Modelling sensory properties against instrumental measurements by PLS-Path Modeling: application to dairy products

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Abstract
In the present article, Partial Least Squares Path Modelling (PLS-PM) was used to investigate sensory perceptions of yogurts and explain them with their composition and instrumental properties. The main objective was to find out the latent variables including nutritional content (sugar, proteins and lipids), instrumental texture and structure properties and color, which could explain texture and flavor perceptions, as assessed by a trained panel (12 judges). Results show the interest of PLS-PM, which brings two main advantages: i) a good communication tool with a better visualization of the the links between explained and explaining variables; ii) a more accurate model in our problematic since PLS-PM fit the results on each variable individually rather than as a group, as for classical PLS, where the model is more of a compromise, possibly not well adapted to all variables.

Keywords: PLS-PM, texture, dairy product, sensory

1. Introduction

Consumer acceptance of food products is highly dependent on their texture properties (Bourne, 2002; Gilbert et al., 2013). As described by Szczesniak (2002), texture could be defined such as 1) a sensory property of food that is perceived by humans; possibly involving several senses; and 2) a multi-parameter property including food structure at different length scales (molecular, microscopic and macroscopic). A lot of studies aim to study and characterize i) the structure and texture properties of products by instrumental measurements and ii) texture perceptions by sensory analyses, and iii) the links between both. For instance, to characterize dairy products, several sensory and instrumental methods were carried out in literature (Everette & Auty, 2008). One way to understand perception of products and to go further in rationalized formulation is thus to study the links between sensory variables and those relating to the composition and the instrumental texture characteristics (Soukoulis et al., 2010; Pascua et al., 2013; Kraggerud et al., 2014 or Sonne et al., 2014). To study these relationships, different statistical methods are used in literature: for example, determination of correlation coefficient or, use of Principal Component Analysis (PCA) on instrumental variables with sensory attributes added as supplementary variables. But these approaches did not allow to predict sensory properties from instrumental variables. One way to go further will be to use methods based on linear regression methods. PLS is considered useful when there are many explanatory variables and comparatively little sample data (Hoskuldsson, 1988). As suggested by Wold. S. in 2001, when the Y's are correlated, they should be analyzed together. If the Y's really measure different concepts which are fairly independent, a single PLS model tends to have many components and can be difficult to interpret. Then a separate modelling of the Y's gives a set of simpler models with fewer dimensions, which are easier to interpret. However, this requires realizing as many models as the number of variables to explain. This approach does not achieve a simpler overall picture of all the Y. For these reasons, we decided to explain sensory perceptions from instrumental and composition data with a PLS-PM approach. This method allows investigating in a same model, different variables to be explained by using latent variables. In this context, the objective of the present study is to find out the latent variables including nutritional content (sugar, proteins and lipids, as stated on the packaging), instrumental texture and structure properties and color, which could explain texture and flavor perceptions, with a statistical method such as PLS-PM.

2. Material and methods

2.1 Products

Eight commercial yogurts were studied. They were selected to be representative of the French market of yogurts, including set and stirred yogurts, with or without bifidus source (health segment or not), and with various fat contents (from 0.1g to 3.5 g/100g of yogurt). Yogurts were stored at 4 °C and they spend 30 min out of the fridge before each evaluation. Samples were at approximately 10 °C when they were tested.

2.2 Rheological characterization

The physico-chemical properties of the yogurts were assessed measuring the water content (105°C), the Brix index (refractometer PAL-1. ATAGO), pH at 10 °C (pH meter Mettler Toledo) and the color (spectrophotometer BYK) using the CIEL method based on L*/a*/b* representation of light and colors. Rheological properties were also characterized: 1) maximal normal force Fmax (N), original slope E (N.mm-1) and area under the curve A (N.mm), all measured by back extrusion test (TAXT2, Stable Micro Systems) at 25°C, using a 5 kg-cell and a steel plane (4 cm diameter) with pre-test speed = 1 mm.s-1, test speed = 0.5 mm.s-1, and distance (d) in the product = 20 mm; 2) viscosity η (Pa.s) and the shear-thinning index n, deduced from the slope (n-1) of the curve log(viscosity) = log(shear rate) (MCR 301 rheometer, Anton Paar) of pre-sheared with a spoon (ηS, nS) or not (ηNS, nNS), at 25°C using a 5 cm diameter striated plane/Peltier plane system, with a 1.5 mm gap where samples were submitted to five shearing rates: 5, 10, 50, 100 and 250 s-1. Finally, particle size was measured (Mastersizer granulometer, Malvern), using the refractive index of milk of 1.46. All measurements were triplicated.

2.3 Sensory characterization

A group of 12 panelists were selected according to their motivation, and their ability to describe products. Six training sessions were designed to help panelists in perceiving, recognizing and quantifying the sensory properties of yogurts. Attributes generation was carried out during one specific session. The panelists agreed on a reduced list of 27 attributes related to the visual aspect, to the texture in mouth, to the odors, to the taste to the flavor and to the aftertaste. Their definitions and protocols for evaluation were established by the panel. Finally, panelists were trained in the use of the 10-cm unstructured linear scale to quantify the perceived intensities of the 27 attributes. After training of panel, sample evaluation was carried out in four sessions (two replicates).

2.4 Data analysis

The statistical analysis of data were performed using XLSTAT 2014.5.02 software (Addinsoft, Paris, France) and SAS 9.4 software (SAS Institute, Carry, New Orleans, USA).
Instrumental data (rheological and pH data) were investigated by non-parametric tests (Kruskal–Wallis test; pval < 0.05).
For sensory data, two-way analysis of variance (ANOVA) with product, subject effects and product*subject interaction was applied in order to determine the discriminating attributes and investigate the performance of the panel. When significant differences were revealed between products ($p<0.05$), mean intensities were compared using the Newmans Keuls multiple comparison test.
To assess connections between sensory and instrumental variables, PLS-PM method was performed. The instrumental and composition variables were used for the matrix X. Two PLS-PM were used: i) one PLS-PM with sensory attributes relating to visual texture and appearance as matrix Y, ii) another PLS-PM with attributes relating to perception in mouth (i.e. aroma, flavor, aftertaste and texture in mouth) as matrix Y. Three VARCLUS analyses were performed to define each latent variable (LV): one for instrumental measurements, one for composition measurement and one for sensory attributes. Reflective modes were used and composite reliability, item reliability, discriminant validity and convergent validity were checked for the outer model. Partial Least Squares Regression (PLSR) were used to estimate path coefficients and centroid scheme was used for the inner model. Only the LV with a VIP superior to 1 were kept in the model. For each regression coefficient, bootstrap was performed to identify confident interval associated to each coefficient.

3. Results

3.1. Sensory and instrumental data

Concerning panel performance, the homogeneity of the panel was determined by evaluating the interaction between the product and panelist for each attribute. Significant product*subject interactions ($p <0.05$) were observed for five attributes. However, the good discriminating ability of the panel ($p <0.0001$ for the product effect) demonstrated that disagreements between panelists were mainly due to differences in the use of the scoring scales. The discriminatory power of the panel was then determined with the product effect resulting from two-way ANOVA. The results revealed no significant differences between the yogurts for 8/27 attributes ($p >0.05$), so they were not interpreted further. The yogurts were therefore perceived to be significantly different with respect to 19/27 attributes.
According to the Kruskal–Wallis test, all the instrumental variables allow to significantly discriminate at least one product from the others (pval < 0.005).

3.2. Explaining sensory properties using PLS-PM

Figure 5 presents the final model to predict sensory tasting attributes with instrumental data. Four sensory LV presented a value of R^2 superior to 0.8 (fat perception, acid perception, sweet taste, mouth coating). Only the LV “thickness” have a R^2 inferior to 0.5.
Numerous relationships could be established. For instance, the LV related to “fat perception” is positively impacted by the LV lipids and negatively impacted by salt content, water content and size and quantity of particles. The LV “acid perception” is mainly impacted by the pH with a regression coefficient of -0.871. The LV “sugar perception” is obviously impacted by the sugar content, but also

by the two LV related to the texture of the yogurts. The LV “firmness, viscosity” impact four LV. All these results show the key role of texture properties on the perception of dairy products.

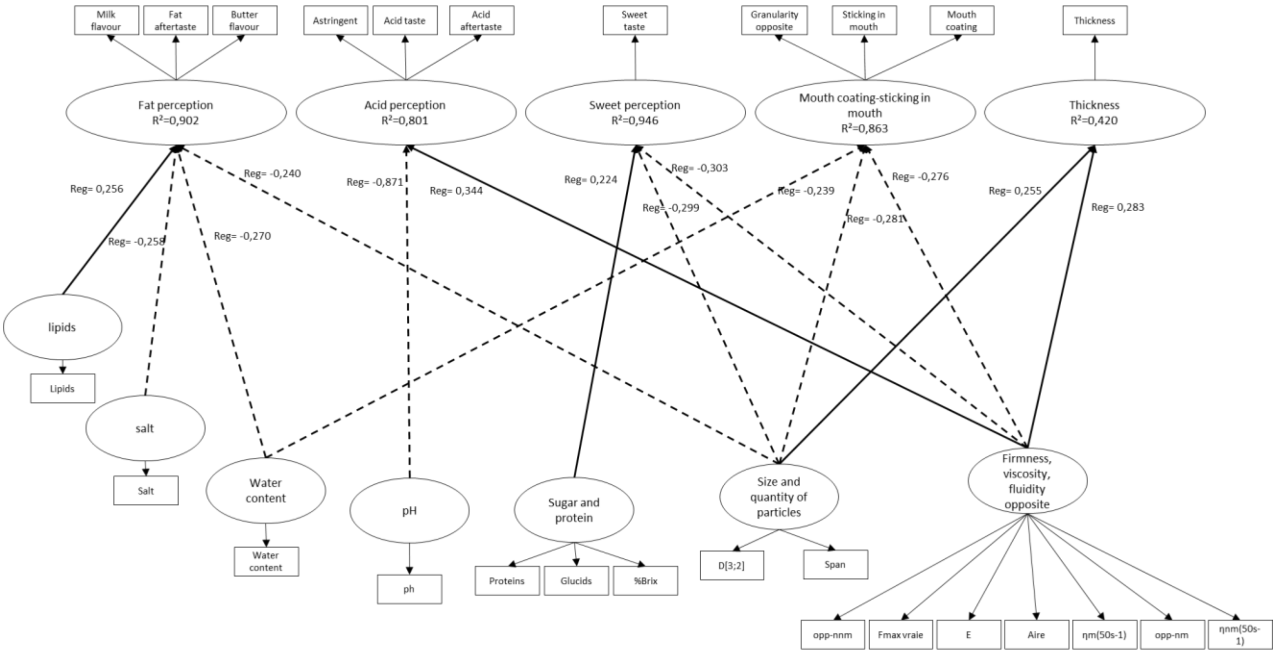

Figure 1: PLS-PM model for the sensory tasting attributes

4. Discussions

Texture of yogurts is one of the most essential components of their quality. To improve it, it seems necessary to better understand the relative contribution of composition or process on yogurt structure and texture and to be able to measure it.

PLS-PM gives an overall picture of all the variables studied, which is a good tool for communication. Like the PLSR, the PLS-PM approach with a PLSR for the structural model allows to remove the problem of co-linearity between variables.

For example, and as observed in our results, mouth coating perception was predicted with the LV related to the water content, size and quantity of particles and the instrumental measurements related to firmness and viscosity. This highlights complexity of this sensory dimension. Besides, perceptions as thickness could not be correctly predicted from instrumental measurements, whatever the statistical methods used (from simple correlation coefficient to PLS-PM). Indeed, sensory prediction from instrumental measurements can reveal some limits (Chen, 2014). Food consumption is complex and induced multimodal variables. Instrumental measurements can hardly mimic physicochemical parameters involved during eating process, such as the impact of thermal variation, saliva hydration, surface and interface of oral cavity etc.

From a methodological perspective, the statistical analysis outlined in this study illustrates the potential of the method of PLS-PM to better understand the determinants of sensory perception of plain yogurts. Results illustrated the interest to measure some parameters such as components and rheological measurements to predict texture sensory variables. On an instrumental point of view, further studies including tribology and bolus kinetics during consumption should provide greater understanding of the texture-structure perception.

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