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Comparison of different ways of handling L-shaped data for integrating sensory and consumer information

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ABSTRACT

Different approaches for handling L-shaped data are compared for the first time in a study conducted with Norwegian consumers. Consumers (n = 101) valuated eight different yoghurt profiles varying in three intrinsic attributes such as viscosity, particle size, and flavour intensity following a full factorial design. Sensory attributes, consumers' liking ratings, and consumer attributes were collected. Data were analysed using two different approaches of handling L-shaped data: approach one used two-step Partial Least Square (PLS) Regression using L-shaped data including the three blocks such as sensory attributes, consumers' liking ratings, and consumer attributes, while approach two was based on one-step simultaneous L-Partial Least Square (L-PLS) Regression model of the same three blocks of data. The different approaches are compared in terms of centering, step procedures, interpretations, flexibility, and outcomes. Methodological implications and recommendations for academia and future research avenues are outlined.

1. Introduction

The most common approach to integrate sensory and consumer information is to simply ask consumers to rate their overall degree of liking of a large set of food products and characterize the sensory attributes of the same products using a trained assessors' panel (Ares, Varela, Rado, & Giménez, 2011). Then, both types of data (i.e., sensory attributes, and consumers' liking ratings) are combined using regression analysis (e.g., preference mapping techniques) to identify the sensory attributes of the most liked product (van Trijp, Punter, Mickartz, & Kruithof, 2007).

However, an important challenge is to identify which consumer attributes (e.g., socio-demographics, habits, attitudes, etc.), drive liking differences among consumers, beyond varying preferences for the sensory attributes of a food product (Kergoat et al., 2010). This information is crucial for product developers and marketers of new food products to improve product properties, product communication, and marketing strategies. Indeed, consumer attributes related to specific aspects affecting preferences, are commonly investigated (see for example, Asioli, Wongprawmas, et al., 2018; Carrillo et al., 2013; Menichelli et al., 2014).

The integration of three types of data, also called L-shaped data, such as sensory attributes (**X**), consumers' liking ratings (**Y**), and consumer attributes (**Z**) can provide a large amount of information useful for understanding the relationships among the different data sets (Martens et al., 2005). The concept of L-shape analysis comes from the shape of the whole data structure as depicted in Fig. 1.

One possible approach which simultaneously takes into account all data is the so-called L[1]-Partial Least Square (L-PLS) regression method (Martens et al., 2005). In L-PLS regression, consumers' liking ratings are approximated by a sum of 'interactions' between linear combinations of the sensory attributes, and the consumer attributes (Vigneau, Endrizzi, & Qannari, 2011). L-PLS applications in consumers' food studies are given in a number of research papers (Frandsen, Dijksterhuis, Martens, & Martens, 2007; Giacalone, Bredie, & Frøst, 2013; Kühn & Thybo, 2001; Mejlholm & Martens, 2006; Pohjanheimo & Sandell, 2009; Thybo, Kühn, & Martens, 2004).

Another possible approach is to use a two-step sequential procedure,

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[1] L- is referred to the shape of data, such as the three blocks (i.e., sensory attributes, consumers' liking ratings, and consumer attributes).

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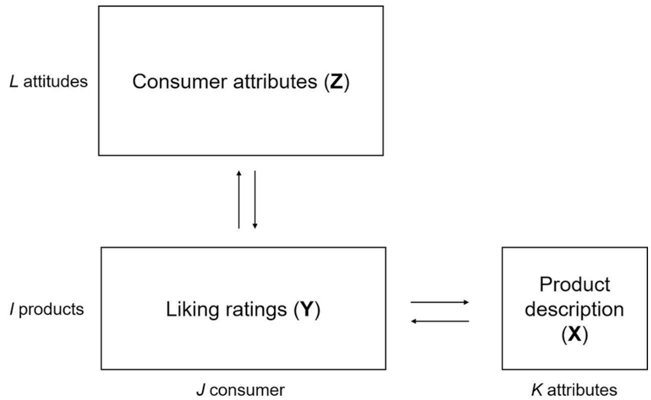

Fig. 1. L-shape data: product description (X) (i.e., sensory attributes), liking ratings (Y) (i.e., consumer liking ratings), and consumer attributes (Z).

based on first analysing the relation between sensory attributes and consumer liking ratings, using PLS or Principal Component Regression (PCR). Then, the consumer loadings are related to the consumer attributes, also using PLS.

The one-step approach (i.e., L-PLS) may have possible advantages over the two- step approach (i.e., PLS) since it is only based on one step, but on the other hand its properties are not well understood yet. The two-step approach has the advantage that it is based on sequential use of better-established and explored techniques, although the properties of the combined approach has not been explored. To the best of the authors knowledge, how the one-step and two-step approaches compare to each other in practice has been very little explored.

To fill this void, the aim of this paper is to compare the two-step PLS regression and one-step L-PLS approaches, using data from an experiment investigating sensory properties, and consumers' preferences for yoghurts in Norway. Issues related to centering, interpretations, flexibility, and outcomes of the two approaches will be compared and discussed.

The paper is structured as follows: firstly, the statistical methods used are briefly described, secondly, the implemented methodological approach is explained, including experimental design, and data analysis, thirdly the obtained results from the analysis are presented. Finally, we discuss the results and provide methodological implications, and recommendations for academia as well as outline some future research avenues.

2. Theory: statistical methods

In this section we will briefly present the theories of the statistical methods used in this paper, such as the PLS regression, preference mapping, and more extensively the L-PLS regression.

In the L-shaped data set, the matrix $\boldsymbol{Y}(I \times J)$, represents the liking ratings data given by J consumers for I products, the descriptive sensory attributes data will be denoted by $\boldsymbol{X}(I \times K)$, containing intensities for K descriptors of the same I products. The data set containing the L descriptors for the J consumers (i.e., consumer attributes) will be denoted by $\boldsymbol{Z}(L \times J)$.

2.1. L-shaped data

In recent years, a number of data analysis approaches have been suggested to handle L-shaped data set (see e.g. Vinzi, Guinot, & Squillacciotti, 2007). The first part of the present sub-section will be devoted to the two-step approach (PLS regression, see e.g. Geladi & Kowalski, 1986), while the second part will be focused on the one-step approach (L-PLS regression).

2.1.1. Two-step approach based on PLS regression

For a detailed description of two-step approach we refer to Næs, Varela, & Berget (2018). Briefly, the two-step PLS approach is performed according to the following procedure. In *step 1* (*for horizontal direction in the L-shape,* Fig. 1*)*, PLS regression is used for relating preference data ($\boldsymbol{Y}$), and sensory attributes ($\boldsymbol{X}$). This can be done using either $\boldsymbol{Y}$ or $\boldsymbol{X}$ as response, corresponding to external and internal preference mapping, respectively. We refer to Næs et al. (2018) for a discussion of advantages and drawbacks of the two approaches.

In *step 2* (*for the vertical direction in the L-shape,* Fig. 1), a PLS regression model is again used for relating the consumer loadings from the first analysis (*step 1*) to the consumer attributes in $\boldsymbol{Z}$. In more detail, the consumer loadings are organised with different loadings as columns, consumers as rows, and the consumer attributes matrix is transposed. A PLS analysis is then used in the standard way. One can use several PLS loadings simultaneously using a PLS2 approach or handle each of them separately (Næs et al., 2018). Alternatively one can use segmentation on the consumer loadings, and relate the consumer attributes to the segments using the classification variant of PLS, such as Partial Least Square – Discrimination Analysis (PLS-DA) based on a dummy response matrix (Almli et al., 2011; Asioli et al., 2014). This opportunity will not be handled in this paper but will be discussed briefly in the discussion part.

2.1.2. One-step approach (L-PLS regression)

There are some different approaches for analysing L-PLS data in one step, e.g., Löfstedt, Eriksson, Wormbs, & Trygg (2012); however, we focus only the approaches related to the two-step approach for further comparison. The L-PLS Regression approach introduced by Martens et al. (2005) is based on one single analysis combining all the three blocks of data (Vinzi et al., 2007). The matrices $\boldsymbol{X}$ and $\boldsymbol{Z}$ are supposed to be centered ($\boldsymbol{X}$ for each sensory attribute, and $\boldsymbol{Z}$ for each consumers' attribute), while matrix $\boldsymbol{Y}$ is supposed to be centered with respect to both its rows and its columns (double centered). The L-PLS regression method used here is based on a Singular Value Decomposition (SVD) of $\boldsymbol{X}'\boldsymbol{Y}\boldsymbol{Z}'$ with deflation between each component. As an alternative to SVD, a Nonlinear Iterative Partial Least Squares (NIPALS) based algorithm for each component can be used, see e.g., Martens (2005).

Generally, L-PLS regression can be arranged as *endo-L-PLS* or *exo-L-PLS*, where the *endo* approach reflects the *inward-pointed regression* of a single response matrix $\boldsymbol{Y}$ from two outer predictors ($\boldsymbol{X}$ and $\boldsymbol{Z}$) as illustrated in Martens et al. (2005), and Mejlholm & Martens (2006); the *exo* approach is characterized by a *simultaneous outward regression* of two responses from a single predictor $\boldsymbol{Y}$ as highlighted in Martens (2005) and Sæbø et al. (2010). The direction of prediction is defined through the deflation step discussed in the next paragraph. The underlying idea of having two variants is that in some cases one is more interested in describing variability in $\boldsymbol{Y}$ and how its main components relate to the other two data sets (*exo*-L-PLS), while in other cases the opposite is the case (*endo*-L-PLS). The direction of regression (*endo* or *exo*) may be based on causal assumptions, or merely a choice of convenience if the purpose is data exploration (Sæbø et al., 2010).

For each component $a(a = 1, \cdots, A)$ the SVD of the $\boldsymbol{X}'\boldsymbol{Y}\boldsymbol{Z}'$ is for both methods calculated (directly for a = 1, and on deflated matrices for a > 1). For the *endo* method, the left and right singular vectors are used as weights for calculating $\boldsymbol{X}$ scores and $\boldsymbol{Z}$ scores which again are used for deflation of the matrices $\boldsymbol{X}$ and $\boldsymbol{Z}$, see Martens (2005). This deflation means that the prediction direction is inwards. This is equivalent to the standard PLS regression where deflation of the input block is a crucial step. For the *exo*-version, the same SVD is used as a basis, but here also scores for $\boldsymbol{Y}$ are calculated. These are used for deflation of all blocks and therefore the prediction direction is considered outwards. The scores are here non-orthogonal, so deflation is done with respect to all previous components. The distinction between the *endo*- and *exo*-variants resembles the distinction between external, and internal preference mapping, respectively.

Plotting of the different parts of $\boldsymbol{X}$, $\boldsymbol{Y}$, and $\boldsymbol{Z}$ is done as suggested in

Martens et al. (2005) using correlation loadings. For the *endo*-L-PLS, the correlation loadings for ***X*** are obtained by correlating the ***X***-variables onto ***X***-scores and the same is done for ***Z***. For ***Y***, the correlation loadings are obtained by both regressing the columns and rows of ***Y*** onto the two sets of scores. For the *exo*-L-PLS the scores in the ***X*** and ***Z*** directions for ***Y*** are used as basis for the correlation loadings (see Sæbø et al. (2010) for details). The obtained correlation loadings for all three blocks are unit free and presented in the same plot.

It is beyond the scope of the present paper to discuss details of *endo*- and *exo*-L-PLS, but interested readers are referred to Sæbø et al. (2010).

3. Materials and methods

3.1. Participants

A sample of 101 consumers was recruited in the region south of Oslo (Norway) in October 2017. Only consumers who regularly consumed yoghurt at least once a month were included in the study. The final sample of consumers was composed by 72.27% females and 27.73% males, aged ranging between 18, and 77 years old. A recruitment questionnaire was used to collect general consumers' information (i.e., age, gender, BMI, consumption, and usage), and to select them based on yoghurt consumption frequency. Each participant got a reward of NOK 300 that was attributed to the leisure time organisation or club of their choice. All data were collected with EyeQuestion (Logic8 BV, The Netherlands).

3.2. Samples

Eight yoghurt samples were prepared from an experimental design based on the same ingredients and composition, but varying in texture, obtained by using different processing strategies. A full factorial design was used in this study, including three intrinsic attributes with two levels each: viscosity (thin/thick), particle size (flake/flour), and flavour intensity (low/optimal). The samples thus had the same calories and composition, and they were designed for the study of consumers' satiety and liking as related to sensory attributes, see Nguyen, Næs, & Varela (2018) for more details. Table 1 shows the samples with different levels of viscosity, particle size, and flavour intensity.

3.3. Consumer test

The consumer test was held in the sensory lab of Nofima AS (Ås, Norway). Consumers rated their hunger, fullness levels, and their attitudes toward health and taste of foods. In the second session, consumers were asked to taste each of the eight samples, and rate their liking ratings using a Labeled Affective Magnitude (LAM) scale (Schutz & Cardello, 2001).

All the sensory evaluations were conducted in standardized individual booths according to ISO 8589:2007. Samples were served in plastic containers coded with 3-digit random numbers, and in a sequential monadic manner following a balanced presentation order. Thirty grams (i.e., 30 gr.) of each sample (i.e., yoghurt) was served to each assessor for all the evaluations.

Table 1
Formulation of yoghurt samples and the symbols used in plots.

Sample	Viscosity	Particle size	Flavour intensity
P1 (t-F-l)	Thin	Flakes	Low
P2 (T-F-l)	Thick	Flakes	Low
P3 (t-f-l)	Thin	Flour	Low
P4 (T-f-l)	Thick	Flour	Low
P5 (t-F-o)	Thin	Flakes	Optimal
P6 (T-F-o)	Thick	Flakes	Optimal
P7 (t-f-o)	Thin	Flour	Optimal
P8 (T-f-o)	Thick	Flour	Optimal

3.4. Quantitative descriptive analysis (QDA®)

Nofima's sensory panel was used to obtain the sensory profiling of the eight samples using generic quantitative descriptive analysis (QDA®) (Lawless & Heymann, 2010; Stone, Bleibaum, & Thomas, 2012). The descriptive terminology of the products was created in a pre-trial session using two extreme samples (T-f-l and t-F-o) for stretching the sensory space. After a 1-hour pre-trial session, the descriptors and definitions were agreed upon by the assessors; all assessors were able to discriminate among samples, exhibited repeatability, and reached agreement with other members of the group. The final list of sensory attributes used in the experiment included six odour attributes (*intensity, acidic, vanilla, stale, sickening,* and *oxidized*), three taste attributes (*sweet, acidic,* and *bitter*), six flavour attributes (*intensity, sour, vanilla, stale, sickening,* and *oxidized*), and six texture attributes (*thick, full, gritty, sandy, dry,* and *astringent*) (see in the supplementary material S1)

3.5. Consumer attributes

Several consumer attributes were also collected using a questionnaire. Firstly, consumers' attitudes toward the health and hedonic characteristics of foods were assessed through the Health and Taste Attitudes Questionnaire (HTAQ) using a 7-point Likert scale (Roininen, Lahteenmaki, & Tuorila, 1999) by including (1) three health-related factors (*general health interest*, *light product interest*, and *natural product interest*); (2) three taste-related factors (*craving for sweet foods*, *using food as a reward*, and *pleasure*). In addition, consumers' socio-demographics such as age, and gender were collected. Table 2 shows a summary of consumer attributes.

The complete questionnaire is available in the supplementary material S2.

3.6. Statistical data analysis

To investigate L-shaped data, we used three different types of datasets such as sensory attributes (***X***), consumers' liking ratings (***Y***), and consumer

attributes (***Z***).

Prior to further analysis, the sensory attributes, which are the sensory attributes that are not significantly different among samples, were eliminated using the software PanelCheck (Ås, Norway).

3.6.1. Two-step approach (PLS regression)

In PLS regression for sensory attributes vs. consumer liking (*step 1*), two options of centering/ standardisation will be handled: (i) *Option 1*: sensory attributes (which include only significant attributes) are mean centered and standardised, consumers' column-wise mean centered, not standardised while (ii) *Option 2*: the same data analysis as in Option 1, but consumers' liking ratings are double-centered. The latter is done for the comparison with L-PLS since this uses double centered consumer data. It should be mentioned that centering prior to analysis is not needed since standard PLS does that automatically.

In *step 2*, PLS regression for consumer attributes vs. PLS loadings of the components 1 and 2 (derived from *step 1*), consumer attributes are mean centered and standardised. Furthermore, PLS loadings were also centered and scaled prior to analysis. We used PLS2.

3.6.2. One-step approach (L-PLS regression)

Preceding the extraction of latent vectors, the $\boldsymbol{X}(I \times K)$ and $\boldsymbol{Z}(L \times J)$ are centered and standardized, ***X*** for each sensory attribute, and ***Z*** for each consumers' attribute. The matrix $\boldsymbol{Y}(I \times J)$ is subjected to a double centering across both rows and columns. This corresponds to option 2 for the two-step approach.

The computations of L-PLS regression are done in R version 4.0.4 (R Core Team, 2021) using the package *lpls* (Sæbø, 2018), while PLS regression is done by Python using library *hoggorm* (Tomic, Graff, Liland,

Table 2
Consumer attributes and codes used in the plots.

Attribute	Definition
gen_1R	The healthiness of food has little impact on my food choices
gen_2	I am very particular about the healthiness of food I eat
gen_3R	I eat what I like and I do not worry much about the healthiness of food
gen_4	It is important for me that my diet is low in fat
gen_5	I always follow a healthy and balanced diet
gen_6	It is important for me that my daily diet contains a lot of vitamins and minerals
gen_7R	The healthiness of snacks makes no difference to me
gen_8R	I do not avoid foods, even if they may raise my cholesterol
lig_1R	I do not think that light products are healthier than conventional products
lig_2R	In my opinion, the use of light products does not improve one's health
lig_3R	In my opinion, light products don't help to drop cholesterol levels
lig_4	I believe that eating light products keep one's cholesterol level under control
lig_5	I believe that eating light products keeps one's body in good shape
lig_6	In my opinion by eating light products one can eat more without getting too many calories
nat_1	I try to eat foods that do not contain additives
nat_2R	I do not care about additives in my daily diet
nat_3	I do not eat processed foods, because I do not know what they contain
nat_4	I would like to eat only organically grown vegetables
nat_5R	In my opinion, artificially flavoured foods are not harmful for my health
nat_6R	In my opinion, organically grown foods are no better for my health than those grown conventionally
cra_1R	In my opinion it is strange that some people have cravings for chocolate
cra_2R	In my opinion it is strange that some people have cravings for sweets
cra_3R	In my opinion it is strange that some people have cravings for ice-cream
cra_4	I often have cravings for sweets
cra_5	I often have cravings for chocolate
cra_6	I often have cravings for ice-cream
rew_1	I reward myself by buying something really tasty
rew_2	I indulge myself by buying something really delicious
rew_3	When I am feeling down I want to treat myself with something really delicious
rew_4R	I avoid rewarding myself with food
rew_5R	In my opinion, comforting oneself by eating is self-deception
rew_6R	I try to avoid eating delicious food when I am feeling down
ple_1R	I do not believe that food should always be source of pleasure
ple_2R	The appearance of food makes no difference to me
ple_3	When I eat, I concentrate on enjoying the taste of food
ple_4	It is important for me to eat delicious food on weekdays as well as weekends
ple_5	An essential part of my weekend is eating delicious food
ple_6R	I finish my meal even when I do not like the taste of a food
Age	Age
Gender	Gender (1-male, 0-female)

Note: *gen* refers to general health interest; *lig* refers to light product interest; *nat* refers to natural product interest; *cra* refers to cravings for sweet foods; *rew* refers to using food as a rewards; *ple* refer to pleasure; and, *gender* and *age* refer to the socio-demographics gender and age.
The negative attributes are marked with 'R' after their abbreviations. For each negative attribute, the new score is calculated by subtracting original score from 7.

& Næs, 2019).

3.6.3. ANOVA of consumer liking data

Since double centered data do not provide information about differences in the true liking of the different products (only relative liking), an Analysis of Variance (ANOVA) with effects for products and consumers together with a multiple comparison was used. This analysis is useful for comparison with the two-step approach, and in general also as an add-on to the general L-PLS approaches. Interactions will be confounded with errors, and therefore only main effects are used. A fixed effects analysis for this model gives the same results as a mixed effects model.

The computations of ANOVA model are done in R version 4.0.4 (R Core Team, 2021) using the package *mixlm* (Liland, 2019).

4. Results

4.1. Two-way ANOVA model: consumers' liking ratings

First, for a complete view of consumer liking ratings, we performed ANOVA for comparison of the means. Double centered data only contain information about the relative liking ratings of products for different consumers, while consumers' liking ratings before double centering also contain information about which samples are most/least liked for each consumer. The ANOVA table (see in the supplementary material S3) shows that both effects, *product,* and *consumer,* were strongly significant for liking with p-values of < 0.001. The confidence intervals for the Tukey test are shown in the supplementary material S4.

Average liking ratings of the different products are depicted in Fig. 2. There were essentially three groups of products: *thick* products (T-F-l, T-f-l, T-F-o, T-f-o), *thin-optimal flavour* products (t-F-o, t-f-o), and *thin-low flavour* products (t-F-l, t-f-l); thicker samples were the most liked. Considering the thin ones, the products with optimal flavour intensity (t-F-o, t-f-o) were rated higher in liking than the ones with low flavour intensity (t-F-l, t-f-l). This indicates that, for thin products, consumers on average liked the products with optimal flavour intensity more than the rest, regardless of particle size (flakes vs flour). Particle size seems less important for average consumer liking.

4.2. Two-step approach (PLS regression)

4.2.1. Internal vs. External mapping

In this section we present the results from the internal and external preference mapping from PLS. Both internal and external mapping are used since both *endo*- and *exo*-PLS use either inwards or outwards predictions.

4.2.2. PLS internal preference mapping

Fig. 3) and 4) exhibit the correlation loadings and scores plots, respectively for PLS internal preference mapping. In Fig. 3, we can see that both component 1 (22.7%, 55.6%), and component 2 (31.2%, 21.8%) contribute to the liking pattern. The bottom-right quadrant is the dominating one for liking. We can notice that the majority of consumers

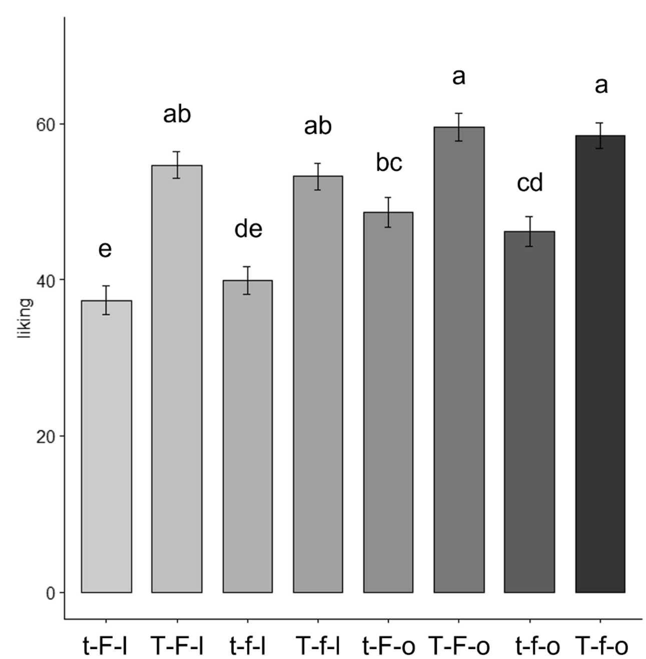

Fig. 2. Liking ratings and Tukey test values of the samples. Error bar represents standard error of the mean (SEM).

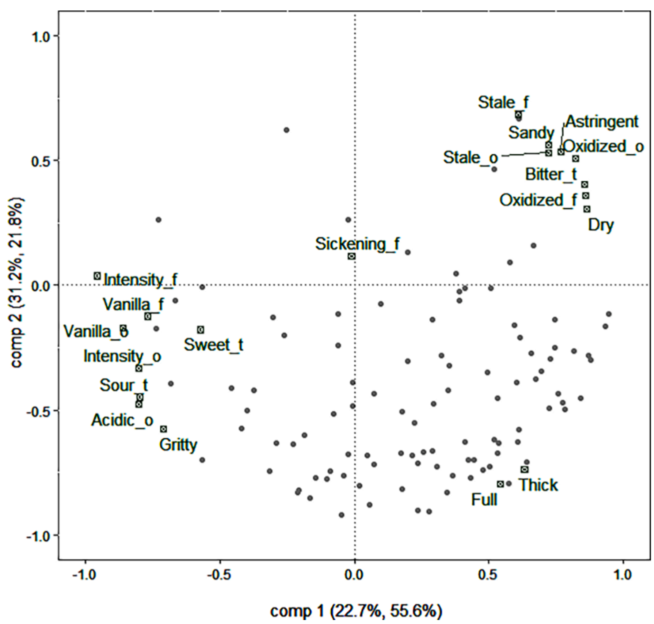

Fig. 3. PLS internal preference mapping: correlation loadings. Sensory data (X) – *responses*: standardized, and column-centered. Consumer data (Y) – *predictors*: column-centered. The first percentage in the parentheses below the horizontal axis and along the vertical axis refers to explained variance of consumer data and the last number corresponds to the explained variance of the sensory data (for PLS component 1 and 2).

have strong preference for the texture attributes *thick* and *full* (lower-right part of the plot) which correspond to the products T-F-l, T-f-l, T-F-o, and T-f-o (Fig. 4).

The samples in the upper and left part of the plot represent the thinner samples. Samples t-f-l and to some extent t-f-o, were characterized by the sensory attributes to the upper side of the plot, related to attributes linked to the thin samples containing flour, i.e., towards the upper-right (e.g., *oxidized*, *bitter*, *sandy, dry*, etc.), while the samples t-F-l and t-F-o tended more towards the sensory attributes on the left-side of the correlation loading plot (e.g., *vanilla*, *intensity*, *sweet*, etc.). This shows that the texture attributes were the main drivers of liking of the products, added to the fact that the negative flavour and mouthfeel attributes imparted by the flour seemed to come through easier in the thin samples (i.e., *oxidized*, *bitter*, *sandy*, *dry)*. However, there are some flavour attributes to the right of the plot which some consumers favored. It should be noted that sickening had a very weak relation to the consumer data, either because the attribute was not related to consumer preferences (or lack of preference) or because it is not perceived by consumers in the same way as for the trained panel.

All these results correspond well to the ANOVA results, the advantage here is that the sensory drivers of liking are pinpointed, and that the individual variability among consumers is visible.

4.2.3. PLS external preference mapping

Figs. 5 and 6 show the correlation loadings and scores plots for PLS external preference mapping for the column-centered consumer data. Furthermore, Figs. 7 and 8 illustrate the correlation loadings, and scores plot for PLS external preference mapping for the double-centered consumer data.

Figs. 5 and 6 are highly similar (only with a slight rotation) to the corresponding figures for the internal preference mapping (Figs. 3 and 4). Thus, the results are similar to the PLS internal preference mapping above (see section 4.2.2).

Regarding the correlation loading plots, we can see that the two plots (Figs. 5 and 7) are quite similar regarding the explained variances. In the double centered plot (Fig. 7) consumers are spread out over the whole region. In this type of plots there is no indication of which samples are liked better than others, only about which consumers like the different products more or less than the average consumers. For instance, the consumers in the upper right corner are consumers which have a higher preference for product 3 than the rest, not that they prefer product 3 (see for instance Fig. 3). This spread of consumers over the whole region is

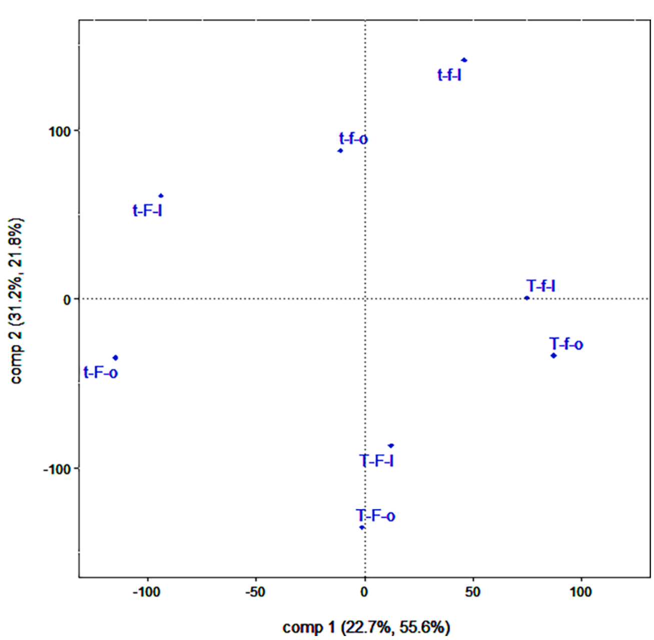

Fig. 4. PLS internal preference mapping: scores. Sensory data (X) – *responses*: standardized and column-centered. Consumer data (Y) – *predictors*: column-centered. The first percentage in the parentheses below the horizontal axis and along the vertical axis refers to explained variance of consumer data and the last number corresponds to the explained variance of the sensory data (for PLS component 1 and 2).

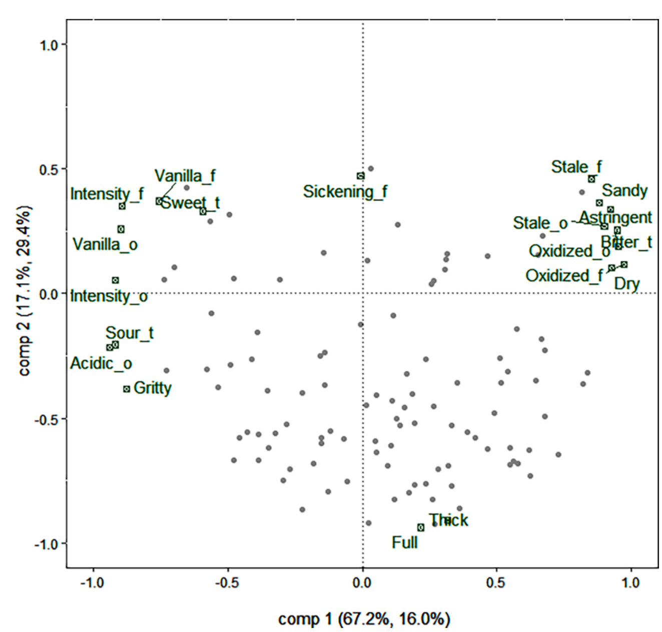

Fig. 5. PLS external preference mapping, correlation loadings. Sensory data (X) – *predictors*: standardized and column-centered. Consumer data (Y) – *responses*: column-centered. The first percentage in the parentheses below the horizontal axis and along the vertical axis refers to explained variance of sensory data and the last number corresponds to the explained variance of the consumer data (for PLS component 1 and 2).

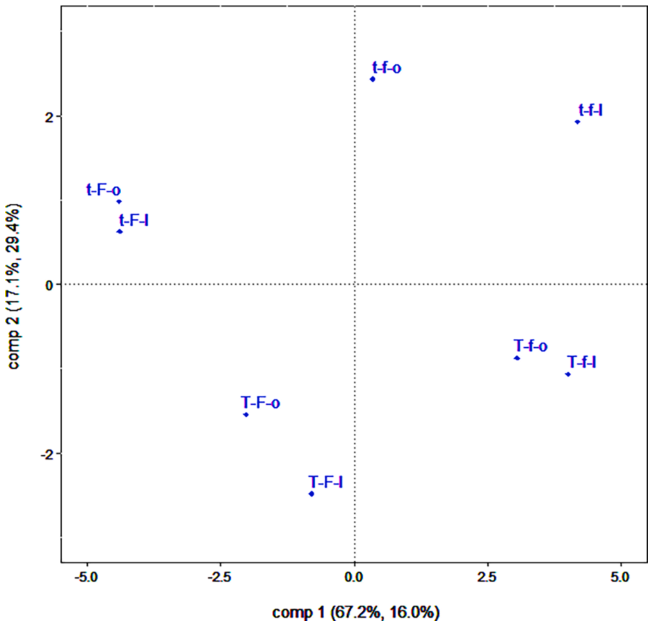

Fig. 6. PLS external preference mapping, scores. Sensory data (X) – *predictors*: standardized and column-centered. Consumer data (Y) – *responses*: column-centered. The first percentage in the parentheses below the horizontal axis and along the vertical axis refers to explained variance of sensory data and the last number corresponds to the explained variance of the consumer data (for PLS component 1 and 2).

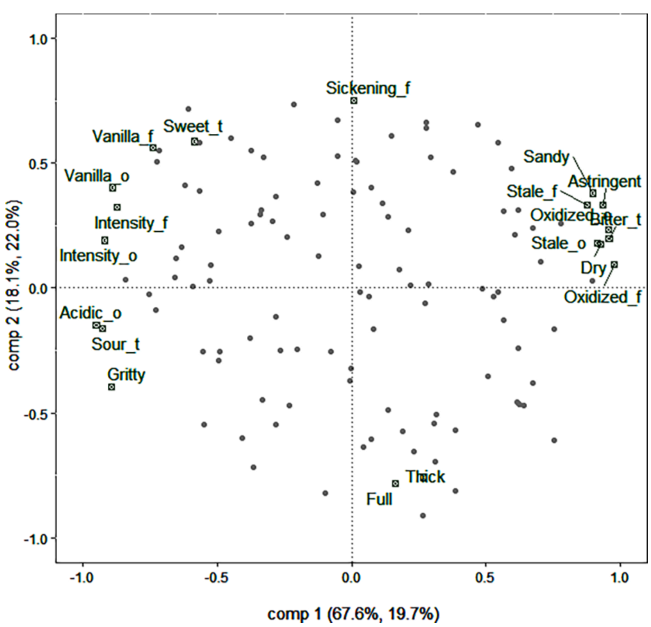

Fig. 7. PLS external preference mapping, correlation loadings. Sensory data (X) – *predictors*: standardized and column-centered. Consumer data (Y) – *responses*: double-centered. The first percentage in the parentheses below the horizontal axis and along the vertical axis refers to explained variance of sensory data and the last number corresponds to the explained variance of the consumer data (for PLS component 1 and 2).

natural since the origin is now the center of both samples, and consumers. The sensory attributes are roughly at the same place in the perceptual space. The same is the case for the scores in Figs. 6, and 8.

4.2.4. Relating consumer loadings to consumer attributes

The results correspond to *step 2* of the two-step approach, that is, PLS regression model is fitted with the *first two consumer liking loadings* from *step 1* as response and the transposed matrix ***Z*** of *consumer attributes* as predictors.

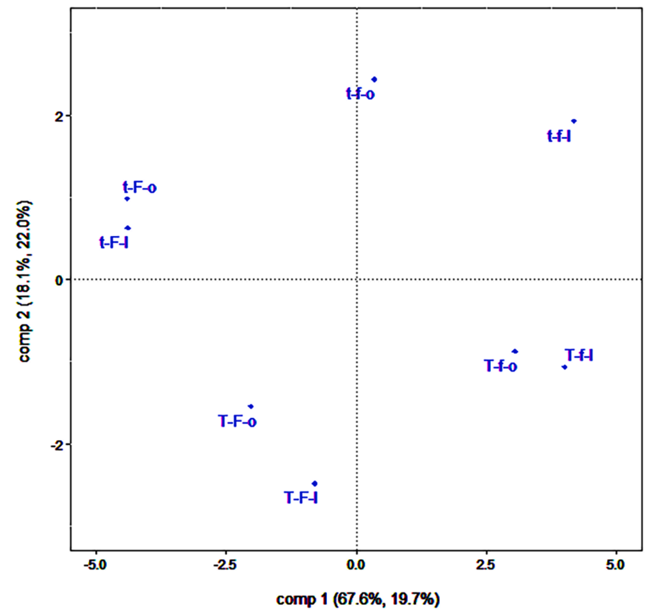

Fig. 8. PLS external preference mapping, scores. Sensory data (X) – *predictors*: standardized and column-centered. Consumer data (Y) – *responses*: double-centered. The first percentage in the parentheses below the horizontal axis and along the vertical axis refers to explained variance of sensory data and the last number corresponds to the explained variance of the consumer data (for PLS component 1 and 2).

Fig. 9 shows the map for consumer attributes linked to components 1

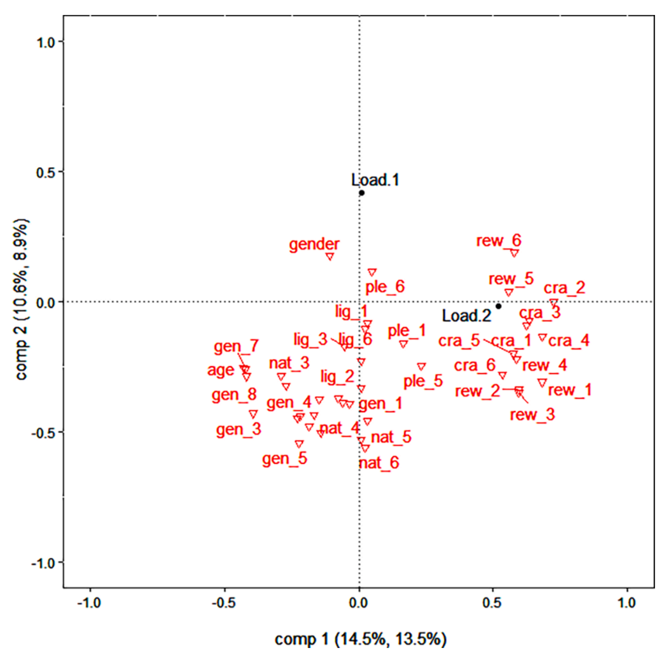

Fig. 9. Consumer attributes vs. Consumer liking loadings 1 and 2: the results are based on results presented in Figs. 5 and 6. For this analysis consumer attributes and loadings from Fig. 5 are centered and standardized before PLS regression. The first percentage in the parentheses below the horizontal axis and along the vertical axis refers to explained variance of consumer attributes, and the last number corresponds to the explained variance of the consumer loadings.

and 2 (standardized and centered) with column-centered and standardized consumer attributes (results taken from Figs. 5 and 6). The two components from the consumer loadings (Load.1 and Load.2) represent an axis each, Load.1 along the vertical axis, and Load.2 along the horizontal. As it is shown from the percentages on the axes, the second consumer loading (Load.2) represents a substantially stronger relation to consumer attributes, which is not surprising since component 2 above was the most dominating for liking.

The consumer attributes basically split in two groups, and interpretation should be performed in comparison with the plots in Figs. 5 and 6. Group one (right side of the plot), with a high value of consumer loadings 2 (Load.2, corresponding to low liking values for most consumers, Fig. 5) is characterized by consumer attributes related to two types of taste-related factors such as using food as a reward (e.g., *rew_5, rew_6,* etc.), and craving for sweet foods (e.g., *cra_4, cra_5,* etc.). The first group of consumer attributes is related to low values of thick and full (Fig. 5), and particularly samples t-f-l and t-f-o (Fig. 6). Conversely, samples T-F-l, T-f-l, T-F-o, and T-f-o (described by the sensory attributes *thick* and *full*) liked by consumers is negatively related to the consumer attributes *reward* and *craving for sweet foods.* In principle, it may appear counter-intuitive that consumers that reward themselves with food and have cravings will not be associated with typically more indulgent samples with thicker textures, but the explanation may lie on the *sickening* flavour, potentially providing a more intense, cloying experience, which some consumers with craves may enjoy.

Consumer attributes in group two (middle-lower left side of the plot in Fig. 9), which tends to have lower values of Load.1 and Load.2, is mainly characterized by consumer attributes related to health-related factors such as general health interest (e.g., *gen_3, gen_4,* etc.), light product interest (e.g., *lig_2, lig_3,* etc.), and natural product interest (e.g., *nat_4, nat_5*, etc.). The comparison with Figs. 5 and 6 shows that the second group of consumer attributes is related to samples T-F-l and T-F-o, but also to samples t-F-l and t-F-o. These are the flakes samples. Consumers more interested in health and natural attributes could have been driven by the flakes, linking them to higher fibre content. These samples are related in particular to *gritty*, *acidic* and *sour*, but also to the attributes *vanilla_f, vanilla_o, intensity_f*, and *intensity_o*.

4.3. One-step approach (L-PLS regression)

4.3.1. Endo-L-PLS regression

The sensory description in Fig. 10 shows that the first component (Comp.1) is interpreted by both texture attributes (*sandy, dry* on the right vs *gritty* on the left), and flavour attributes (*oxidized, bitter* on the right vs *sour, acidic* on the left). Note that the attributes *vanilla*, and *sweet* are located on the left of the component 1, in some extent, related to *sour,* and *acidic*. The second component (Comp.2) is described by texture attributes *full* and *thick* vs the property *sickening flavour*. *Sickening* (cloying) *flavour* was more intense in the samples with flour (small particles), and it may have been more distinguishable in the thin viscosity samples (t-f-l and t-f-o).

As expected from the sensory attributes, the products t-F-l, T-F-l, t-F-o, and T-F-o, on the left of the component 1, are flakes products (see Table 1), the rest of the samples, on the right-hand side of the component 1, are flour products. Coupled with sensory description, samples with flakes were characterised by higher values of *gritty* (imparted by the need to somehow chew the flakes within the yoghurt mass), and some of the typical "yoghurt with cereal flavours" *sour, acidic, vanilla,* and *sweet.* On the other hand, the flour containing products t-f-l, T-f-l, t-f-o, and T-f-o were associated to textures imparted by the smaller particles *dry, sandy,* and *bitter, stale,* and *oxidized* flavours. On the second component (Comp.2), the products were separated in terms of their yoghurt consistency. Products T-F-l, T-f-l, T-F-o, and T-f-o (*think,* and *full*) are contrasted to products t-F-l, t-F-o, and t-f-o, the thinner samples that were associated with low values of *thickness*, *fullness,* and high values of *sickening* flavour attribute.

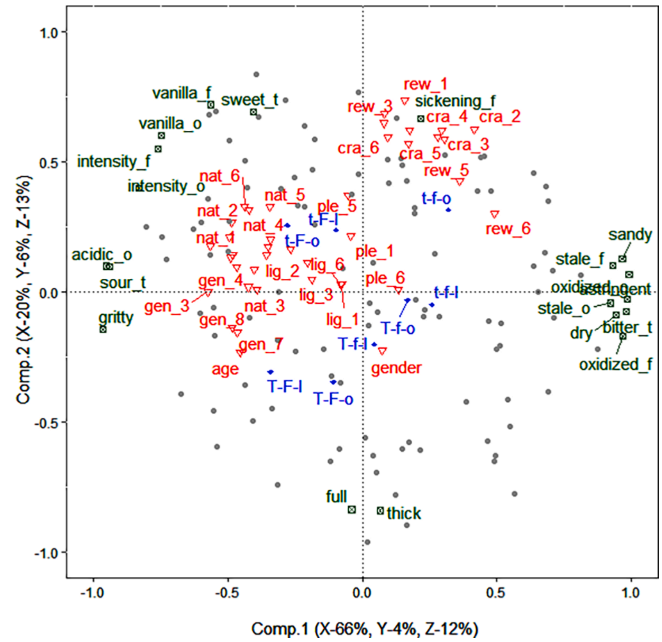

Fig. 10. Endo-L-PLS. Sensory data (X): centered and standardized for each sensory attribute. Consumer data (Y): double-centered. Consumer attributes (Z): centered, and standardized for each consumer attribute.

Sickening flavour is located opposite to thick and full. Those consumers who lie in this direction, thus, may like sickening flavour samples, or else, liking for those consumers could be driven by yoghurt consistency, and they may favour thinner yoghurts, low in *thick,* and *full*. Since double centered consumers' liking ratings only represent relative differences between products, it is the more or less liking of full and thick in contrast to sickening flavour which is the dominating aspect here. We also refer to Fig. 5 which clearly shows that very few consumers are located in the direction of sickening flavour.

The consumer attributes were essentially split in two groups, a group containing the attributes related to reward (e.g., *rew_1,* etc), craving (e.g., *cra_4,* etc), and another group containing the rest of the measured attributes, linked to health interest and pleasure (e.g., *nat_2, lig_1* and *ple_1*). The former group lies in the direction of sickening flavour and that could respond to the fact that consumers more inclined to cravings could enjoy intense cloying flavours; meanwhile, the latter group tends more towards the flake products (t-F-l, T-F-l, t-F-o, and T-F-o) and the attributes that characterise these. Consumers preferring these samples, are more interested in natural and healthy food choices, and yoghurts where more visible fibre (flakes) and more typical yoghurt flavour (sour, vanilla, sweet) could have been associated to healthier, more natural characteristics. Consumer liking ratings data were spread quite evenly over the actual region.

4.3.2. Exo-L-PLS regression

The results of *exo*-L-PLS regression in Fig. 11a (see also Fig. 11b for clearer view of the consumer attributes) have the same trend with those of *endo*-L-PLS regression. The splitting of consumer attributes in two distinct groups is less clear here. This may indicate that the split is more due to a split (segmentation) in the original consumer attributes data set than in their relations with consumers' liking ratings. The components are here not fully independent (orthogonal) of each other, and this could also be a possible explanation.

As can also be seen, the consumer attributes are closer to the center which is natural since now the deflation is done for consumer liking ratings, and the predictive relations are outwards.

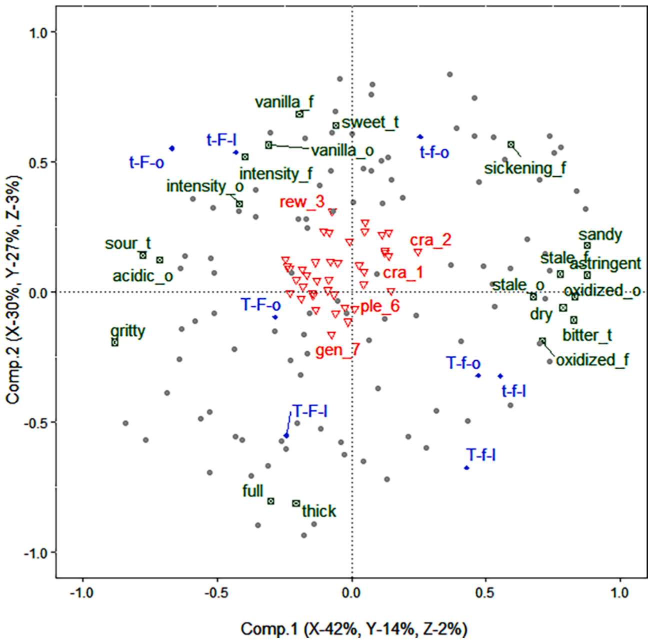

Fig. 11a. Exo-L-PLS. Sensory data (X): centered, and standardized for each sensory attribute. Consumer data (Y): double-centered. Consumer attributes (Z): centered, and standardized for each consumer attribute.

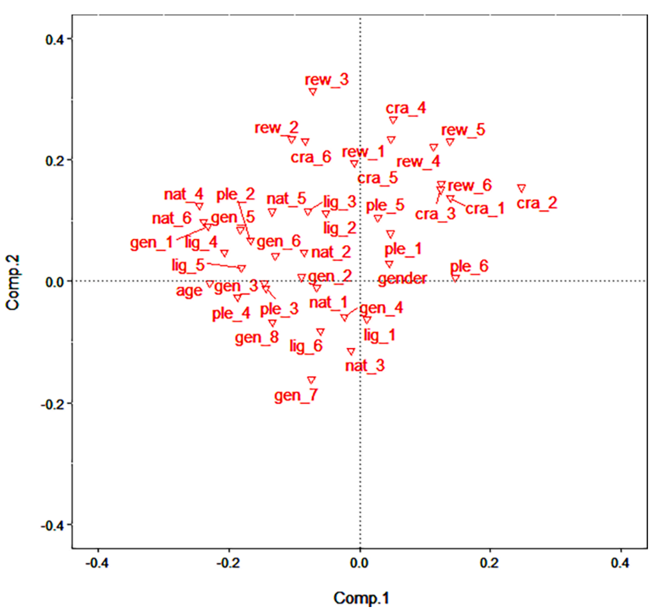

Fig. 11b. Exo-L-PLS. Sensory data (X): centered, and standardized for each sensory attribute. Consumer data (Y): double-centered. Consumer attributes (Z): centered, and standardized for each consumer attribute. *Consumer attributes are zoomed in.*

4.3.3. Comparison of endo- and exo-L-PLS

Table 3 shows that *exo*-L-PLS explains more of ***Y*** than the *endo*-L-PLS (14% and 27% as compared with 4% and 6%). This is as expected, since the *exo*-L-PLS defines the latent structures in terms of its bi-linear components from ***Y***, while the *endo*-L-PLS defines them from the ***X***- and Z'-components. Moreover, it shows that the sensory attributes data in ***X*** are in general better modelled than the consumer attributes data in ***Z'*** (for both *endo*- and *exo*-L-PLS). Importantly, using *exo*-L-PLS, consumer attributes (Z') are not well explained with 2% and 3% explained sum-of-squares in component 1 and 2, respectively. This is a quite standard finding in this area, the relation between sensory, and consumer liking ratings is stronger than between liking ratings and consumer attributes. It explains why consumer attributes are more or less located in the middle (Fig. 11a) whereas it does not happen for *endo*-L-PLS (Fig. 10), as was already discussed above.

Table 3
Percent sum-of-squares in the three blocks explained by the first two components.

	Component 1 (%)	Component 2 (%)
Endo-L-PLS		
X	66	20
Y	4	6
Z'	12	13
Exo-L-PLS		
X	42	30
Y	14	27
Z'	2	3

4.4. Comparison of the two-step PLS regression and one-step L-PLS regression

4.4.1. Interpretation

Comparing the outcomes of the two approaches we can see that the PLS external mapping with consumer data double-centered (Fig. 7) is very similar to both the *endo*-L-PLS (Fig. 10), and *exo*-L-PLS maps (Fig. 11) in terms of samples, sensory attributes, and consumers' liking ratings with slightly more dispersed (and visible) sensory attributes especially for *exo*-L-PLS regression. We can also see that the effect of double-centring shows that in both approaches consumers are well spread in the space, which is natural because of the pre-treatment. For the preference mapping approaches, the relation between the sensory attributes and samples is similar regardless of whether one uses double-centered consumer liking data or not. This means that when concerns interpretation of the relation between samples and sensory attributes, all approaches give similar results.

Concerning the consumer attributes and how they relate to the other data sets, the L-PLS methods lead also in this case to similar interpretation as the approach based on using standard preference mapping with subsequent regression of consumer loadings (from the first step) vs. consumer attributes. In particular this is true for the *endo*-L-PLS since two groups of attributes can be clearly identified. For *exo*-L-PLS, consumer attributes appear to be not so well spread.

It is worth noting that the consumer loadings for the L-PLS methods (because of double-centring) contain no information about the overall differences in preference for the different products. The standard external, and internal preference mapping is more useful in this respect. This means that the L-PLS methods need to be supplemented by an additional analysis in order to reveal the actual differences in liking between products. A possibility here is to use standard ANOVA as shown above. The results from the ANOVA give similar conclusions about liking of product differences as the external preference mapping. The two-step approach pinpoints, however, more explicitly individual differences in product liking differences (given in the original units).

4.4.2. User-friendliness and flexibility

Regarding interpretation of all methods covered here, the focus is on scores plots and loadings plots of different style. In that sense, interpretation goes along the same lines. The one-step approach, however, has the advantage that everything can be read out of one single plot, while the two-step approach needs plots for both steps 1 and 2. The advantage of the latter is that the interpretation can be done in sequence using standard methods for which interpretation is well known. The sequential interpretation may be important in practice. If for instance one detects an interesting pattern among consumers in the plots in *step 1*, one can place the consumers in clusters, and then use PLS-DA (Almli et al., 2011; Asioli et al., 2014) in order to investigate the relation between consumer attributes and the clusters. This procedure is less obvious with direct use of the one-step approach.

5. Discussion & conclusions

This paper investigates and compares for the first time the two-step PLS and one-step L-PLS regression approaches using data from an experiment investigating consumers' preferences for yoghurts in Norway. We found some interesting outcomes. First, the two approaches, one step and two step methods, show very similar results. Second, the two approaches differ in the way interpretation is done. Indeed, in the one-step L-PLS approach the results are visible all in one plot which can make the interpretation easier at a first instance, but the method is less understood than the standard PLS regression approach used in the two-step PLS approach. However, the interpretation of the consumer liking ratings is less straightforward in the one-step L-PLS since double centered liking data are used. Therefore, an additional ANOVA is required. More research is needed to better explore the properties of the L-PLS regression methods because they are generally less understood than for the standard PLS regression.

In both approaches (two step and one step), the interpretation of the consumer attributes vs the sensory attributes of the sample were by times not easy, in particular when trying to relate consumer attributes as measured by their attitudes to health and taste. As an example, results showed that consumers that usually have cravings and use food as reward, were those less preferring thicker, full yoghurts, usually associated to more indulgent experiences. However, the experimental design in this case study was originally designed to study satiety perception with regards to preference and eating behaviour, keeping composition constant, not to have extreme samples in terms of indulgency. Further studies with more different or extreme samples should be conducted and analysed by the same methods as treated here.

In conclusion, this paper shows that the two-step PLS and the L-PLS regression approaches provide similar results when integrating sensory, and consumer information. However, the two-step PLS regression approach provides more direct interpretation of individual differences in liking.

CRediT authorship contribution statement

Daniele Asioli: Methodology, Formal analysis, Software, Validation, Writing - original draft. **Quoc Cuong Nguyen:** Methodology, Formal analysis, Software, Validation, Writing - original draft. **Paula Varela:** Funding acquisition, Project administration, Writing - review & editing. **Tormod Næs:** Conceptualization, Methodology, Supervision, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.foodqual.2021.104426.

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