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Assessing the use of different chemometric techniques to discriminate low-fat and full-fat yogurts

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ABSTRACT

This study proposes a new approach to discriminate low and full-fat yogurts using instrumental analysis and chemometric techniques. One hundred twenty six strawberry flavored yogurts were subjected to instrumental analysis of pH, color and firmness. Exploratory methods, such as Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA), and supervised classification methods, such as K-nearest neighbors (KNN), soft independent modeling of class analogy (SIMCA), and Partial Least Square Discriminant Analysis (PLSDA) were used for assessing the data. The results showed that low- and full-fat yogurts presented different with regard to all the variables analyzed. It was not possible to obtain total separation between the samples using PCA and HCA. KMN and PLSDA presented excellent performance toward the full-fat category, with 100% correct prediction which suggests only low-fat yogurts to be subjected to the traditional fat content determination methods. This approach can be incentivized by the health agencies aimed to optimize materials and financial resources.

1. Introduction

Chemometric is a science of multidisciplinary nature which involves multivariate statistics, mathematical modeling and information technology, specifically applied to chemical data. Actually, these methods are useful tool in the quality control of dairy products (Gaspardo, Lavrenčič, Levart, Del Zotto, & Stefanon, 2010; Hammami et al., 2010; Karoui, Mounem, Rouissi, & Blecker, 2011; Lerma-García, Gori, Cerretani, Simó-Alfonso, & Caboni, 2010; Ochi et al., 2010; Sacco et al., 2009; Sola-Larrañaga & Navarro-Blasco, 2009; Souza et al., 2011).

Quality control of low/reduced fat food products has become a common procedure of increasing importance in food industry, since the information displayed on the label often does not correspond the real values present in the food product composition. This is emphasized in several Brazilian surveys (Esper, Bonets, & Kuaye, 2007; Silva, Batista, Cruz, Moura, & Carvalho, 2008), which introduces unreliability to both health authorities and consumers. Despite official methods for determination of fat level in dairy products – Bacok, Gerber and Mojonier – are simple, they require preparation of samples and chemical reagents. In addition, they need glassware and specific pieces of equipment and instruments, such as butyrometers and centrifuges, all of which require minimally trained personnel. Finally, these methods generate chemical waste which requires adequate disposal (Brasil, 2006).

This study proposes a new approach to distinguish yogurts toward their fat content using instrumental analysis such as: pH, color and firmness, using chemometric methods (Principal Component Analysis (PCA), Hierarchical Cluster Analysis (HCA), K-nearest neighbors (KNN), Soft independent modeling of class analogy (SIMCA), and Partial Least Square Discriminant Analysis (PLSDA)).

2. Materials and methods

2.1. Sampling

One hundred and twenty six strawberry-flavored set yogurts (83 full-fat and 43 low-fat yogurts), from 12 commercial brands and different batches were used in this work. The composition of the products was obtained from their labels, with exception of the fat levels that were determined analytically. In the class of full fat

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yogurts, the protein, fat and carbohydrates contents were 1.8–3.5, 2.0–5.4 and 17–27, respectively. In all the yogurts collected, the stabilizers are gelatin and xanthan gum. In the class of low fat yogurts, the protein, fat and carbohydrates contents were 4.3–7.2, 0.9–2.2 and 6.9–7.4, respectively. Five samples from each commercial brand were purchased randomly at different supermarkets in the city of Campinas, São Paulo, Brazil and kept under refrigeration (3–5 °C). All the commercial brands analyzed correspond to 100% of the Brazilian yogurt market.

2.2. Analytical procedures

The fat in the yogurts were determined by the Blen-Dyer Method (Brasil, 2006). The pH, instrumental firmness and instrumental color (L^*, a^*, b^*) (Cielab, Hunterlab, Virginia, USA) of yogurts were performed using techniques commonly described for fermented milk products. Details about the methods are published elsewhere (Cruz, Walter, Cadena, Assis, Bolini & Fratini, 2009).

2.3. Chemometric techniques

The data analyses were performed using the software PIROUETTE 2.2 (Infometrix, Seattle, WA). The yogurt data set consisted of a 126 × 5 matrix, in which rows represented the yogurt samples, and columns the instrumental analysis values: pH, instrumental firmess and instrumental color parameters (L^*, a^*, b^*). Each sample was represented in the multidimensional space by a data vector, which was an assembly of the 5 features in yogurt samples. Data vectors belonging to the same category (full-fat, F and low-fat, L) were analyzed using chemometric procedures: PCA, HCA, KNN, SIMCA, PLSDA (Abdi, & Williamns, 2010; Alonso-Slaces et al., 2005, 2006; Granato, Katayma, & Castro, 2010).

The classification rules achieved by the supervised chemometric techniques were validated by dividing the complete data set into a training set and an evaluation set. Samples were assigned randomly to a training set, consisting of 75% of them, and the test set, composed by the remaining 25% of the samples. These percentages are sufficient to perform this study. All data were autoscaled before the analysis, which means that each column data matrix was mean-centered and scaled to unit variance. Indeed, a pre-processing of the data is required in order to avoid the effect of different scales of the variables.

3. Results and discussion

3.1. Analytical results

Table 1 shows the average values obtained from the instrumental analysis of the yogurts. Significant differences were observed for all the parameters analyzed ($p < 0.05$). These findings can be due the different starter and probiotic cultures used by the manufacturers (each one with its own metabolic profiles) and the control of the operational parameters used in the yogurt processing, such as homogenization milk pressure, heat-related variables, type and amount of stabilizer used in the product formulation as well as final pH of fermentation.

The manufacture of yogurt is relatively simple, being produced in several small and medium-sized processing facilities. In many of them, the control of the inherent processing parameters is not performed. These parameters include the fat level obtained by skimming the milk, the amount of milk powder added to standardize the total solids, the heat treatment of the milk, the inoculum level of starter culture and the stabilizer used (Mortazavian, Ehsani, Mousavi, Sohrabvandi, & Reinheimer, 2006; Mortazavian, Khosrokhavar, Rastegar, & Mortazaei, 2010; Peng, Horne, & Lucey, 2009; Soukoullis, Panagiotidis, Kourell, & Tzia, 2007). In the case of probiotic yogurts, there are additional parameters to be considered, such as the compounds used to supplement the milk (Lucas, Sodini, Monnet, Jolivet, & Corrieu, 2004), interaction between probiotic and starter cultures (Vinderola, Mocchiutti, & Reinheimer, 2002), the inoculation rate of the probiotic culture and its moment of addition during the yogurt processing (Kaur, Mishra, & Kumar, 2009), the quantity of water available during processing (Oliveira & Damin, 2003), oxygen level (Cruz et al., 2010; Cruz et al., 2012a,b) and the supplementation with a prebiotic ingredient (Oliveira, Perego, Oliveira, & Converti, 2009, 2011; Debon et al., 2012).

Table 1
Results obtained in the instrumental analysis of the yogurts.

	Full fat	Low-fat
pH	4.15^b	4.38^a
Hardness (N)	77.50^a	70.82^b
L^*	70.05^a	59.02^b
a^*	13.94^a	8.89^b
b^*	2.95^a	2.10^b

[a,b]Values followed by the same letter and in the same row do not differ significantly according to the Tukey test ($p < 0.05$).

3.2. Chemometric techniques

3.2.1. Cluster analysis and principal component analysis

The Euclidean distance and incremental linkage methods were used in the pre-processing to elaborate the HCA. The presence of three distinct segments is observed as shown in the dendogram (Fig. 1). The upper segment (Cluster 1), correspond exclusively to low-fat yogurts, comprising 32 samples, while in the lower segment are found 24 samples corresponding to full-fat yogurts. Finally, in the mid-section of the figure it is noted 70 samples of both low-fat and full-fat yogurt (59 samples of full-fat yogurt, which corresponds to 84.3% of the total, and 11 samples of low-fat yogurt, corresponding to the remaining 15.7%). These results suggest that yogurt manufacturers still need to make significant investments in research and development to produce low-fat yogurts that are similar to their full fat counterparts.

Five principal components (PC) were necessary to explain the variation of the data with principal components 1 and 2 explaining

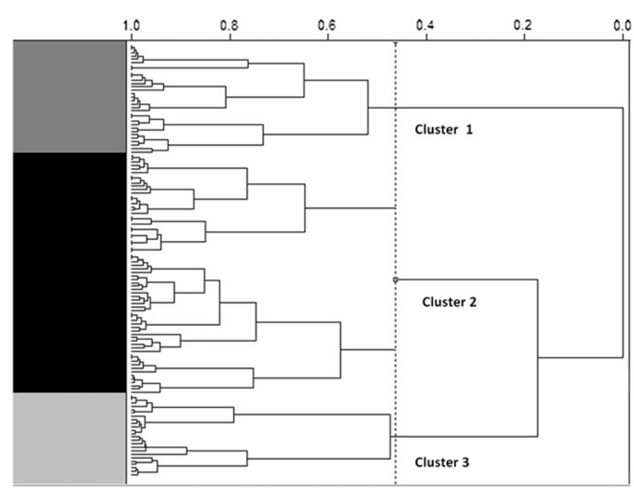

Fig. 1. Dendrogram of cluster analysis of the yogurt data. Cluster 1 = 32 samples, (100% low fat yogurt), Cluster 2 = 70 samples (84.3 full fat and 15.7% low fat, respectively), Cluster 3 = 24 samples (100% full fat yogurt).