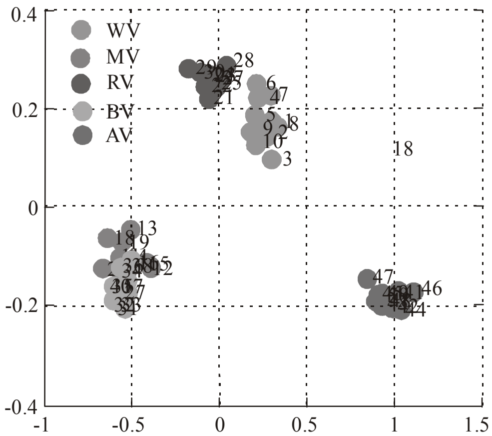

Fig. 7a: 2D

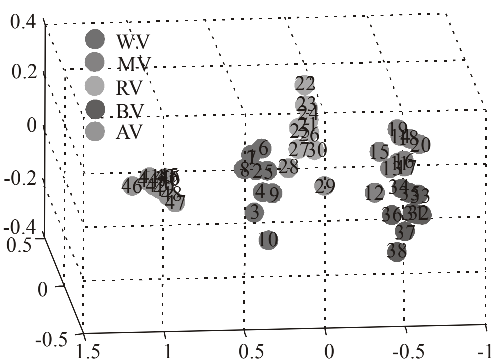

Fig. 7b: 3D LDA score scatter plots

classification model has a higher classification accuracy.

CONCLUSION

In conclusion, electronic nose is developed to identify different flavor vinegar based on neural networks. Fingerprint information of vinegar can be acquired effectively with sensor arrays which are different characteristic and highly sensitive. LabVIEW is used to control the measurement process. PCA and LDA are used to recognize vinegar samples and MLP model has achieved high classification accuracy rate. It provides a better quality analysis tools and the online monitoring for vinegar fermentation process maybe possible.

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