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A sensor array optimization method of electronic nose based on elimination transform of Wilks statistic for discrimination of three kinds of vinegars

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ABSTRACT

In order to discriminate three kinds of Chinese vinegars using an electronic nose (E-nose), an E-nose sensor array optimization method based on elimination transform with pivoting of Wilks Λ-statistic is put forward. With the help of the elimination transform some sensors with high discriminant ability are orderly selected step by step, and an ordered set of the selected sensors is simultaneously obtained by the selected sequence. Although the ordered set is not necessarily optimization array, the optimization array can be easily obtained by further exploring the discrimination results of sub-arrays which are composed by the first two, three, four and more sensors of the ordered set. In the discrimination of three kinds of vinegar samples, 9 sensors were selected in sequence and consisted of the ordered set using the method, and these vinegar samples could be well discriminated by principal component analysis (PCA). Furthermore, the first two sensors were selected and their PCA result was better than that of the 9 sensors. This illuminates that the array optimization method is very suitable and effective.

1. Introduction

As a favorite condiment, a large amount of vinegar is produced and consumed every year in China. And the discrimination of vinegars has attracted the increasing attention of people. Due to the innumerable compounds in vinegar, the conventional chemical analysis methods cannot be used in a straightforward manner. In addition, sensory assessment of vinegars has numerous problems like inaccuracy or non-repeatability. In recent years, there are many applications of food discrimination using different E-noses which mimic the olfactory receptor in human nose, such as the quality assessment of Chinese spirits (Li et al., 2011), the quality prediction of peach (Zhang et al., 2012), instrumental testing of tea (Banerjee(Roy) et al., 2012), screening contamination in beef (Balasubramanian et al., 2012), fruit classification (Breijo et al., 2013). These applications show that the E-noses are still attractive in the field of food discrimination analysis. Moreover, Falcone et al. (2007) pointed out that volatile components could be used to distinguish high quality wine vinegars from defective or adulterate samples. So based on the above-mentioned practices, an E-nose was employed to classify three kinds of Chinese vinegars, which are favorite vinegars for consumers in Luoyang city of China and the details of three kinds of vinegars can be seen in Section 2. In our previous work (Yin et al., 2008), a kind of features based on wavelet packet analysis was used to discriminate the other three kinds of vinegars, but it is not competent for the classification of these vinegars in this investigation. In this investigation, the discrimination practice has been accomplished successfully by optimizing sensor array of the E-nose, and then a sensor array optimization method is put forward.

Due to the natural complexity and variability of vinegar composition as well as the cross-reactivity of the sensors in the array, the redundant information is yielded inevitably which affects greatly the identification performance. In order to reduce redundant information and to improve identification performance of the sensor array, it must be optimized. Therefore, choosing optimal sensor set is very important for the successful application of an E-nose. Theoretically, the optimal sensor array can be obtained by testing different sub-arrays, i.e. full factorial design (Alizadeh, 2010). The method is practicable when the amount of sensors is less, but with more sensors, the possible amount of sub-arrays and the computational complexity will increase distinctly. Sensor array can be optimized by testing degree of relevance or approximation between sensors (Zhang et al., 2008,2009), which is a conventional method. Recent years, genetic algorithm (GA) belongs to global optimization method, it is more and more employed to optimize sensor array (Xu and Lu 2011; Xu et al., 2010). But some disadvantages of this method were pointed out, such as parameters initialization and calculation time problems of GA (Alizadeh, 2010). In fact, the current sensor

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array optimization methods could get different optimized application-specific sensor arrays. For some reasons, we did not try aforementioned methods in our investigation. Petersson et al. (2009) presented an array optimization method by multivariate forward selection. Their investigation inspired us to think of a new idea for sensor array optimization, i.e. the optimizing process of sensor array is actually a process of selecting sensor and each sensor can be regarded as a variable, so this process of selecting sensor also is regarded as a process of selecting variable step by step from a mathematics viewpoint.

Gas sensors have a prominent characteristic that is the broad spectrum response characteristic to compounds, so these so-called variables are not independent. But the sensors' discriminant ability to vinegars is different because of their different sensitivity and selectivity. Therefore, some sensors can be sequentially selected by assessing their discriminant ability to vinegars based on a pivot elimination transform of Wilks Λ-statistic and consist of an ordered sensors set. The ordered sensors set is not a necessarily optimization array, but the optimization array can be easily obtained by further exploring the discrimination result of some sub-arrays which are composed by the first two, three, four and more sensors of the ordered set. This method is basically consistent with a viewpoint of multivariate discriminant analysis.

Therefore we think this is an effective and straightforward method for the selection of optimization sensor array. This study not only focused on how to select sensors using Wilks Λ-statistic but also on how to find an optimal sub-array by this method for the three kinds of Chinese vinegars classification.

2. Experimental

2.1. Materials

Three kinds of commercial Chinese vinegars were selected as discriminated objects, i.e. Zhenjiangxiangcu, Luoyangshiziguocu and Shanxilaochencu, and they were labeled as XC, GC and CC for convenient expression, respectively. Their fermentation methods are all solid fermentation. The sample label, type, raw materials, total acidity and production area are listed in Table 1.

2.2. Original gas sensor array

The original gas sensor array of the E-nose was composed of 13 TGS sensors made in Japan (Figaro Engineering Inc.). They were TGS-800, TGS-812, TGS-813, TGS-821, TGS-822, TGS-824, TGS-825, TGS-826, TGS-830, TGS-831, TGS-832, TGS-842 and TGS-880. The original array was placed in a stainless steel test chamber, the size of which was 2.0 l volume or so, 20.0 cm diameter and 7.0 cm height. In addition, in order to compensate the effects of temperature and humidity on the gas sensor responses, the test set also appended a humidity sensor and a temperature sensor. The humidity sensor and the temperature sensor are a integration subassembly made in China (AoSong Ltd.), its model number is DHT11, and the temperature measuring range is 0–50 °C, the humidity measuring range is 20–90% RH. So totally there are 15 sensors for the original gas sensor array of the test set.

A 16-channel and 12-bit high precision data acquisition system (DAS) was employed for the 13 TGS sensors, the humidity sensor and the temperature sensor. The DAS was made in China (Beijing Art Technology Development Co., Ltd.) and its model number was USB2008. Heater voltage of each gas sensor was 5 ± 0.05 V, the circuit voltage was 10 ± 0.01 V, and the circuit voltages of a humidity sensor and a temperature sensor were also 10 ± 0.01 V.

2.3. Measurement method

2.3.1. Sampling

Accurate quantity of samples is the foundation of analysis during the measurement. But the volatile of vinegar is compressible gas and has diffusion activity, so it is quite difficult for us to carry out sampling accurately. According to Yin et al. (2008), in order to carry out sampling accurately, we directly sampled fixed amounts of vinegar into the test chamber, and the amount of each testing sample was 5.0 ml. The sampling procedure was that: each sample was sampled with a pipette of 5.0 ml from sample bottle to an evaporating dish of 10.0 cm diameter, and then the evaporating dish was quickly put into the test chamber.

For each kind of vinegar, 35 samples were prepared, totaling 105 samples for the three kinds of vinegars. During the measurement of vinegar sample, the sample was selected in random sequences for every test so as to avoid chained analysis of samples.

2.3.2. Testing method and test results

The dynamic responses were selected as test signals. Moreover, in order to partially reduce the effect of white noise, one response result of each sensor was the mean of triplicate response values captured in rapid succession by DAS, and the interval between two neighboring response results was 1 s. Fig. 1 shows the response curve of TGS-813 to one sample GC. From the Fig. 1, the response results of each sensor in 1500 s can reflect basically its process of dynamic response. Thus the total number of response results of a sensor to one vinegar sample was 1500 (i.e. 1500 data). It took 1500 s for the 1500 data. In addition, it took 15 min or so to recuperate these sensors before every measurement of vinegar. The recuperation was carried out by cleaning the test chamber with clean air.

To reduce the effects of temperature and humidity on the gas sensor responses, two steps were adopted. Firstly, the response of each sensor to ambient air in our lab was tested before measurement to vinegar sample, giving a baseline value. Then, the baseline value was subtracted from the 1500 response data of each sensor to one sample, and 1500 difference values were obtained. The one difference value was called as one test result of each sensor to one sample. This treatment method is named "baseline-removing pretreatment". Secondly, the response values of temperature and humidity of ambient air to one sample were simultaneously measured so as to further compensate their effects, i.e. the test results of gas sensor array, humidity sensor and temperature sensor were considered as input data of pattern recognition system in the

Table 1
The details of three kinds of vinegar samples utilized in the experiment.

Sample label	Type	Raw materials	Total acidity (g/100 ml)	Production area
CC	Mature vinegar	Water, broomcorn, barley, pea, wheat bran, sodium benzoate	5.0	Shanxi province
XC	Aromatic vinegar	Water, rice, wheat bran, sugar, salt, yeast for making hard liquor, polished glutinous rice	5.5	Jiangsu province
GC	Fruit vinegar	Spring water, persimmon, wheat mouldy bran, sodium benzoate	3.5	Henan province