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Intelligent sensing sensory quality of Chinese rice wine using near infrared spectroscopy and nonlinear tools

Qin Ouyang [a,b], Quansheng Chen [a,b,*], Jiewen Zhao [b]

[a] Institute of Agricultural Engineering, Jiangsu University, Zhenjiang 212013, PR China
[b] School of Food and Biological Engineering, Jiangsu University, Zhenjiang 212013, PR China

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ABSTRACT

The approach presented herein reports the application of near infrared (NIR) spectroscopy, in contrast with human sensory panel, as a tool for estimating Chinese rice wine quality; concretely, to achieve the prediction of the overall sensory scores assigned by the trained sensory panel. Back propagation artificial neural network (BPANN) combined with adaptive boosting (AdaBoost) algorithm, namely BP-AdaBoost, as a novel nonlinear algorithm, was proposed in modeling. First, the optimal spectra intervals were selected by synergy interval partial least square (Si-PLS). Then, BP-AdaBoost model based on the optimal spectra intervals was established, called Si-BP-AdaBoost model. These models were optimized by cross validation, and the performance of each final model was evaluated according to correlation coefficient (R_p) and root mean square error of prediction (*RMSEP*) in prediction set. Si-BP-AdaBoost showed excellent performance in comparison with other models. The best Si-BP-AdaBoost model was achieved with $R_p = 0.9180$ and $RMSEP = 2.23$ in the prediction set. It was concluded that NIR spectroscopy combined with Si-BP-AdaBoost was an appropriate method for the prediction of the sensory quality in Chinese rice wine.

1. Introduction

Chinese rice wine, also known as yellow wine, is a traditional fermented alcoholic beverage brewed directly from glutinous rice and wheat *Qu*. It is one of the three ancient alcoholic beverages in the world [1]. Except for physical and chemical indicators, sensory attributes are the other important factors for assessment of Chinese rice wine quality. The sensory quality plays a major role in product acceptability by directly influencing the success of a product in the marketplace [2]. Its sensory quality is generally estimated by human sensory analysis that employs the human senses to provide information about color, aroma, taste and style, as well as the overall quality and acceptance of Chinese rice wine. However, there are some disadvantages of human sensory analysis, such as the high cost of training the panel, the reproducibility of the evaluation, the standardization of the measurements, and the low comparability between panels, which makes it unattractive for routine analysis [3]. Therefore, it is crucial to seek faster and directly applicable methods following the necessity of real-time monitoring sensory quality in the Chinese rice wine industry.

Near infrared spectroscopy (NIR), as an instrumental measurement technique, has been proven to be fast, objectively and routinely applicable alternatives for qualitative and/or quantitative determination of food quality. Although most NIR studies deal with determining chemical composition or physical properties [4], a growing number of papers report the use of NIR to evaluate sensory attributes [5]. There are several reports in the literature demonstrating the potential of NIR in predicting the sensory attributes of food, such as, tea [6], virgin olive oil [7], grapes [8] and beans [9]. In Chinese rice wine, NIR spectroscopy was mainly applied by researchers to predict chemical composition or physical properties [10–14]. While, the prediction of sensory attributes of Chinese rice wine using NIR spectroscopy technique remains scarce.

In model calibration, it is of great significance to select appropriate algorithms for establishing the relationship between NIR spectra data and sensory quality of Chinese rice wine, to acquire robust models with good performance. Synergy interval partial least squares (Si-PLS), as an efficient spectra variables selection method, has been widely-applied and has shown its potential for modeling with good precision [15,16]. On the other hand, sensory scores from experts, which is a comprehensive understanding about the Chinese rice wine, influenced by the interaction among senses (sight, smell and taste, etc) [17]. In consequence, the relationship between the NIR spectra and the sensory scores maybe complicated, which is inclined to be nonlinear rather than linear. Linear methods may not completely present the relationship between the NIR spectra and the sensory scores. Back propagation artificial neural network (BPANN) combined with adaptive boosting (AdaBoost) algorithm, namely BP-AdaBoost, as a novel nonlinear algorithm, which is recently proposed and applied in modeling, has shown good capability [18].

* Corresponding author at: Institute of Agricultural Engineering, Jiangsu University, Zhenjiang 212013, PR China.
E-mail address: qschen@ujs.edu.cn (Q. Chen).

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In this sense, the main goal of this work is to demonstrate the capability of NIR spectroscopy technique to mimic the human sensory perception and provide an analytical tool for sensory assessment of Chinese rice wine. In model calibration, first, Si-PLS was used to select the optimal spectra intervals; then, BP-AdaBoost was employed to build calibration model based on the optimal spectra intervals for predicting the sensory quality, and this model was called Si-BP-AdaBoost.

2. Materials and methods

2.1. Samples collection

Totally, 75 samples from different bottles of Chinese rice wine were provided by "Danyang" brand, Jiangsu province Danyang winery Co., ranged from 9 to 14%/V V^{-1}. Danyang rice wine is well-known in China which is made from high-quality glutinous rice and wheat. These samples covered all types of semi-sweet products in this winery. The same product included two or three samples but from different manufacturing dates.

2.2. Reference sensory analysis

The reference sensory analysis of Chinese rice wine samples was performed by human panel test, which was conducted in the Sensory Laboratory at Jiangsu Danyang winery at a controlled room temperature (25 °C). The sensory panel consisted of four trained panelists. All of them were professional and with decades of experience in evaluating the Chinese rice wine. The human sensory analysis about the samples was in accordance with the relevant occupation standard and enterprise standard. The full sensory scores for the color, aroma, taste and style sensory attributes according to their respective impact factors were 10, 25, 50 and 15, respectively. The score of each sensory attribute for one sample will be obtained by subtracting the corresponding scores about the undesirable sensory quality from the respective full sensory scores, more details can refer to the reference [19]. The overall score summed from the scores of the four sensory attributes was taken for the further analysis, where a higher score meant better sensory characteristics. Overall, 17 sessions were scheduled throughout the experiment in order to avoid a saturation effect in tasters. In each session, four or five Chinese rice wine samples were randomly presented to the panelists. The mouths were rinsed with mineral water between samples. After sensory analysis, the samples were kept in sealed containers in the refrigerator at 4 °C before next analysis. Pearson correlation analysis using SPSS 14.0 for Windows (SPSS Inc.) was utilized to test the validity and uniformity of the sensory scores from the four experts.

2.3. Spectra collection

The NIR spectra of Chinese rice wine samples were acquired using the Antaris II Near-infrared spectrophotometer (Thermo Electron Co., USA) with a transmittance module. The samples were measured in a quartz cuvette with 5 mm optical path length that is a standard accessory from this spectrophotometer. The cuvette was first washed by distilled water when each sample was finished, then rinsed by the sample for measurement at least three times before spectra collection. Each spectrum was the average of 16 scanning spectra. The range of spectra was from 4000 to 10,000 cm^{-1} in every 3.856 cm^{-1} resolution, which resulted in 1557 variables. The spectra data were collected as absorbance values [log(1/T)], where T = transmittance. Result Software (Antaris II System, Thermo Electron Co., USA) was used in NIR spectra data acquisition. The room temperature was kept at around 25 °C to avoid the influence of the outer environmental condition on the spectrophotometer. Each sample was measured in triplicate, and the results were averaged to generate a single spectrum for each sample used for the subsequent analysis.

2.4. Spectral data preprocessing methods

Raw spectra acquired from NIR spectrometer contained background information and noises besides sample information. The spectra should be preprocessed before the model calibration, in order to achieve a reliable, accurate and stable model. In this work, mean centering (MC) was applied to process the raw spectra, subtracting the average from each variable that ensures all results will be interpretable in terms of variation around the mean [20].

2.5. Multivariate analysis

In model calibration for predicting sensory attribute, all the samples were divided into two subsets, namely, calibration set and prediction set. Samples in the calibration set were used to establish the model; while samples in the prediction set were applied to test the robustness of the established model. To avoid bias in subset division, this division was made as follows: all samples were sorted according to their respective y-values (viz. the reference overall sensory scores). One spectrum from every three samples was selected into the prediction set. Thus, the calibration set contained 50 samples, the prediction set 25 samples.

First, synergy interval partial least squares (Si-PLS) was used to select the optimal variables from the whole spectrum and develop models for predicting the sensory quality of Chinese rice wine. Then, BP-AdaBoost model was established based on the optimal spectra variables selected by Si-PLS. The correlation coefficient (R_c) and the root mean square error of calibration (*RMSEC*) of the calibration set and the correlation coefficient (R_p) and the root mean square error (*RMSEP*) of the prediction set were used to evaluate models. Generally, good models should have higher R_c and R_p values and lower *RMSEC* and *RMSEP* values. In addition, the difference between R_c and R_p or between *RMSEC* and *RMSEP* should be small. A minor difference between *RMSEC* and *RMSEP* indicates that the robustness of the models is satisfactory [21]. All data processing and analysis were conducted in Matlab Version 7.10.0 (MathWorks, Natick, USA) using Microsoft Windows 7.

3. Results and discussions

3.1. Reference sensory analysis result

Pearson correlation analysis was used to test the validity and uniformity of the sensory scores from the four experts. The results in Table 1 indicated that the reference overall sensory scores among the four different experts and their average had significant correlation. So, the scores that were averaged from the four experts were used as the final sensory score for one sample, and used for the further analysis. Table 2 shows the reference overall sensory scores for all the samples

Table 1
Pearson correlations of reference overall sensory scores among the four experts and their average.[a, b, c, d, e]

	P1[a]	P2[b]	P3[c]	P4[d]	Average[e]
P1	1	.856**	.800**	.821**	.916**
P2		1	.885**	.857**	.960**
P3			1	.888**	.949**
P4				1	.944**
Average					1

[a] P1: The score of the first expert.
[b] P2: The score of the second expert.
[c] P3: The score of the third expert.
[d] P4: The score of the fourth expert.
[e] Average: The mean score of the four experts.
** Correlation is significant at the 0.01 level (2-tailed).