



Classification of non-alcoholic beer based on aftertaste sensory evaluation by chemometric tools

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ABSTRACT

Sensory evaluation is the application of knowledge and skills derived from several different scientific and technical disciplines, physiology, chemistry, mathematics and statistics, human behavior, and knowledge about product preparation practices. This research was aimed to evaluate aftertaste sensory attributes of commercial non-alcoholic beer brands (P1, P2, P3, P4, P5, P6, P7) by several chemometric tools. These attributes were bitter, sour, sweet, fruity, liquorice, artificial, body, intensity and duration. The results showed that the data are in a good consistency. Therefore, the brands were statistically classified in several categories. Linear techniques as Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA) were performed over the data that revealed all types of beer are well separated except a partial overlapping between zones corresponding to P4, P6 and P7. In this research, for the confirmation of the groups observed in PCA and in order to calculate the errors in calibration and in validation, PLS-DA technique was used. Based on the quantitative data of PLS-DA, the classification accuracy values were ranked within 49–86%. Moreover, it was found that the classification accuracy of LDA was much better than PCA. It shows that this trained sensory panel can discriminate among the samples except an overlapping between two types of beer. Also, two types of artificial networks were used: Probabilistic Neural Networks (PNN) with Radial Basis Functions (RBF) and FeedForward Networks with Back Propagation (BP) learning method. The highest classification success rate (correct predicted number over total number of measurements) of about 97% was obtained for RBF followed by 94% for BP. The results obtained in this study could be used as a reference for electronic nose and electronic tongue in beer quality control.

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1. Introduction

The evaluation is a process that analyzes elements to achieve different objectives such as quality inspection, design, marketing exploitation and other fields in industrial companies. In many of these fields the items, products, designs, etc., are evaluated according to the knowledge acquired via human senses (sight, taste, touch, smell and hearing), in such cases, the process is called *sensory evaluation*. In this type of evaluation process, an important problem arises as it is the modeling and management of uncertain knowledge, because the information acquired by our senses

throughout human perceptions involves uncertainty, vagueness and imprecision. Sensory evaluation is a scientific discipline used to evoke measure, analyze and interpret reactions to those characteristics of foods and materials as they are perceived by the senses of sight, smell, taste, touch and hearing. This definition represents an obvious attempt to be as inclusive as is possible within the framework of food evaluation.

As the definition implies, sensory evaluation involves the measurement and evaluation of the sensory properties of foods and other materials. Sensory evaluation also involves the analysis and the interpretation of the responses by the sensory professional; that is, that individual who provides the connection between the internal world of technology and product development and the external world of the marketplace, within the constraints of a product marketing brief. This connection is essential such that the processing and development specialists can anticipate the impact of product changes in the marketplace (Haseleu, Intelmann, &

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Hofmann, 2009; Yin & Ding, 2009). Similarly, the marketing and brand specialists must be confident that the sensory properties are consistent with the intended target and with the communication delivered to that market through advertising. They also must be confident that there are no sensory deficiencies that lead to a market failure.

Although the brewing of beer has a history extending back some 800 decades, it is only in the past 150 years that the underlying science has been substantially unraveled (Bamforth, 2000). Brewing and aging of beer are complex processes during which several parameters have to be controlled to ensure a reproducible quality of the finished product (Rudnitskaya et al., 2009; Arrieta, Rodriguez-Mendez, de Saja, Blanco, & Nimubona, 2010). These include chemical parameters that are measured instrumentally and taste and aroma properties that are evaluated by the sensory panels. Sensory quality and its measurement are complex issues which have received a large amount of attention in the sensory literature.

Brands of non-alcoholic beer are presently being marketed and sold. It is typical that a non-alcoholic beer has a restricted final alcohol by volume content lower than 0.5% (Porretta & Donadini, 2008). Non-alcoholic beers can offer several opportunities that can be exploited by marketers. This is true especially in a context where more strict regulations are likely to ban or restrict alcoholic products from classical usage situations. This is the case of wherein administrators are enforcing a renewed battle against alcohol misuse and abuse. A list of positivities for a beer with a zero alcohol level is summarized as follows: (a) no restriction for sale by hours and by places of consumption; (b) no warning on labels for sensitive consumer subgroups such as pregnant women; (c) health benefits of beer can be promoted; (d) no social judgment in the case of heavy drinking out of the home; (e) no excise duty or a reduced one is charged (Porretta & Donadini, 2008).

The consumer's perception of non-alcoholic beer quality is usually based on a reaction to a complex mix of expectations, which are associated with the effects of some sensory attributes such as color, foam, flavor and aroma, mouthfeel and aftertaste. Many of these perceptions are outside the control of the brewer, but for those factors directly influenced by the brewing and packaging processes, the control of beer flavor and aroma are the most significant. Whilst the various analytical and microbiological methods referred to earlier provide fairly objective tools for identification and quantification, the very nature of the differing responses by the senses to different flavors and aromas makes this identification and quantification difficult. Despite this fundamental limitation, brewers and flavor analysts have developed robust procedures that enable sensory analysis to be a valuable tool in the monitoring and control of beer quality.

One of the most important sensory attributes in beer to consumers is known *Aftertaste* attributes. Although there are some researches on alcoholic beer sensory evaluation in the literature (Daems & Delvaux, 1997; Langstaff, Guinard, & Lewis, 1991; Mejlholm & Martens, 2006), but there is not any work on aftertaste sensory evaluation of non-alcoholic beer. So, the current research focuses on the sensory evaluation of aftertaste attributes of commercial non-alcoholic beer brands.

2. Materials and methods

2.1. Samples

One-hundred and fifty samples of commercial non-alcoholic beers of different types were provided. Samples from different production batches which were brewed within intervals of 1–2 months were available for the seven brands. Samples were kept in dark bottles of 500 mL, which were stored in a dry dark cool

room (1 °C) before the experiments. Each bottle was opened prior to the measurements and used the same day.

2.2. Panel of judges

A panel of seven judges consisting of students and staff were selected on the basis of interest and availability. All persons had previous experience on sensory-analysis panels. All the meetings were made in the English language (the panelists speak English fluently). The training of the panel took place in six sessions of 1 h each. During these sessions, the panel trained on all the non-alcoholic beer of the study.

2.3. Experimental design and procedure

The judges assessed the 150 commercial beers in duplicate in three sessions over a 3-week period. In each session, from four to six beers were randomly presented to the panelists. The testing sessions took place in a room at a controlled temperature (25 °C). Beer was cooled down to 10 °C and served in dark glasses (Rudnitskaya et al., 2009). Selection of a scale for use in a particular test is one of the several tasks that need to be completed by the sensory professional before a test can be organized. Determining test objective, subject qualifications, and product characteristics will have an impact on it and should precede method and scale selection. Nominal scale was considered for this research. In such scales, numbers are used to label, code, or otherwise classify items or responses. The only property assigned to these numbers is that of non-equality; that is, the responses or items placed in one class cannot be placed in another class. Letters or other symbols could be used in place of numbers without any loss of information or alteration of permissible mathematical manipulation. In sensory evaluation, numbers are frequently used as labels and as classification categories; for example, the three-digit numerical codes are used to keep track of products while masking their true identity. It is important that the product identified by a specific code not be mislabeled or grouped with a different product. It is also important that the many individual servings of a specific product exhibit a reasonable level of consistency if the code is used to represent a group of servings from a single experimental treatment.

The beer samples were coded and served in a random manner. Panel members scored the beer samples for aftertaste attributes by marking on a 9 cm line, where 0 to 9 represented poor to excellent. These attributes consisted of bitter, sour, sweet, fruity, liquorice, artificial, body, intensity and duration. For eliminating fatigue and carrying over effects of beer taste, the judges applied water to rinse the mouth and ate a piece of bread between subsequent samples (Rudnitskaya et al., 2009).

2.4. Data analysis

In this study, for analyzing the results obtained, several chemometric tools were addressed. The use of chemometrics implies the use of multivariate data analysis that is based on the fact that complex systems need multiple parameters to be described and thus more information about the analyzed system can be retrieved by using a multivariate approach. One of the drivers for the use of chemometrics is the potential of simple objective measurements coupled with multivariate data analysis methods to replace expensive sensory information. A critical question that should be addressed is to what extent an analytical method coupled with soft modeling can ever give results that agree with sensory studies. There is a tendency for studies to offer optimistic views of the ultimate use of a particular method. Description and explanation of the chemometric tools used are presented at the following text. Matlab v7.6 (The Mathworks

Inc., Natick, MA, USA) and The Unscrambler 9.2 (Camo, Norway) and SPSS 13 were the softwares used for data analysis in this study.

Intensity scores (average scores of seven panelists and three replicates) for each nine attributes was calculated from the sensory sheets for each of the beer samples. Statistical analysis was done applying the analysis of variance (ANOVA). The *F* test was used to determine significant effects of beer brands and assessors, and the Duncan's multiple ranges test was used to separate means at a 5% level of significance.

Based on this statistical analysis, the seven non-alcoholic beer brands were ranked in point of view of each attribute and the categories for each attribute were developed. The polar plots for each panelist and each brand showing aftertaste attributes mapping were prepared as well.

There are many possible techniques for classification of data. Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA) are two commonly used techniques for dimensionality reduction of data and allow plotting the measurements in a graph in order to see the discrimination capability of the sensory panel. Linear Discriminant Analysis easily handles the case where the within-class frequencies are unequal and their performances have been examined on randomly generated test data. This method maximizes the ratio of between-class variance to the within-class variance in any particular data. The use of Linear Discriminant Analysis for data classification is applied to classification problem in food recognition (Ghasemi-Varnamkhasti, Mohtasebi, Siadat, Ahmadi, et al., 2011).

In this study, Principal Components Analysis (PCA) is used as a data reduction methodology. The objective of PCA is to reduce the dimensionality (number of variables) of the dataset while retaining most of the original variability (information) in the data. This is performed through the construction of a set of principal components which act as a new reduced set of variables. Each principal component is a linear combination of the original variables and they are all orthogonal to each other. For a given data set with *N* variables, the first principal component has the highest explanatory power (it describes as much of variability of the data as possible), whereas the *N*th principal component has the least explanatory power. Thus, the *n* first principal components are supposed to contain most of the information implicit in the attributes.

For the confirmation of the groups observed in Principal Components Analysis and in order to calculate the errors in calibration and in validation, PLS-DA technique was used. This technique is a frequently used classification method and is based on the PLS approach (Barker & Rayens, 2003). The basics of PLS-DA consist firstly in the application of a PLS regression model on variables which are indicators of the groups. The link between this regression and other discriminant methods such as LDA has been shown. The second step of PLS-DA is to classify observations from the results of PLS regression on indicator variables. The more common used method is simply to classify the observations in the group giving the largest predicted indicator variable.

By the way, the mean ratings of the seven beer brands for nine attributes rated were then analyzed by Principal Component Analysis (PCA). PCA results are confirmed with a more powerful pattern recognition method. Then, the results were confirmed with the prediction made with Probabilistic Neural Networks (PNN) with radial basis activation function. Also, confusion matrix obtained in validation and the success rates were included.

We decided to implement an algorithm for LDA in hopes of providing better classification compared to Principal Components Analysis. The prime difference between LDA and PCA is that PCA does more of feature classification and LDA does data classification. In PCA, the shape and location of the original data sets changes when transformed to a different space whereas LDA

does not change the location but only tries to provide more class separability and draw a decision region between the given classes. This method also helps to better understand the distribution of the feature data.

LDA results are confirmed with the prediction made with Radial Basis Function (RBF) and Back Propagation networks (BP). Also, confusion matrices obtained in validation and the success rates were included.

2.5. Probabilistic Neural Networks (PNN)

Probabilistic Neural Networks possess the simplicity, speed and transparency of traditional statistical classification/prediction models along with much of the computational power and flexibility of back propagated neural networks (Dutta, Prakash, & Kaushik, 2010; Hsieh & Chen, 2009; Specht, 1990). A PNN can be realized as a network of four layers (Fig. 1).

The input layer includes *N* nodes, each corresponding to one input attribute (independent variable). The inputs of the network are fully connected with the *M* nodes of the pattern layer. Each node of the pattern layer corresponds to one training object. The $1 \times N$ input vector x_i is processed by pattern node *j* through an activation function that produces the output of the pattern node. The most usual form of the activation function is the exponential one:

$$o_{ij} = \exp\left(-\frac{\|x_j - x_i\|^2}{\sigma^2}\right)$$

where σ is a smoothing parameter. The result of this activation function ranges between 0 and 1. As the distance $\|x_j - x_i\|$ between the input vector x_i and the vector x_j of the pattern node *j* increases, the output of node *j* will approach zero, thus designating the small similarity between the two data vectors. On the other hand, as the distance $\|x_j - x_i\|$ decreases, the output of node *j* will approach unity, thus designating the significant similarity between the two data vectors. If x_i is identical to x_j , then the output of the pattern node *j* will be exactly one. The parameter σ controls the width of the activation function. As σ approaches zero, even small differences between x_i is identical to x_j will lead to $o_{ij} \approx 0$, whereas larger values of σ produce more smooth results.

The outputs of the pattern nodes are passed to the summation layer that consists of *K* competitive nodes each corresponding to one class. Each summation node *k* is connected to the pattern nodes that involve training objects that belong to class *k*. For an input vector x_i , the summation node *k* simply takes the outputs of the pattern nodes to which it is connected with to produce an output $f_k(x_i)$ as follows:

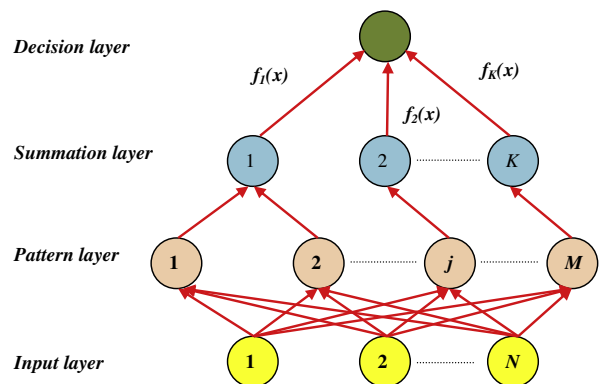


Fig. 1. Architecture of a Probabilistic Neural Network.

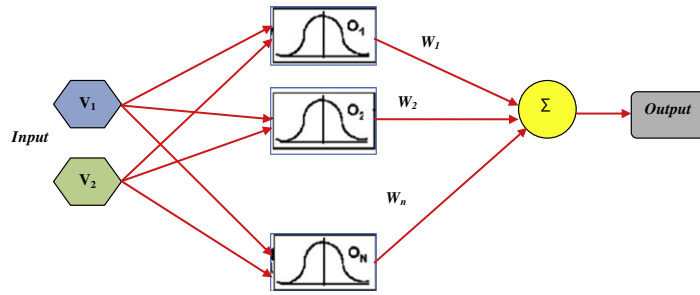


Fig. 2. Architecture of a Radial Basis Function network.

$$f_k(x_i) = \frac{1}{M_k} \sum_{\forall x_j, y_k} o_{ij}$$

where y_k is the class label corresponding to the summation node k and M_k is the number of training objects that belong to this class. Assuming that all data vectors are normalized to unit length (i.e., $\|x\| = 1$), $f_k(x_i)$ can equivalently be written as:

$$f_k(x_i) = \frac{1}{M_k} \sum_{\forall x_j, y_k} \exp\left(\frac{x_j x_i^T - 1}{\sigma^2}\right)$$

and the outputs of the summation nodes can be easily transformed to posterior class membership probabilities:

$$P(y_i = k|x_i) = \frac{f_k(x_i)}{\sum_{k=1}^K f_k(x_i)}$$

On the basis of these probabilities, a classification rule is employed at the decision layer, which consists of a single node, to assign the input vector x_i to a particular class. The obvious approach is to assign x_i to the class where it is most likely to belong (i.e., the class with the maximum $P(k|x_i)$). In a two class case with $y = \{0, 1\}$ it is possible to define a cut-off probability point c , such that x_i is assigned to class 0 if and only if $P(y_i = 0|x_i) \geq c$. The specification of this cut-off point is based on the prior probabilities of class membership and the misclassification costs.

2.6. Radial Basis Function (RBF)

A Radial Basis Function network is a neural network approached by viewing the design as a curve-fitting (approximation) problem in a high dimensional space. Learning is equivalent to finding a multidimensional function that provides a best fit to the training data, with the criterion for “best fit”

being measured in some statistical sense. Correspondingly, regularization is equivalent to the use of this multidimensional surface to interpolate the test data. This viewpoint is the real motivation behind the RBF method in the sense that it draws upon research work on traditional strict interpolations in a multidimensional space. In a neural network, the hidden units form a set of “functions” that compose a random “basis” for the input patterns (vectors). These functions are called *Radial Basis Functions*. Different types of Radial Basis Functions could be used, but the most common is the Gaussian function (Riverol-Canizares & Pilipovik, 2010; Tudu et al., 2009; Vrankar, Kansa, Ling, Runovc, & Turk, 2010).

RBF networks have three layers: Input layer – There is one neuron in the input layer for each predictor variable. In the case of categorical variables, $N - 1$ neurons are used where N is the number of categories. The input neurons (or processing before the input layer) standardize the range of the values by subtracting the median and dividing by the interquartile range. The input neurons then feed the values to each of the neurons in the hidden layer. Hidden layer – This layer has a variable number of neurons (the optimal number is determined by the training process). Each neuron consists of a Radial Basis Function centered on a point with as many dimensions as there are predictor variables. The spread (radius) of the RBF function may be different for each dimension. The centers and spreads are determined by the training process. When presented with the x vector of input values from the input layer, a hidden neuron computes the Euclidean distance of the test case from the neuron’s center point and then applies the RBF kernel function to this distance using the spread values. The resulting value is passed to the summation layer. Summation layer – The value coming out of a neuron in the hidden layer is multiplied by a weight associated with the neuron (W_1, W_2, \dots, W_n), as shown in Fig. 2, and passed

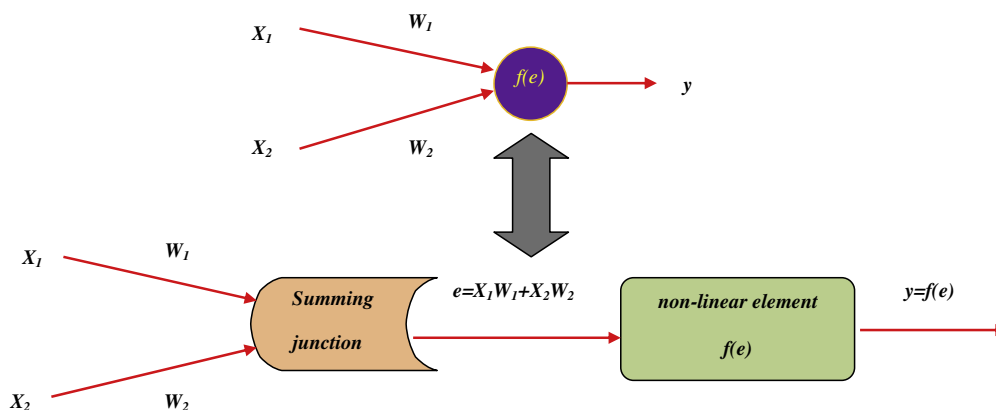


Fig. 3. Architecture of Back Propagation.

Table 1
Statistics on aftertaste attributes of non-alcoholic beer.

Attribute	Non-alcoholic beer brand							Mean	Standard deviation [*]
	P1	P2	P3	P4	P5	P6	P7		
Bitter	2 (0.272)**	2.04 (0.23)	1.33 (0.384)	1.43 (0.417)	4.05 (0.448)	1.95 (0.23)	1.19 (0.262)	2	0.968
Sour	0.19 (0.262)	0.09 (0.162)	0.67 (0.272)	0.09 (0.162)	0 (0)	0.23 (0.37)	0.33 (0.33)	0.23	0.22
Sweet	0.95 (0.23)	0.19 (0.262)	0.23 (0.418)	1.9 (0.37)	1.14 (0.179)	0.14 (0.179)	0.24 (0.371)	0.69	0.671
Fruity	0.95 (0.3)	0.28 (0.355)	0.86 (0.178)	0 (0)	0.95 (0.126)	0.09 (0.162)	2.09(0.252)	0.75	0.72
Liquorice	0.62 (0.23)	0.09 (0.163)	0.14 (0.262)	0.09 (0.163)	0.05 (0.126)	0.19 (0.262)	0.14 (0.178)	0.19	0.194
Body	4.76 (0.252)	1.43 (0.317)	4.05 (0.3)	4.14 (0.325)	5.24 (0.371)	2.28 (0.23)	4.09 (0.499)	3.71	1.362
Artificial	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0.28 (0.3)	0.24 (0.252)	0.07	0.128
Duration	5.81 (0.262)	5.19 (0.378)	4.05 (0.126)	2 (0.192)	3.90 (0.163)	1.95 (0.126)	1.71 (0.356)	3.52	1.658
Intensity	5.86 (0.325)	5.05 (0.23)	4.05 (0.405)	1.86 (0.262)	3.95 (0.356)	2 (0.192)	2.05 (0.405)	3.54	1.607

* Standard deviation was the square root of the error variance of ANOVA.

** The numbers in parenthesis are standard deviation.

to the summation which adds up the weighted values and presents this sum as the output of the network. Not shown in this figure, it is a bias value of 1.0 that is multiplied by a weight W_0 and fed into the summation layer. For classification problems, there is one output (and a separate set of weights and summation unit) for each target category. The value output for a category is the probability that the case being evaluated has that category. These parameters are determined by the training process: The number of neurons in the hidden layer, the coordinates of the center of each hidden-layer RBF function, the radius (spread) of each RBF function in each dimension and the weights applied to the RBF function outputs as they are passed to the summation layer (Pretty, Vega, Ochando, & Tabares, 2010).

2.7. Back Propagation (BP)

Since the real uniqueness or ‘intelligence’ of the network exists in the values of the weights between neurons, we need a method of adjusting the weights to solve a particular problem. For this type of network, the most common learning algorithm is called Back Propagation (BP). As shown in Fig 3, the multiplayer perceptron (MLP) model using the Back Propagation (BP) algorithm is one of the well-known neural network classifiers which consist of sets of nodes arranged in multiple layers with connections only between nodes in the adjacent layers by weights. The layer where the inputs information is presented is known as the input layer. The layer where the processed information is retrieved is called the output layer. All layers between the input and output layers are known hidden layers. For all nodes in the network, except the input layer nodes, the total input of each node is the sum of weighted outputs of the nodes in the previous layer. Each node is activated with the input to the node and the activation function of the node (Chen, Chen, & Kuo, 2010).

The input and output of the node i (except for the input layer) in a MLP mode, according to the BP algorithm, is:

$$\text{Input : } X_i = \sum W_{ij}O_j + b_i \tag{1}$$

$$\text{Output : } O_i = f(X_i) \tag{2}$$

where W_{ij} : the weight of the connection from node i to node j , B_i : the numerical value called bias, F : the activation function.

The sum in Eq. (1) is over all nodes j in the previous layer. The output function is a non-linear function which allows a network to solve problems that a linear network cannot solve. In this study the Sigmoid function given in Eq. (3) is used to determine the output state.

$$F(X_i) = 1/(1 + \exp(-X_i)) \tag{3}$$

Back Propagation (BP) learning algorithm is designed to reduce an error between the actual output and the desired output of the

network in a gradient descent manner. The summed squared error (SSE) is defined as:

$$SSE = 1/2 \left(\sum_{pi} \sum O_{pi} - T_{pi} \right)^2 \tag{4}$$

where p index the all training patterns and i indexes the output nodes of the network. O_{pi} and T_{pi} denote the actual output and the desired output of node, respectively when the input vector p is applied to the network.

A set of representative input and output patterns is selected to train the network. The connection weight W_{ij} is adjusted when each input pattern is presented. All the patterns are repeatedly presented to the network until the SSE function is minimized and the network “learns” the input patterns (Zhu et al., 2010). An application of the gradient descent method yields the following iterative weight update rule:

$$\Delta W_{ij}(n + 1) = \eta(\delta_i O_i + \alpha \Delta W_{ij}(n)) \tag{5}$$

where Δ : the learning factor, α : the momentum factor, δ_i : the node error, for output node i is then given as

Table 2
Variance analysis of the interaction effects of assessor, non-alcoholic beer brands on bitterness sensory evaluation.

Source of variations	Degree of freedom	Sum of square	Mean square	F
Assessor	6	6.09	1.01	3.11 ^b
Beer brand	6	118.09	19.68	60.27 ^a
Assessor × beer brand	36	7.80	0.21	0.66 ^b
Error	98	32	0.33	–

^a Corresponding to confident of interval 95%.

^b Corresponding to no marked difference.

Table 3
Classification of non-alcoholic beer brands based on Duncan’s multiple range test.

Attributes	Categories (class) [*]					
	A	B	C	D	E	F
Bitter	P5	P1, P2, P6	P3, P4	P7		
Sour	P3	P7	P6	P1	P2, P4	P5
Sweet	P4	P5	P1	P3, P7	P2	P6
Fruity	P7	P1, P3, P5	P2	P6	P4	
Liquorice	P1	P6	P3, P7	P2, P4	P5	
Body	P1, P5	P3, P4, P7	P2, P6			
Artificial	P6	P7	P1, P2, P3, P4, P5			
Duration	P1	P2	P3, P5	P4, P6	P7	
Intensity	P1	P2	P3, P5	P4, P6, P7		

* The classes are in descending order, i.e. Classes A and F have the greatest and the lowest values of an attribute, respectively.

$$\delta_i = (t_i - O_i)O_i(1 - O_i) \tag{6}$$

The node error at an arbitrary hidden node is

$$\delta_i = O_i(1 - O_i) \sum_k \delta_k W_{ki}$$

Each neuron is composed of two units. First unit adds products of weights coefficients and input signals. The second unit realizes non-linear function, called neuron activation function. Signal e is adder output signal, and $y = f(e)$ is output signal of non-linear element. Signal y is also output signal of neuron.

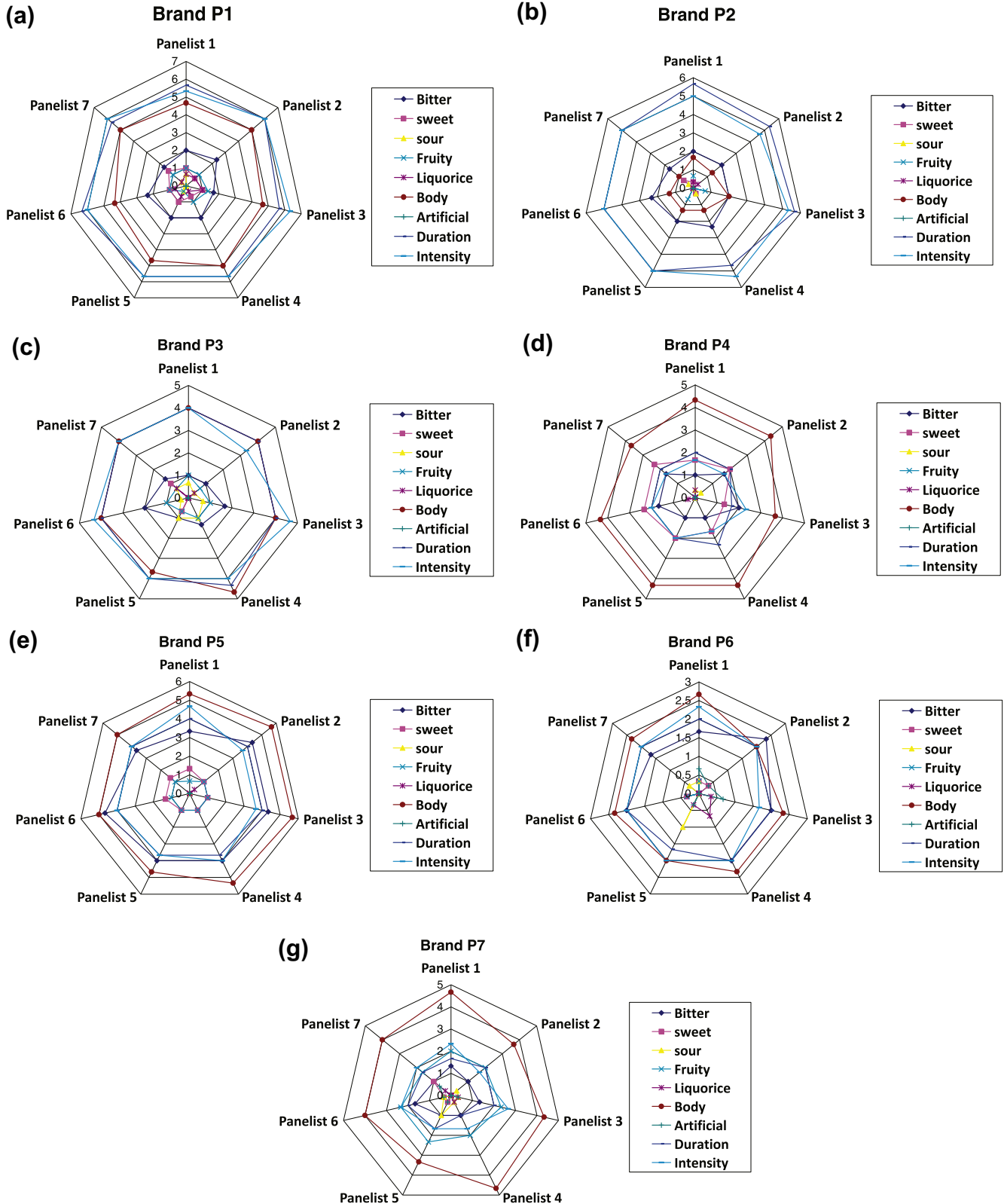


Fig. 4. Polar plots of the panelists response to aftertaste attributes of seven non-alcoholic beer brands: (a) brand P1, (b) brand P2, (c) brand P3, (d) brand P4, (e) brand P5, (f) brand P6, (g) brand P7.

3. Results and discussions

3.1. Statistical analysis

Results from the ANOVA showed significant differences ($p < 0.05$) between the seven beer brands (P1, P2, P3, P4, P5, P6,

P7) for all sensory attributes. Statistics on non-alcoholic beer attributes are given in Table 1.

No important interactions between panelists and samples were observed. For example, about bitter attribute analysis of variance is shown in Table 2.

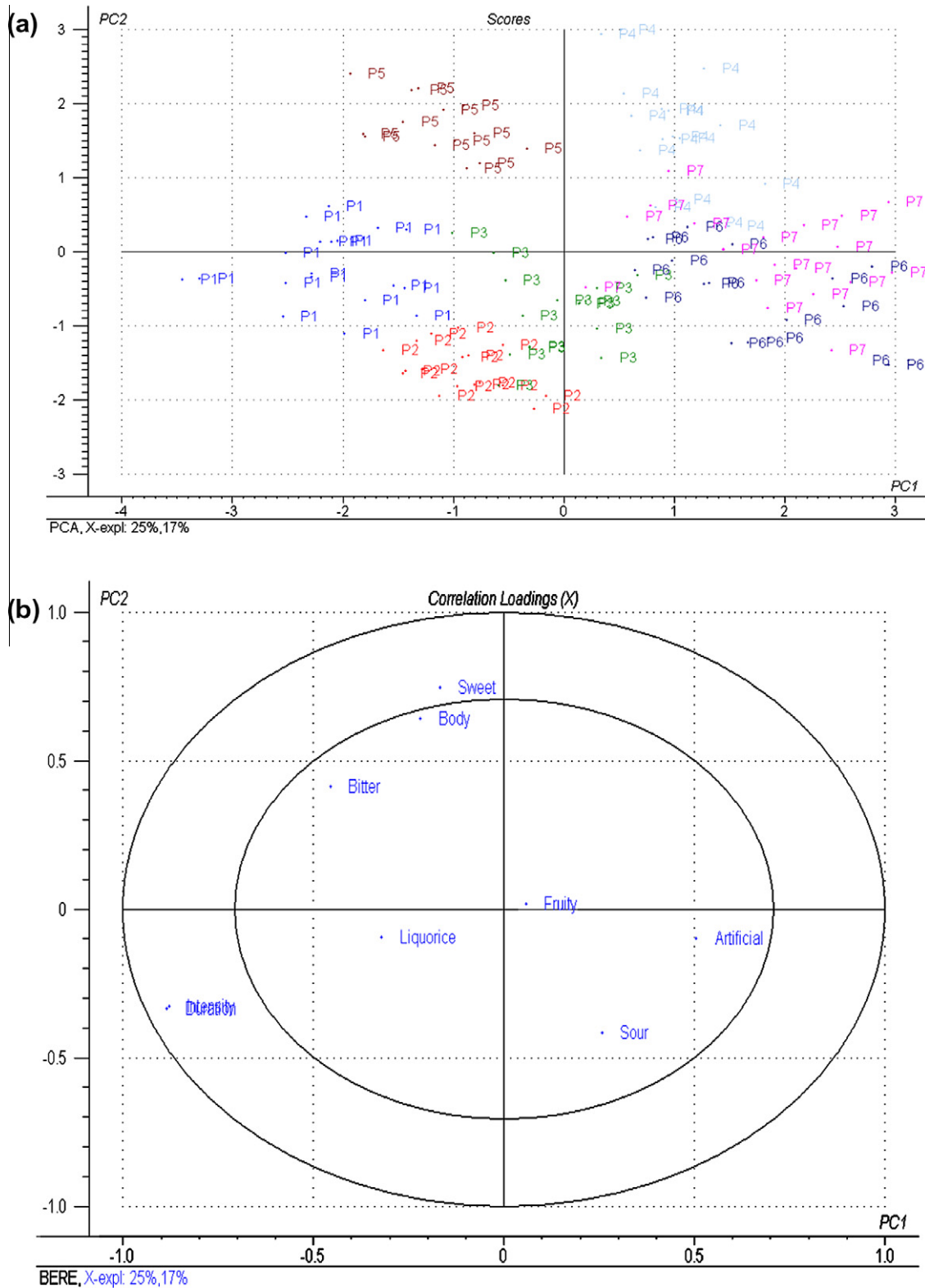


Fig. 5. PCA plots of aftertaste sensory evaluation for non-alcoholic beer: (a) score plot and (b) loading plot.

Therefore, Duncan's multiple ranges test was performed for means comparison among the beer brands. This statistical test was used for all nine attributes to develop the categories. The categories are given in Table 3. It is clear from this table that the products with similar letter have not significant difference for a specific aftertaste attribute.

An awareness of these categories could be of interest to brewers; for example about bitter, the information obtained on bitterness value could give an insight into process control to brewer, since the causes of bitter taste is: content and alpha strength; length of hop boil; presence of dark malts, alkaline water and it can be reduced by lower alpha hops, hops added at stages through

boil, filtration, high temperature ferment. So, a brewer can check the beer production line that whether bitterness value of the beer processed is within the categories considered or not. Then, beer production manager decide about these items: How long hops are boiled, type of hop, fermentation temperature (high temperature and quick fermentation decrease bitterness), filtration reduces bitterness.

The polar plots of the average scores of the panelists for nine aftertaste attributes in seven non-alcoholic beer brands are shown in Fig. 4, in terms of relative response changes. The contour of these polar plots differs from one sample to another, illustrating the discrimination capabilities of the panel. These contour could be com-

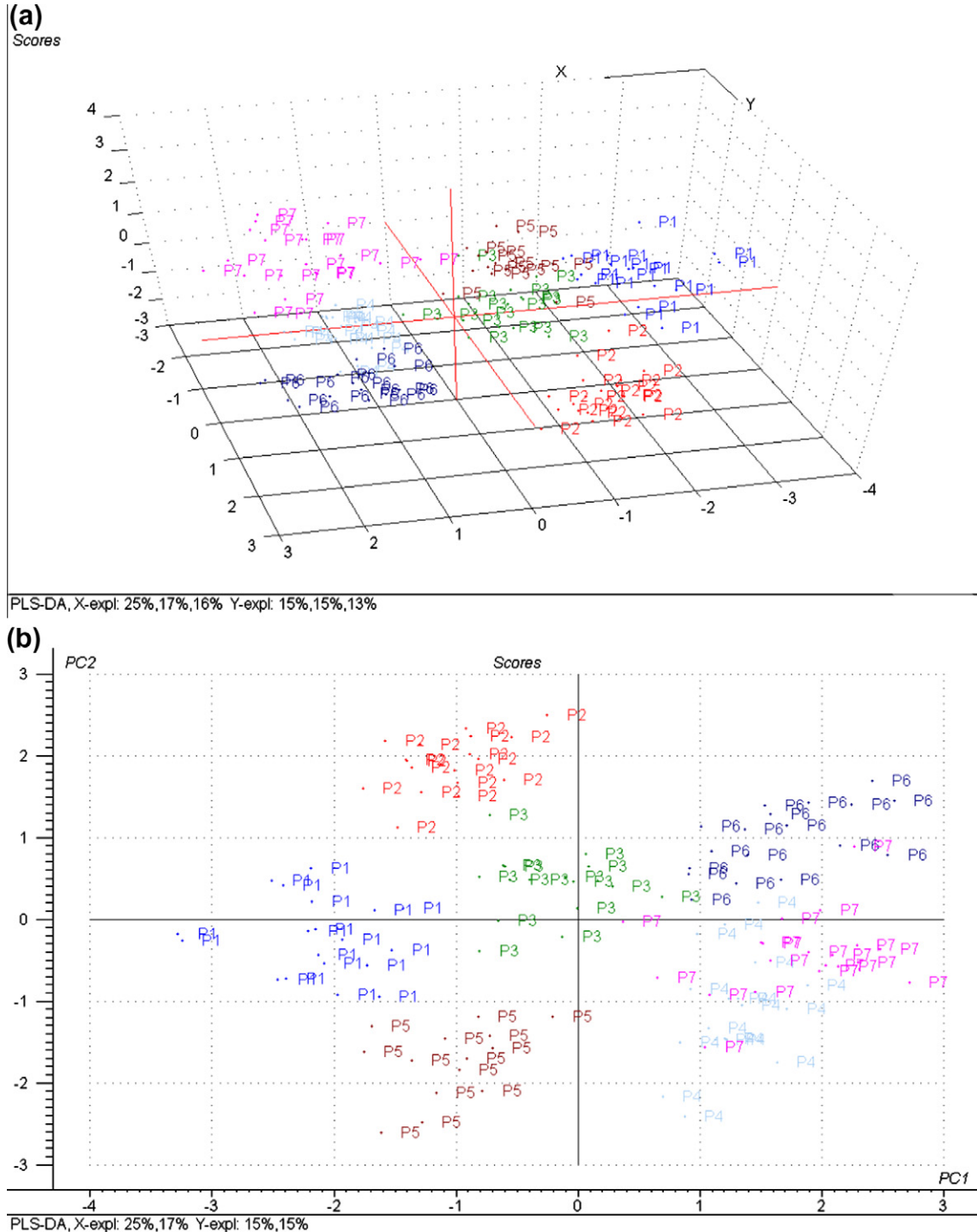


Fig. 6. PLS-DA score plot corresponding to the classification of non-alcoholic beers.

Table 4
Quantitative data of PLS-DA for each non-alcoholic beer brand.

Beer	Calibration				Validation (prediction)			
	Slope	Offset	Correlation	RMSEC	Slope	Offset	Correlation	RMSEP
P1	0.550	0.064	0.7416	0.2347	0.528	0.067	0.708	0.247
P2	0.648	0.050	0.805	0.207	0.628	0.052	0.780	0.218
P3	0.302	0.099	0.550	0.292	0.271	0.106	0.490	0.305
P4	0.719	0.040	0.848	0.185	0.702	0.042	0.829	0.195
P5	0.726	0.039	0.852	0.183	0.712	0.041	0.835	0.192
P6	0.536	0.066	0.732	0.238	0.497	0.071	0.691	0.253
P7	0.773	0.032	0.879	0.166	0.743	0.035	0.859	0.178

pared and correlated to the fingerprint obtained from electronic nose and electronic tongue (the analytical tools) in such a way, the sensors of these systems are replaced by the panelist. Such works have done by some researchers (Lozano et al., 2007; Rudnitskaya et al., 2009).

3.2. Classification

To carry out beer prediction, the responses have been analyzed using Principal Component Analysis technique. Principal Component Analysis (PCA) is a well known technique which provides insight into the structure of a dataset. PCA produces a set of new orthogonal variables (axes), the principal components, which are linear combinations of the original variables (Ding, Tian, & Xu, 2010). The maximum amount of variance in the original dataset (information) is contained in the first principal component. The components that account for a large variation in the data are used as the new axis to obtain plots of the samples (score plots). Together with samples also the original variables may be displayed in the same plot by the values of their coefficients of the eigenvector equations, named loadings. The loadings indicate the relative contribution of the variables to each principal component: the higher the loading of a variable on a principal component, the more the variable has in common with this component. The chemical meaning of a component can be derived from the variables forming it.

By means of this technique we tried to separate the non-alcoholic beer brands in different classes. The PCA results of the aftertaste sensory evaluation are illustrated in Fig. 5. It can be seen that all types of beer are well separated except a partial overlapping between zones corresponding to P4, P6 and P7. It shows that this trained sensory panel can discriminate among the samples except an overlapping between three brands of beer. As shown in Fig. 5, the scores plot and correlation loadings plot show that beers of P4 and P5 have strong body and sweetness, while brand of P1 has much duration. Much artificial variation could be found for P6 and P7 as well. Samples in one spot of the 2-vector score plot has, in general, much of the properties of the variables pointing in the same direction in the loading plot, provided that the plotted PCs describe a large portion of the variance.

In this study, prediction models based on PLS-DA were constructed as well. Fig. 6 shows the result of the PLS-DA calculated for the beer brands. Also, quantitative data of PLS-DA for all brands are given in Table 4. As observed, both the calibration and validation values for brands of 4, 5, and 7 involved a good-quality modeling performance (slope near 1, off-set near 0 and large correlation between aftertaste attributes and categorized variables). Moreover, as seen in Fig. 6, the relative location of the samples retains the general structure of the PCA score plots shown in Fig. 5, confirming the previous observations.

Fig. 7 illustrates the attributes for each panelist. As seen in the figure, P4, P6 and P7 could be distinguished for the panelists as found in Fig. 5 for PCA.

LDA can be considered, as PCA, as a feature reduction method in the sense that both, LDA and PCA, determine a smaller dimension

hyper plane on which the points will be projected from the higher dimension. However, whereas PCA selects a direction that retains maximal structure among the data in a lower dimension, LDA selects a direction that achieves maximum separation among the given classes. The results obtained by LDA provided a more appropriate classification compared to PCA. Fig. 8 shows the plot of the discriminant scores for all the beer samples. In this method, the variance between beer categories as well as the variance within beer categories is maximized. It merely looks for a sensible rule to discriminate between them by forming linear functions of the data maximizing the ratio of the between-group sum of squares to the within-group sum of squares. The linear functions are constrained to be orthogonal. Once the linear functions have been found, an observation is classified by computing its Euclidean distance from the group centroids, projected onto the subspace defined by a subset of the linear functions. The observation is then assigned to the closest group. To assess the performance of this method, the group centroids are estimated using a 'leave one out' cross validation method. Each observation is removed in turn from the data set and the group centroids calculated without reference to the missing data point. The excluded observation is then classified using these new group centroids. The data point is then replaced and the next observation removed from the data set. This process is repeated until all observations have been left out in turn. Thus, the percentage of observations correctly classified can be ascertained by comparing the true class membership with that estimated by LDA. This provides a good indication of the reliability of the classification method (Zhao, Wang, Lu, & Jiang, 2010).

3.3. Artificial neural network methods

A Probabilistic Neural Network (PNN) was used for prediction purposes. The PNN was composed by three layers: the input one had three neurons, corresponding to the three principal components; the hidden layer, with radial basis transfer functions, had the same number of neurons that number of training vectors and a competitive layer in the output (Duda, Hart, & Stork, 2001). Leave one out (LOO) cross validation method was applied to the network in order to check the performance of the network. LOO consists of training N distinct nets (in this case, N is number of measurements) by using $N - 1$ training vectors; while the validation of the trained net is carried out by using the remaining vector, excluded from the training set. This procedure is repeated N times until all vectors are validated (Bishop, 1999). Also, Radial Basis Function (RBF) and Back Propagation (BP) methods were performed. As stated earlier, this study was organized in three sessions. So, the confusion matrix for the neural networks studied for overall session and individual session are shown in Table 5–8 (for individual sessions, PNN results are presented here). The success rate (correct predicted number over total number of measurements) for each table is shown. For instance, in session 3, the results were more acceptable with success rate of 82%. In this session, all the beer brands corresponding to P1, P2, P3 and P6 are well-classified. The network only confuses one sample of P7 and P4 and one of P5 that classify like P1.

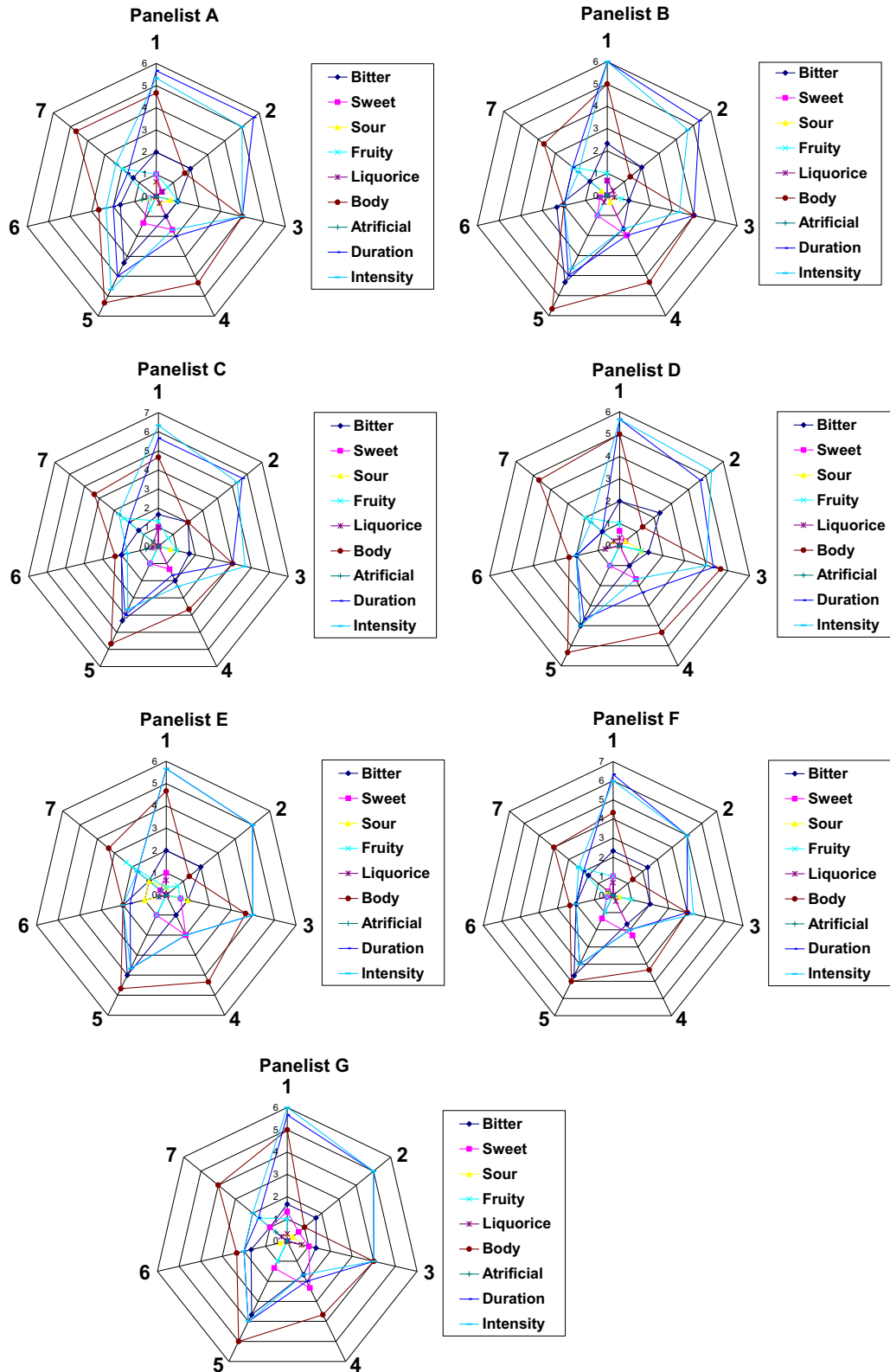


Fig. 7. Polar plots of the panelists' response to aftertaste attributes of seven non-alcoholic (the numbers around the plots are the beer brands).

The highest success rate to classify the beer brands was obtained in RBF approach as 0.9727 as seen in Table 9.

The BP network topology was formed by three layers: the input layer has two neurons corresponding to the first two components, a variable number in hidden layer, and seven neurons in the output layer corresponding to the seven beer brands. The network

processes the inputs and compares its outputs against the desired outputs. Errors are then propagated back through the system, causing the system to adjust the weights that control the network. This process occurs over and over as the weights are continually tweaked. During the training of a network the same set of data is processed many times as the connection weights are always

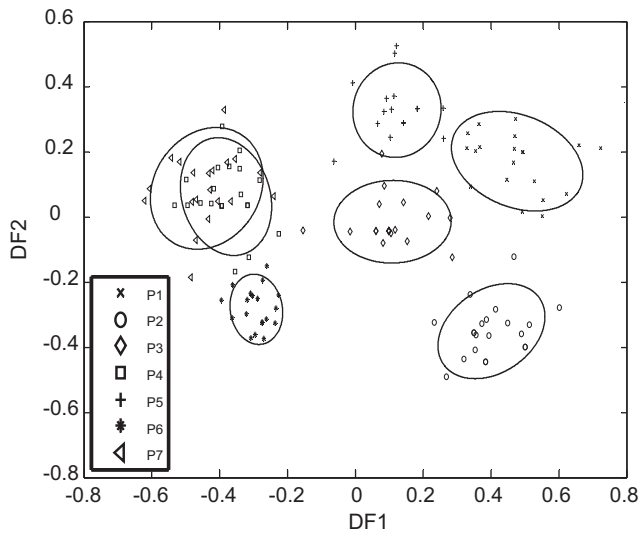


Fig. 8. Score plots of seven different non-alcoholic beer brands by LDA.

Table 5
Confusion matrix for the PNN prediction for whole sessions.

Real/predicted	P1	P2	P3	P4	P5	P6	P7
P1	18	1	1	0	1	0	0
P2	0	21	0	0	0	0	0
P3	0	0	20	0	0	0	1
P4	0	0	0	9	0	2	10
P5	1	0	0	0	20	0	0
P6	0	0	0	2	0	19	0
P7	0	0	0	8	0	1	12
Success rate	0.80952381						

Table 6
Confusion matrix for the PNN prediction for session 1.

Real/predicted	P1	P2	P3	P4	P5	P6	P7
P1	5	1	1	0	0	0	0
P2	1	6	0	0	0	0	0
P3	1	0	5	1	0	0	0
P4	0	0	0	3	0	1	3
P5	0	0	0	0	7	0	0
P6	0	0	0	1	0	6	0
P7	0	0	0	3	0	1	3
Success rate	0.714286						

Table 7
Confusion matrix for the PNN prediction for session 2.

Real/predicted	P1	P2	P3	P4	P5	P6	P7
P1	7	0	0	0	0	0	0
P2	0	7	0	0	0	0	0
P3	0	0	7	0	0	0	0
P4	0	0	0	2	0	1	4
P5	0	0	0	0	7	0	0
P6	0	0	0	0	0	5	2
P7	0	0	0	4	0	1	2
Success rate	0.755102						

refined. The samples were divided into two groups training set and the testing set. In the training of the network, different number of neurons in the hidden layer has been tested in two proofs. The result is shown in Fig 9. The optimal number turned out to be 14 neurons by several times tested. The classification success is

Table 8
Confusion matrix for the PNN prediction for session 3.

Real/predicted	P1	P2	P3	P4	P5	P6	P7
P1	7	0	0	0	0	0	0
P2	0	7	0	0	0	0	0
P3	0	0	7	0	0	0	0
P4	0	0	0	3	0	1	3
P5	1	0	0	0	6	0	0
P6	0	0	0	0	0	7	0
P7	0	0	0	4	0	0	3
Success rate	0.81632653						

Table 9
Confusion matrix for the RBF prediction for whole sessions.

Real/predicted	P1	P2	P3	P4	P5	P6	P7
P1	21	0	0	0	0	0	0
P2	0	21	0	0	0	0	0
P3	1	0	20	0	0	0	0
P4	0	0	0	19	0	1	1
P5	0	0	0	0	21	0	0
P6	0	0	0	0	0	21	0
P7	0	0	1	0	0	0	20
Success rate	0.97278912						

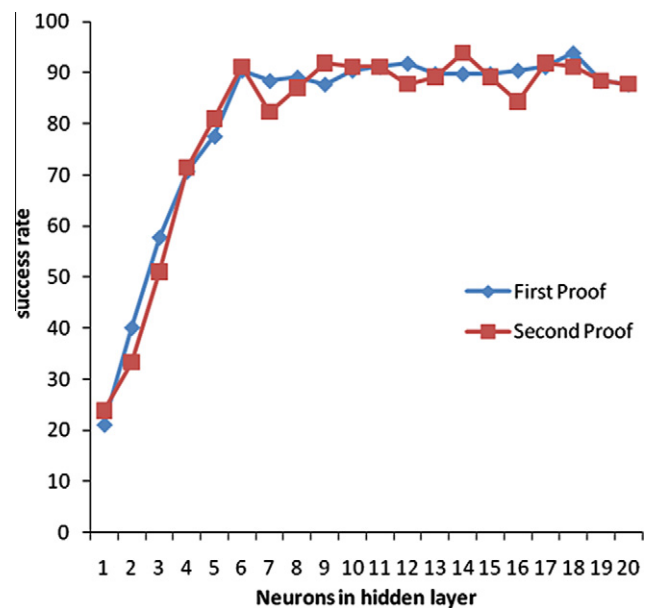


Fig. 9. Success rate values in different neurons number in hidden layer in Back Propagation method.

Table 10
Confusion matrix with 14 neurons in hidden layer for the RBF prediction for whole sessions.

Classification	P1	P2	P3	P4	P5	P6	P7
P1	20	0	0	0	1	0	0
P2	1	20	0	0	0	0	0
P3	1	0	20	0	0	0	0
P4	0	1	0	20	0	0	0
P5	1	0	0	1	19	0	0
P6	1	0	0	0	0	20	0
P7	0	0	0	0	1	0	20
Success rate	0.945578231						

100% for the training set in total and 97% for the testing set in total. The result of the testing set is shown in Table 10.

All together, among the methods used, Radial Basis Functions (RBF) showed the greatest accuracy in beer classification. This approach has attracted a great deal of interest due to their rapid training, generality and simplicity. When compared with traditional multilayer perceptrons, RBF networks present a much faster training, without having to cope with traditional Back Propagation problems, such as network paralysis and the local minima. These improvements have been achieved without compromising the generality of applications.

The results obtained in the current study could be correlated with biomimetic-based devices such as electronic nose and tongue systems (Ghasemi-Varnamkhasti, Mohtasebi, Rodriguez-Mendez, Lozano, et al., 2011; Ghasemi-Varnamkhasti, Mohtasebi, Rodriguez-Mendez, Siadat, et al., 2011; Ghasemi-Varnamkhasti, Mohtasebi, & Siadat, 2010; Wei, Hu, et al., 2009; Wei, Wang, & Liao, 2009). Since sensory evaluation tests are time consuming and require complex and expensive equipment. Then, e-tongue and e-nose as innovative analytical tools could be used instead of sensory evaluation. It is hoped that the correlation of these results with e-tongue and e-nose to be promising. According to the bibliography, such works have shown a very good correlation with human gustatory sensation (Kovacs, Sipos, Kantor, Kokai, & Fekete, 2009; Lozano et al., 2007; Uchida et al., 2001). A similar approach is the adsorption and desorption of beer and coffee on a lipid membrane simulating the bitter reception of the tongue. The measurement of bitter intensities and durations showed good correlation to sensory experiments (Kaneda & Takashio, 2005; Kaneda, Watari, Takshio, & Okahata, 2003).

At the end of this paper, this is worth mentioning that bitterness is the most important organoleptic characteristic of non-alcoholic beer and not only the intensity but also the duration affects the bitter quality of beer in a sensory evaluation. Bitterness is one of the flavor items in the matching test and a criterion for the descriptive ability, used for selection and training of assessors. As emphasized in the literature (Kaneda, Shinotsuka, Kobayakawa, Saito, & Okakata, 2000), the time-intensity rating of bitterness provides a category scaling and additional information, including rates of increase and decrease of bitterness, persistence of maximum intensity, changes caused by swallowing, and duration of after-taste.

The above issues are recommended to be studied in future. Since practical problems associated with the sensory assessment of non-alcoholic beer and other foodstuffs are well known, training and maintaining of the professional sensory panels is necessary for ensuring reproducibility of the results but expensive. Another problem is a rapid saturation of the assessors meaning that only a limited number of samples may be assessed during the same tasting session (Rudnitskaya et al., 2009). As a consequent, sensory analysis is notorious for being slow, expensive and sometimes suffering from irreproducibility even when professional panels are involved. It is stated that significant efforts are being directed to the development of instrumental methods for routine analysis of taste attributes of foodstuffs and beer in particular (Rudnitskaya et al., 2009). However, sensory analysis suffers from an objective, unbiased, and reproducible evaluation, this necessitate the statistical handling of the data. Recently, taste and odor evaluations using membrane sensors, which are supposed to reflect olfactory and gustatory characteristics of the human nose and tongue, have been actively studied (Ghasemi-Varnamkhasti, 2011; Ghasemi-Varnamkhasti et al., 2010; Hayashi, Chen, Ikezaki, & Ujihara, 2008; Peres, Dias, Barcelos, Sa Morais, & Marchado, 2009; Rodriguez-Mendez et al., 2004; Rudnitskaya et al., 2006; Wei, Hu, et al., 2009; Wei, Wang, et al., 2009). An electronic aroma detector has been introduced for quality control in the brewing industry,

e.g., for differentiation between beers and for recognition of the presence of important beer aromas and variety/quality parameters. The results obtained from the current study could be considered as a reference data in such systems (e-tongue and e-nose). There are many reports on the correlation of the output of electronic noses and tongues to sensory data, and in many the sensory part of the data is implied rather than measured. However, the prospects for these kinds of devices are very good, and we expect to see many variants of machine smell/taste/sight systems in the future.

4. Conclusions

The sensory evaluation of non-alcoholic beer plays a relevant role for the quality and properties of the commercialized product. In this contribution, we did a sensory evaluation of aftertaste attributes for non-alcoholic beer. We used seven beer brands to evaluate nine attributes by a trained sensory panel. The results showed that the data are in consistent. Therefore, the brands were statistically classified in some categories. Effect of panelist was found to be statistically insignificant. Also, neural network methods showed a promising result for prediction of beer brands in such a way the success rate (correct predicted number over total number of measurements) was found to be acceptable. Among the methods used, Radial Basis Functions (RBF) showed the greatest accuracy in beer classification.

It is important that a proper grounding in basic experimental design and statistics is given when training sensory scientists. This will encourage a wider understanding of possible manipulations of data, and ultimately result in better products. This study could be gone on another research in which electronic nose and tongue would be used to evaluate non-alcoholic beer quality (Ghasemi-Varnamkhasti, 2011). As found in this study, the results are suitable as a reliable reference data to be considered in multi arrays of sensors and the results on aftertaste sensory evaluation could be correlated to the data obtained from electronic nose and tongue in a separate research.

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