Exploring the common and unique variability in TDS and TCATA data - a comparison using canonical correlation and orthogonalization

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Highlights

- TDS and TCATA are compared by common and distinct components
- Common components are identified by canonical correlation analysis
- Distinct components are found after orthogonalization
- Results indicate only subtle differences between the methods
- TCATA give better discrimination of samples in all case studies
Abstract
Temporal Dominance of Sensations (TDS) and Temporal Check-all-that-Apply (TCATA) from three different case studies are compared by means of canonical correlation analysis, orthogonalization and principal component analysis of the vertically unfolded data (which means that the matrices compared have samples*timepoints in the rows and attributes in the columns). The multivariate analyses decompose the datasets into common and distinct components. The results showed that the major part of the variation is common between the two methods for the cases investigated, but that there were subtle differences showing better discrimination for TCATA than TDS. TDS showed a more complex data structure and more unique variation. The unique variation in TDS is, however, difficult to interpret. The methods are more different towards the end of the mastication, this can be explained both by the difficulty of assessors to agree on the dominant attributes at the bolus stage for TDS, and that assessors may forget to unclick attributes in TCATA. This work builds on recent methodological studies on temporal methods that aim to better understand differences among methodologies and ultimately to identify what methods could be better for answering different objectives.
1 Introduction

Sensory perception is a dynamic process as the perceived sensory characteristics of products change during consumption due to several complex processes, such as chewing, breathing, salivation, tongue movements and swallowing (Lawless & Heymann, 2010). Methods for tracking changes in sensory perception over time have been used since the beginnings of sensory science (Holway & Hurvich, 1937; Sjostrom, 1954). The first methodological approach for temporal sensory measurement was time-intensity, which aims at measuring the perceived intensity of a given attribute continuously over time (Lee & Pangborn, 1986). Although this methodology provides detailed information on the dynamics of sensory perception, it has several drawbacks that limit its application in many situations, including its time-consuming nature, differences in how assessors respond to the task, and dumping effects due to attribute restriction (Lawless & Heymann, 2010).

To overcome these limitations, multi-attribute temporal methods that rely on the description of the sensory characteristics of products over time have been developed, including Temporal Dominance of Sensations (TDS) (Pineau, Cordelle & Schlich, 2003) and Temporal Check-all-that-apply (TCATA) (Castura, Antúnez, Giménez & Ares, 2016). In TDS, assessors evaluate the temporal sensory profile of products by identifying the dominant attribute at each moment of the evaluation (Pineau et al., 2009). Although no standard definition of the dominant attribute exists, most recent studies define dominance as the “ability of sensory attributes to catch assessors’ attention” (Di Monaco, Su, Masi & Cavella, 2014). TDS focuses only on the dominant attribute, not other sensory characteristics that are simultaneously perceived while consuming a product. This could lead to a relevant loss of sensory information when dealing with complex products that require simultaneous evaluation of multiple sensory modalities (Ares & Jaeger, 2015). In TDS data, competitive effects of attributes and modalities may be linked to enhanced dumping or dithering (Varela et al., 2018). To overcome these problems, variations of TDS have been proposed, such as TDS by modality (Agudelo, Varela, & Fiszman, 2015; Nguyen, Næs, & Varela, 2018) and dual TDS (Schlich, 2017).

TCATA proposes a different type of multi-attribute temporal evaluation, in which assessors are asked to identify all the sensory characteristics that describe products at each moment of the evaluation (Castura et al., 2016). This methodology can be regarded as an extension of (static) check-all-that-apply (CATA) questions, which have become one of the most popular methods for sensory characterisation with consumers (Ares & Jaeger, 2015). In TCATA, assessors are allowed to select all the attributes that are perceived simultaneously during product consumption and are asked to uncheck sensory attributes when they are no longer applicable (Castura et al., 2016). A potential problem of TCATA lies in the complexity of the task of selecting and unselecting attributes during the evaluation period; a variant of the method, called TCATA Fading, attempts to simplify the task by having attributes return to an unselected state over a predetermined time period, which frees assessors from needing to deselect attributes manually (Ares et al., 2016).

TDS and TCATA are conceptually different and, therefore, they are expected to differ in the information they provide about the dynamics of the sensory characteristics of products. Information on the similarities and differences between these methodologies can help practitioners to select the methodology that best suits for a particular application. TDS and TCATA have been compared in several studies which have shown that TCATA may give better discrimination or provide more detailed information about how the sensory characteristics of products evolve over time (Ares et al., 2015; Esmerino et al., 2017; Nguyen et al., 2018). In general, both TDS and TCATA identify the most relevant changes in the sensory characteristics of products during consumption. However, in previous studies TCATA has shown better discrimination between samples. In addition, significant differences among samples were found for a larger number of attributes in TCATA than in TDS (Ares et al., 2015). Typically, TCATA also gives longer periods of time with significant differences.
In studies comparing TDS and TCATA, data from the two methodologies have typically been analysed separately and comparisons have been done on the basis of the interpretation of the standard analyses, such as looking into significant differences, PCA trajectories, and TCATA or TDS curves. Recently (Nguyen et al., 2018) compared TDS, TCATA and TDS by modality using Canonical Variate Analysis (CVA) and MANOVA on time intervals as described in (Dinnella, Masi, Næs, & Monte Leone, 2013). They showed that TCATA was more discriminative and assessors were more in agreement, as compared to TDS and TDS by modality.

In the present work, we approach the problem of comparing the TDS and TCATA by using multivariate methods to compare the data structures directly. Many different approaches to compare two or more datasets containing measurements on the same set of samples exist. For instance, Consensus PCA (e.g., see Westerhuis, Kourt, & MacGregor, 1998), Multiple Factor Analysis (MFA; Abdi, Williams, & Valentin, 2013; Escofier & Pagès, 1994) and Canonical Correlation Analysis (CCA; Hotelling, 1936; Mardia, Kent, & Bibby, 1979). In this work we are especially interested in finding common and distinct parts in the multivariate structures of TDS and TCATA and have used the method called PCA-GCA first described in Smilde et al. (2017). This method consists of doing data reduction of single blocks by PCA first, and then using canonical correlation analysis (CCA) to find common components. The method is described in more details in section 2.3.

The aims of the present study are to compare TDS and TCATA using PCA-GCA in order to investigate whether the multivariate structures can give improved insight into differences observed for TDS and TCATA, and to introduce common and distinct component analyses as a tool for the sensory and consumer science field. The concept of separating common and distinct components from multiple datasets for the same set of samples has received little attention in sensory and consumer science. We expect that analysing data with respect to common and distinct components can bring a broader understanding of the relationships between interconnected data sets (e.g. chemical, sensory and consumer data for the same set of samples), or for joint analysis of several types of consumer responses. The common and distinct analysis by PCA-GCA is used to compare TDS and TCATA evaluations performed by a trained panel on yoghurt, cheese and bread samples. The results for the yoghurt data were presented at Sensometrics 2018 (Montevideo, Uruguay) and are presented with other purposes in (Nguyen et al., 2018). The cheese data have not been published before, whereas the bread data example was discussed by Varela et al. (2018).

## 2 Background

### 2.1 Data structures investigated

The data structures obtained from TDS and TCATA are similar in nature but with some obvious differences. In TDS (Pineau et al., 2003; Pineau et al., 2009) assessors are asked to select one attribute, the dominant one, from a list, at each moment. In TCATA (Castura et al., 2016), they are asked to select the attributes that apply to describe a focal product at each moment in time (also from a list) and can select several attributes that are applicable. For both methods, the data for each assessor can be represented as a series of 0’s and 1’s for each point in time, where 1 indicates selection and 0 indicates non-selection of an attribute. More precisely, with J pre-specified attributes the data for each assessor j and sample i can be represented as a matrix of 0’s and 1’s of dimension J*T where T represents the time points. For TDS, there will be only one 1 in each column since only one attribute can be dominant attribute at a given time, whereas for TCATA more than one of the attributes can have a value of 1.

Combining all samples for one assessor gives a three-way data structure (of dimension N*J*T), whereas putting all assessors together provides a four-way data structure. In this paper we will focus on the aggregated data. More specifically, for each sample the dominance rates (TDS) and the citation rates (TCATA) were computed as the average for each attribute for each time point. This leads to a three-way data table of dominance/citation rates (samples*attribute*time). Note that the sum of
TCATA attribute citation rates (for a product at each time point) can be higher than one since several attributes can be co-selected. Data were time standardized according to Lenfant et al. (2009) using the R-package tempR (Castura, 2018). For multivariate analyses the three-way data is unfolded in such a way that the rows represent sample*time and columns represent attributes. These vertically unfolded matrices are mean centred prior to analyses. Data were also smoothed prior to the analyses.

2.2 Time dependent similarity between TDS and TCATA
The time-dependent similarity between the data arising from these two methods are investigated by computing the Pearson correlation and the Euclidean distances between the data vectors obtained for each time point. These vectors have one entry for each sample*attribute combination. Since the range of the data vectors from TDS and TCATA differ with a maximum of one for TDS and higher for TCATA, the vectors where scaled by dividing with the maximum value for each timepoint, as all timepoints include at least one zero for one or more attribute*sample combinations, this make sure that the data vectors from the different methods have the same range after scaling. To account for differences in the number of samples and attributes, distances were normalized by dividing by the square root of number of observations for each time point (number of samples x number of attributes). Plots of time versus distances and correlations were applied to investigate when in the evaluation period the methods are more or less similar. Similar patterns were identified for both the distance and correlation approaches, and the result section focuses on the distance approach.

2.3 Analyzing multiblock data by common and distinct components
In food science and related fields, it is becoming more usual to have several data sets describing the same set of samples. In the present paper, only two such sets (TDS and TCATA) are considered; whereas in other cases there may be more datasets to describe the products: the experimental design, descriptive sensory data and chemical data, or different consumer responses to the same products: liking, intake, emotions elicited and so forth. For researchers, it is of great value to better understand the relationships between different data sets related to the same set of samples. One approach for analyzing multiblock data sets, is to identify common and unique variation for each block. The idea behind this approach is that the observed data for each block can be decomposed into common and distinct components, each of which contribute to the observed variability. Conceptually, the common components describe variations arising from the same underlying phenomena, but that is manifested by different measurements (i.e. data blocks), whereas the distinct components are related to phenomena only “seen” by single data blocks. Smilde et al. (2017) discuss and compare methods for identifying common and distinct components in a common mathematical framework. The performance of the different methods is further discussed by Måge, Smilde, & Kloet (2018). In this work the method named PCA-GCA, which will be described below, was chosen for analyzing common and distinct components in TDS and TCATA data.

2.3.1 Separating common and distinct components: PCA-GCA
The overall procedure of PCA-GCA is illustrated in Figure 1. In the first step, each data block (here TDS and TCATA) is decomposed by PCA. Then canonical correlation analysis (CCA; Hotelling, 1936; Mardia et al., 1979) is applied to find the common components between the datasets. Next, the common information is removed by orthogonalization. Finally, PCA is applied on the remaining part to structure the remaining information labelled as unique. For the general case with more than two blocks, generalized canonical correlation analysis (GCA; Carroll, 1968; Kettenring, 1971) is applied instead of CCA. Since the methodology has been developed and named for the multiset-data case, it is here referred to as PCA-GCA although CCA is applied since we work with only two blocks (TDS and TCATA). Similar approaches have also been applied for regression with multiple blocks of independent variables (Måge, Mevik, & Næs, 2008; Måge, Menichelli, & Næs, 2012).
2.3.2 Canonical correlation analysis (CCA)

Canonical correlation analysis can be defined as finding the linear combinations of $X$ and $Y$ with the maximum correlation. These linear combinations are called canonical variates and represent the common information in the two data sets. First the component with the largest correlation is found, after that new components are extracted using the same criterion under the restriction that the components are uncorrelated.

In more detail, with two blocks $X$ and $Y$, the canonical variates are computed as linear combinations of variables in $X$ and $Y$ such that the correlation between $u=a'X$ and $v=b'Y$ is maximized. The next variate is obtained using the same criterion, but under the restriction of orthogonality. The central results of CCA are the canonical correlations, the canonical coefficients $(a, b)$ (loadings), and the canonical variates $(u, v)$ (scores). Bold letters indicate vectors.

Like all other correlation-based methods, CCA is sensitive to noise and overfitting. When the number of variables exceeds the number of observations (or variables are highly multi-collinear), a data compression (using for instance PCA) is needed before the canonical variates are calculated to avoid overfitting. It should be emphasized that the loadings or the coefficients of the canonical variates are not orthogonal to each other as in PCA.

2.3.3 Common and distinct components

In PCA-GCA (Smilde et al., 2017) the canonical variates with large enough correlation and which explain a considerable part of the variation, represent the variation that is common between the two datasets and will in the following be referred to as the common components.

The common variation can be removed from the data by orthogonalization with respect to the common components. The idea is that what is left after the common part is removed represents unique information for each data set (unique signal plus noise). The orthogonalization can be done in two different ways, either by orthogonalizing $X$ and $Y$ with respect to the common scores $(C_A)$, or with respect to the canonical variates for the respective blocks $(U_A$ and $V_A)$. The latter approach is more natural since the common scores are not in the space defined by $X$ and $Y$ (Langsrud, Jørgensen, Ofstad, & Næs, 2007) and is therefore applied here. This means that $X$ is orthogonalized with respect to the canonical variates obtained from $X$, and that the same is done for $Y$. This means that with this method we identify two separate subspaces that are as similar as possible. In the case of a common component, the parts of $X$ and $Y$ that are orthogonal to the common part, can be computed as

$$X_A^{ort} = X - U_A(U_A'U_A)^{-1}U_A'X$$

$$Y_A^{ort} = Y - V_A(V_A'V_A)^{-1}V_A'Y$$

After orthogonalization, the distinct components are obtained by PCA on $X^{ort}$ and $Y^{ort}$. Differences between TDS and TCATA can then be investigated studying ordinary PCA plots for the unique parts, whereas the similarities are expressed as the common part, given by the canonical variates. Note that distinct components for one block are orthogonal to the common components of the same block, but not necessarily to common or distinct components from the other block.

2.3.4 Interpreting and selecting the number of components

Both common and distinct components can be interpreted and investigated by looking at scores and loadings plots in the same way as for PCA. The canonical scores $(U$ and $V)$ can be studied separately for each block, or as common scores estimated as the average of $U$ and $V$ for each component identified. Score plots for two components at a time can be obtained by plotting the scores in two-dimensional scatter plots. Each point represents one sample*time combination, and the line connecting the scores represent the time trajectory for how the samples evolve during the evaluation period. An alternative to
the two-dimensional score plots with trajectories is to fold the scores into a three-way structure (samples, component, and time), and then plot scores versus time for one component at a time.

The common components can be interpreted by looking at scatter plots of the corresponding canonical coefficients \( \mathbf{a} \) and \( \mathbf{b} \). For distinct components, interpretation can be done using scatter plots of scores and loadings from the PCA. Canonical coefficients for the common part will be investigated by correlation loading plots based on correlations between the original variables (for \( \mathbf{X} \) and \( \mathbf{Y} \) and the corresponding canonical covariates (\( \mathbf{U} \) and \( \mathbf{V} \)). To enhance interpretation of the similarities and differences between TDS data and TCATA data, the correlation loadings for the common components are plotted together (see for instance Figure 6).

The number of components to keep for the initial PCA of each block is not very crucial, as long as enough components are kept for further analysis. When more components are kept in PCA, the canonical correlations tend to be higher. This is natural since canonical correlation analysis only focuses on correlation and with more components there will be more variability to search from. In this paper we decided to focus on components which together explain 90% of the variation. This is large enough for capturing the majority of the variability and small enough to avoid bringing in too much of the noise. It is unlikely that the last 10% of the variability in this type of quite noisy data will contribute in any useful way to interpretation.

A canonical variate with a reasonably large correlation, but with a small explained variance may be considered of little interest for interpretation. Therefore, as a general rule only components with both high canonical correlation and explained variance should be considered to be common components. Typically, one would want the required common components to explain at least 10% of the variance in the data and to have canonical correlations of at least 0.9. Since this study has an explorative character, other choices were also tested and commented on in the case studies below. Although the terminology distinguishes between common and distinct components, it is important to emphasise that in practice it is impossible to find components describing only common or only unique variability. Therefore, this type of methodology should always be used as done here together with interpretations and testing of alternative choices of number of components.

In this work the main aim was to study differences between TDS and TCATA, therefore different combinations of common and unique components were investigated, and the number of components reported were selected to highlight differences between the methods.

### 3 Material and methods

#### 3.1 Panel

The sensory panel at Nofima has six years of experience of using temporal method as TDS and TI and one-year experience with TCATA, with a range of different food products including liquids, solids and semi-solids. The ten assessors were selected and trained according to recommendations in (ISO-8586, 2012) and are regularly trained, tested and monitored for their performance. Tests were performed in a sensory laboratory designed according to guidelines in (ISO-8589, 1988) with separate booths and electronic registration of data, EyeQuestion Software (Logic8 BV, Netherlands).

#### 3.2 Case studies

TDS and TCATA were performed by the trained panel on three different cases with the products yoghurt, cheese and bread. An overview of the samples for each of the cases studies are given in Table 1.

##### 3.2.1 Yoghurt

The data were taken from a previous study (Nguyen et al., 2018) and were presented at Sensometrics 2018 (Montevideo, Uruguay). In the original study, eight yoghurt samples were made based on a \( 2^5 \)
factorial design, with factors texture (thin-Thick), granola addition (flour-Flakes), and flavour (optimal-
low). Samples were evaluated by TDS, TDS by modality, and TCATA. In the present paper we use only
the TDS and TCATA data. For more details of the study, refer to (Nguyen et al., 2018). The design and
the labels used for the different products are shown in Table 1.

Attributes used for both tests were Acidic, Bitter, Cloying, Dry, Gritty, Sandy, Sweet, Thick, Thin, and
Vanilla (J=10).

3.2.2 Cheese
Six different cheese products were bought at a local store the day before analysis. The cheese products
were cut into pieces measuring 1x1x2 cm and put into a 3-digit marked plastic container with a lid.
Samples were served at room temperature.
The attributes included in cheese temporal evaluation were Rubber, Grainy, Nutty, Juicy, Acidic, Sticky,
Soft, Sweet, Salt and Umami (J=10).

3.2.3 Bread
Data were taken from a previous study where results were only discussed qualitatively (Varela et al.,
2018). Seven different bread products were bought and sliced early in the morning in a local store, put
into plastic bags, and stored at room temperature. Immediately before each session, the bread samples
were cut into circles with a diameter of 35 mm and put directly into a plastic container marked with a 3-
digit code and covered with a lid.
The attributes included in bread temporal evaluation were Soft, Chew resistance, Coarse, Doughy, Juicy,
Sweet, Acidic, Salt, and Bitter (J=9).

3.3 Experimental procedure
Attribute lists were developed in previous sessions for the purpose of (static) sensory quantitative
descriptive analysis (denoted QDA). From those lists, the panel selected the attributes that were relevant
for the temporal sensory description of the samples in a preliminary session in which they tasted two
different samples selected by the panel leader. The assessors developed a list of attributes, including
taste/flavour and texture, which was used both for TDS and TCATA tests. For each case study, two pre-
tests were run prior to the evaluations, as described below for each product category.
In both tests, attributes were presented in a circular layout on the computer screen. Assessors were
instructed to put the sample in their mouths and click the “Start” button simultaneously. Then, they
performed the TDS or TCATA test as instructed. The evaluation ended when they clicked the “Stop”
button at the time they were ready for swallowing.
For both TDS and TCATA, samples were served following a balanced rotation order, fully randomized
over assessor, product and replicate.
For the formal assessment, for both TDS and TCATA, products were evaluated in three replicates for
each assessor, with a compulsory 1-minute break between each sample and a 10-minute break between
every four samples tasted.
3.3.1 TDS
For the TDS evaluation, the assessors were instructed to put the whole sample into the mouth (bread or
cheese standardized piece, or a spoonful of yoghurt), and evaluate the most dominant attribute of the
sample at each time until the time for swallowing. Dominance was defined as the sensation that caught
their attention at a given time, not necessarily the most intense (ISO-13299(E), 2016). They were free
to choose as dominant the same attribute for the same sample as often as they deemed necessary.
3.3.2 TCATA
For the TCATA evaluation assessors were instructed to put the whole sample into the mouth (bread or cheese standardized piece, or a spoonful of yoghurt), and check and uncheck all the terms from the list that applied to describe the sensory profile of the sample at each time of the evaluation. They were free to choose the same attribute for the same sample as often as they deemed necessary.

3.4 Data analyses
Each data set was first standardized to 100 standardized time units. Next, attribute dominance rates (TDS) and attribute citation rates (TCATA) were computed and smoothed. Pre-processing steps were performed using the tempR package in R (Castura, 2018).

The time-dependent correlation and distances between the methods were computed as described in section 2.2, before the common and distinct component analysis were performed in Matlab (Matlab, R2017b) using the toolbox PCAGCA which can be downloaded from (https://nofimamodeling.org/software-downloads-list). Readers not using Matlab can easily implement the procedure by combining canonical correlation analysis (CCA), principal component analysis (PCA) and orthogonalization (Equation 2).

The number of common components were selected by looking at the canonical correlation and the explained variance. A general rule is that the canonical correlation should be high, and the canonical covariates should explain a substantial amount of variation (at least 10%) for common components to be of interest. As for all types of multivariate analysis, the model selection (number of components) is not always an easy task. The number of components is discussed separately for each of the case studies.

Stability of solutions from multivariate analyses should in principle be validated. Typical candidates for this are cross-validation and the bootstrap, however, due to the low number of samples and assessors none of these techniques are really suitable here. Instead, solutions from different sets of replicates were compared. More specifically, PCA-GCA was applied for all possible combinations of replicate pairs from TDS and TCATA (nine different combinations). Note that stability of single replicates will be lower than averages, so results will always be on the very conservative side.

To assess the stability of the components, for each data set the Tucker’s congruency coefficient (Lorenzo-Seva, & ten Berge, J, 2006) was computed between the estimated components for all pairwise comparisons for each of the case studies. For each case study, stability was assessed for two different sets of models. For all models PCA with six components was applied in the first step, then stability of common components was first investigated by extracting five common components. Next, stability for both common and distinct components for the models selected for each case was investigated. This gives insight into the identified distinct components for the selected models (the common components will be the same). For each set of models, the percentage of comparisons were the congruency coefficient exceeded 0.85 was computed for each component.

4 Results and discussion
For the yoghurt we refer to (Nguyen et al., 2018), for a detailed description of results obtained for TDS and TCATA. For the two other sets, overviews of results are presented in the appendices. Here we only focus on results from the common – distinct part analyses described in section 2.3.

4.1 Overall comparison
An overall comparison of the methods was performed by a visual comparison of PCA plots of the unfolded data from TDS and TCATA for each of the case studies. In general, the trajectories were similar and could be interpreted in the same way, but with some differences. In the PCA plots for the bread case study (Figure 2), the TDS trajectories are more entangled than the TCATA trajectories. In the beginning of the evaluation the samples were relatively well separated by both methods. For most
samples the TCATA trajectories remained separated throughout the evaluation, whereas for TDS the trajectories ended up in a bundle towards the end (Figure 2). The relative entanglement of TDS trajectories vis-à-vis the TCATA trajectories was most pronounced in the bread case study, but also observed in data from the other case studies (not shown). For the yoghurts and the cheeses, the two or three first components had similar overall patterns. These two datasets were also less complex than the bread study, as some samples were clearly separated from the others also along the first component. Moreover, a larger part of the variation was explained with fewer components for TCATA data than for TDS data (Figure 3). This will be discussed further for each case study below.

PCA-GCA was also tested on raw data without smoothing (not shown). Since the raw data are much more complex, these analyses provided a larger number of components which were more difficult to interpret. With smoothing, a large part of the noise is removed, and the analysis can focus more on the information and real structure in the data. The overall impression of similarities and differences between the data arising from TDS and TCATA methods were similar for the unsmoothed data as for the smoothed data.

4.2 Similarity over time

Figure 4 shows normalized distances between the two data vectors obtained for each method (TDS, TCATA) when looking at single time points. For all three cases, the distance is smallest in the early phase (from t=0 to t=20), then increases between approximately t=20 and t=40. The increase is clearly slower for bread than the other two cases, whereas the distance between TDS and TCATA in early phase is higher for the yoghurt than the other datasets. The time-dependent correlations showed a similar pattern with a drop in correlations between t=20 and t=40 (not shown).

The curves in Figure 4 indicate that TDS and TCATA provide very similar results in the early phase, which is not surprising as the PCA plots (Figure 2) indicated that samples are better separated in the early phase of the evaluation. A possible explanation for good early separation of samples is that textures in the bolus formation tend to be more similar between products within the same product category as compared to intact samples (Peyron et al., 2011). The point where TDS and TCATA start to become more different may be close to the point where the bolus starts to form. Bolus formation has a high inter-individual variability (Panouille, Saint-Eve, Deleris, Le Bleis, & Souchon, 2014; Yven et al., 2012), which may be differently reflected in TDS and TCATA. TCATA has been shown to reflect a more complete sample description than TDS (Nguyen et al., 2018; Ares et al., 2015), so would be assumed to provide a more complete characterization of the dynamic transition from an intact product to a bolus. There may also be variations in when assessors add/remove applicable attributes in TCATA (Meyners & Castura, 2018).

4.3 How many common components?

In each of the case studies, the first six principal components (PCs) were used for input in the common-distinct analysis based on canonical correlation analysis. These components accounted for at least 90% of the variance in the data (Figure 3a). Typically, more components were needed for TDS than TCATA to account for 90% of the variance (Figure 3a). We have, however, chosen to use the same number of components for both methods.

The canonical correlation coefficients are shown in Figure 3a, whereas Figure 3b-d show the explained variance for PCA, and for the common components when computing up to five common components in each of the three examples. The datasets differ in how much of the variation was described by the common components. The common components explained almost as much of the variation as the PCA components, but with some differences between TDS and TCATA, and also between the different cases, which will be discussed below.

Selecting the number of common components can be a difficult task. As the main focus here is to better understand the differences between TDS and TCATA, different combinations of common and distinct
components were investigated by looking at scores for pairs of components (trajectories) or as functions over time (see section 2.3.4). For some combinations it was observed that the distinct components had similar interpretations for both TDS and TCATA in some of the examples. For these cases, more components were selected as common although the canonical correlations were not that high. This strategy was selected since the main aim was to study differences between the two methodologies. This illustrates that the concept of common and distinct components is not black and white, such that components are often neither completely common, nor completely distinct, but something in between. The words common and distinct, are used to label the part of the variation (common or unique) they mostly describe.

Below the three case studies are discussed separately. Since the focus of this work is to find out if there is unique information in either TDS or TCATA, we interpret more components than what is usually done for this type of data.

4.4 Detailed description of the case studies

Prescripts D- and A- are used to denote dominant (TDS) and applicable (TCATA) attributes, respectively; attributes mentioned without prescript are similar for both methods.

4.4.1 Yoghurt

The data from the yoghurt study are summarized in supplementary Figure A1.1. For more info and discussion on the results, please refer to (Nguyen et al., 2018). Figure 4a shows a steady decrease in the canonical correlation from one to five components, without a clear breaking point. The canonical correlations were the lowest among the three case studies.

When looking at PCA results, the explained variance after three components was clearly higher for TCATA than TDS (Figure 3b). Common components 1-3 explained almost as much variation as for the separate PCA models, indicating little extra information in any of the datasets. For TCATA there was a clear breaking point after three components, fitting with three experimental factors, whereas for TDS no such break point existed. Due to this breaking point, we focused on a solution with three common components.

Common components

The three first common components gave similar trajectories as the separate PCAs which were discussed in (Nguyen et al., 2018) The scores for common component 1 (C1) and common component 3 (C3) are given in Figure 5a (TDS) and 5b (TCATA). For both methods, these components gave four classes of trajectories related to thickness of yoghurt (Thick-Thin) and the type of fiber added (Flour-Flakes). Samples were, however, better separated for TCATA than TDS, in particular with respect to low-optimal flavour in C3 for yoghurts with flour (right side of Figure 5 b). Common component 2 (C2) was related to the overall time development and did not separate the yoghurt samples for either of the methods.

Figure 5c) shows the correlation loadings for C1 and C3 from TDS and TCATA data (see section 2.4). For both methods C1 was related to Sandy (positive side) and Gritty (negative side). C3 was related to Thin (positive direction) and Thick (negative direction). In general, the attributes from TDS and TCATA had similar positions. The largest differences were observed for Acidic and Vanilla which may explain the better separation with TCATA. The dominance rate of Vanilla was quite low in TDS and always below the significance level, whereas in TCATA samples with higher Vanilla intensity could be well differentiated from the low-flavour samples (Supplementary Figure A1.1). Also, for Sweet the dominance rate was low in TDS, although a difference between optimal and low flavour yoghurts can be seen during the 20 first time units. With TCATA on the other hand, citation frequency is higher for the optimal flavour yoghurts throughout the whole evaluation. In this case study, TCATA elucidated differences between optimal and low-flavour samples better than TDS. For more detailed info on the complete sensory profiles, please refer to (Nguyen et al., 2018).
Distinct components

The trajectories for C2 and distinct component 1 (D1) (after three common components were extracted) are shown for TDS and TCATA in Figure 6a and b, respectively. The D1 from TCATA separated low-optimal flavour, whereas for TDS this distinct component was difficult to interpret since the trajectories in this plot are completely intertwined. Figure 6c shows the correlation loadings for TCATA C1 and D1, where both Sweet and Vanilla loads on D1, with interpretation aligned with observations in the previous section regarding these two attributes.

4.4.2 Cheese

The data from the cheese study are summarized in Supplementary Fig. A1.2. There was a clear drop in the canonical correlation after two components which are close to 1 (Figure 3a). It is therefore natural to focus on two common components for this data set. Among the three case studies, the canonical correlations are highest for cheese for two first components, but lowest after five components.

From Figure 3c it is evident that TCATA was better explained with fewer components than TDS. For TCATA, the amount of variation explained by the common components was almost the same as for the principal components, whereas there was some additional variability in TDS not explained by the common components.

Common components

TDS and TCATA trajectories for the two first common components (C1 and C2) were quite similar (Figure 7a and b). The C1 separated semi-hard firm cheeses (samples JA and KO) from the rest. The other cheeses were separated by C2 in the first half of the evaluation, then around the mid-point of the evaluation trajectories cross each other, and in the second half they are better separated by C1. The separation is slightly better with TCATA than TDS.

Attributes loading on C1 were Nutty, Rubber, Grainy and Sweet (Figure 7c). These attributes were cited more frequently for JA and KO, but infrequently for the other cheeses (Supplementary Fig. A1.2). In addition, D-Juicy and D-Acidic loads on the positive side for the TDS data, whereas A-Salt for TCATA data is correlated with A-Umami on the negative side of C2 (Figure 7c). The C2 describes a contrast between Soft (start of evaluation) and Sticky/Umami (end of evaluation).

Distinct components

The differences between TDS and TCATA become more apparent when considering trajectories for C2 and the first distinct components (D1 for TDS and D2 for TCATA) as shown in Figure 8a and b for TDS and TCATA respectively. Based on TDS data, the cheeses KO and JA show no dynamics related to these two components (trajectories are only in the middle of the plot and very short). For TCATA data on the other hand, the component D2 is clearly related to dynamical changes in these two cheeses, and trajectories for KO and JA are near vertical. The trajectories are generally better separated in Figure 8b than a, although the D1 explains more of the variability in TDS (19.0%) than D2 does for TCATA (9.1%). The pair NR/GR was not well separated by any of the methods, not even when looking at later components.

The distinct components D1 and D2 are both related to Sweet, Juicy and Acidic, however D-Juicy and D-Acidic also contribute to C2, hence these attributes are located differently in Figure 8c and d. With TDS, D-Soft loads on the negative direction of D1, whereas remaining attributes are in the centre of Figure 8c. With TCATA data the distinct component contrasts A-Nutty and A-Grainy (together with Sweet, Juicy and Acidic), and A-Rubber. The almost vertical trajectories for KO and JA in Figure 7b are related to temporal changes in these attributes.

4.4.3 Bread

The data from the bread study are summarized in Supplementary Fig. A1.3. Canonical correlations were high (>0.7) for up to five common components (Figure 3a), and there was no clear breaking point.
Comparing TDS and TCATA for the full evaluation period

The explained variances for separate PCAs and the common components (Figure 3d) showed a different pattern than for the two previous cases. Both PCA explained higher variances (dotted lines, Figure 3d) than did the curves for the common components (solid lines, Figure 3d), in particular when looking at explained variance for two and three common components. Thus, there was additional variation in each of the data sets which could represent unique information. Distinct components were, however, difficult to identify as the so-called distinct components from TDS and TCATA could be interpreted in the same way, and hence did not represent unique information after all.

There were, however, several indications that TDS and TCATA differed more in the later part of the evaluation period. In the trajectory plots from the separate PCA models (Figure 2), the TDS trajectories (Figure 2a) became intertwined around the mid-point, whereas the TCATA plot (Figure 2b) trajectories were better separated throughout the whole period. Also, when looking at the detailed profiles for the bread (Supplementary Fig. A1.3), Coarse, Softness and in a lesser extent Chew resistance seemed to drive the temporal perception in the beginning of the mastication (before t=50). Towards the end of the evaluation, when the samples had reached a bolus state, TDS becomes more variable. The complexity associated with choosing only one attribute, as well as individual differences in bolus formation (Yven et al., 2012) may explain why the two methods showed fewer common characteristics at this stage of the evaluation. Another possible explanation is that assessors may forget to unselect attributes in TCATA (Ares et al., 2015; Meyners & Castura, 2018).

To get better insight into whether TDS and TCATA provided different information about the bread samples, the analyses on common and distinct components were repeated for data after t=50, coinciding approximately with where the largest differences between methods were observed.

Comparing TDS and TCATA for the second half of the evaluation period

The canonical correlations for the reduced bread data (t>50) are shown in Figure 9, with a clear breaking point after three components. Explained variances for the three first common components were larger than 20% (33.7%, 22.5% and 25.2% for TDS; 34.8%, 25.4% and 21.3% for TCATA). Focus is therefore on a model with three common components. Again, interpretation is important when selecting the number of components and here the focus was on highlighting differences between the methods.

Trajectories for the two first common components are shown in Figure 10a and b, with the corresponding correlation loadings in Figure 10c. Similar to the other examples, the trajectories were more entangled for TDS than TCATA. C1 was dominated by Bitter (negative side) and Juicy, Soft and Acidic (positive side). The C2 was related to texture attributes with Coarse (positive side), and Doughy and Salt (negative side). Attributes from TDS and TCATA were mostly located in the same area of the plot, but with some differences for Doughy, which for TDS was located more on the left side compared to TCATA.

The trajectories for the two first distinct components are shown in Figure 11a and b for TDS and TCATA respectively. It is clear that the separation of samples was better for TCATA than TDS, although not all samples could be discriminated. For TCATA (Figure 11 c), D1 was related to Sweet and Salt, whereas D2, which only explained 7% of the variability, was related to Chew resistance.

4.5 Discussion of all case studies

The present work aimed at exploring the common and unique information provided by TDS and TCATA in order to provide insights to practitioners for selecting the methodology that best suits for a particular application. There were quite large differences between the samples and therefore the common components were often related to single or pairs of samples. With such large differences between samples, the methods were highly similar with respect to explain variation and interpretation of the components. This agrees with previous research comparing TDS and TCATA reporting that the methods provide similar information about the main similarities and differences among samples, particularly when marked differences exist (Ares et al., 2015). More differences are expected for situations where
the samples have more subtle differences, for instance when working with small improvements on existing recipes in product development projects.

For the full data sets in the bread study, the difference between explained variation by common components and PCA components on TDS and TCATA separately was larger than for the other examples (Figure 3d). Nevertheless, it was difficult to extract meaningful distinct components, which may indicate that for both methods there may be substantial noise in the data. When discarding data from the first part of the evaluation and focusing on the period where the sample has turned into a bolus, differences between the methods were clearer. In this part of mastication period the dominating attribute may be more difficult to identify by TDS. The competition between texture and flavour attributes during mastication (before bolus state) is perhaps larger in bread compared to the other examples as it is a solid and relatively dry product.

The separation of common and distinct components when comparing TDS and TCATA provided some interesting results. First of all, the common components explained TCATA better than TDS; which also needed more components to explain the same amount of variation as for TCATA when analyzing the data separately by PCA. One of the reasons of the higher complexity of TDS is more “ups and downs” in the dominance curves compared to the citation rates of TCATA. The differences between the distinct components for these two methodologies can occur due to the greater sensitivity of the TCATA method, that TCATA assessors forget to unselect attributes, or that assessors in TDS have more uncertainty when selecting the dominant attribute (Varela et al., 2018). Each of these explanations are plausible, but the fact that the additional variation in TDS was difficult to interpret may indicate that assessor heterogeneity with respect to conceptualization of dominance is an important factor. The better discrimination ability with TCATA can be explained by a more structured variation, i.e. more variation explained by fewer components.

Using the yoghurt data and hypothesis testing for the different attributes and time points Meyners (2018) concluded that the two methods are very different. One of the main conclusions was that TCATA generally gave smaller p-values than TDS, and significant differences occur more often. Moreover, the duration of significant differences lasted longer with TCATA than for TDS (Meyners, 2018). The results from the multivariate study conducted here, however, showed a large degree in similarity between the methods. It is important to emphasise that this does not necessarily mean a contradiction of the result by Meyners (2018), since both focus, hypotheses, type of results considered, and assumptions of TDS and TCATA methods are different. This paper compares in particular the multivariate structures in order to explore differences in overall discrimination of products. The approach of looking for common and distinct components by applying PCA-GCA shows that the main structures are indeed similar. The similarity in structures of multivariate data was also to be expected since several TDS and TCATA comparisons have concluded that the methods provide similar descriptions, but that the unique components of TCATA seem to discriminate samples better than for TDS. In our point of view, it is also natural that a method which measures whether an attribute is dominant detects significant differences less frequently than a method which measures whether the attribute characterizes the sample; more attributes characterize the sample than are dominant, and it is natural to expect that perceptual characterization will be more stable for dominance, and for longer durations.

4.6 Stability of the common components

PCA-GCA was performed for all combinations of the pairs of replicates as described in section 3.4. For all case studies the explained variance for common components and PCA was similar to the results for the complete data sets (not shown). When discussing stability of common components, we focus on results obtained for models with five common components (see section 3.4). The stability of the distinct components was generally lower than for the common components, but this is to be expected as the explained variation of the distinct components are lower than for the common components.
Nevertheless, in the present comparisons of data from TDS and TCATA the differences between the methods became more evident in these components.

**Yoghurt**

The common components extracted from TCATA were more stable than for TDS according to Tucker’s congruency coefficient. The congruency coefficients for the two first common components exceeded 0.85 in more than 50% of the comparisons for TDS and 70% for TCATA. The third component was considerably less stable. This could indicate that a model with only two common components would be most appropriate for this case study. However, for the model with only two common components the first distinct component had very similar interpretation for both TDS and TCATA, demonstrating that the transition from common to distinct variation often is gradual. When applying the model with three common components, the first distinct components (Figure 6c) highlighted better the differences between the methods. This shows that interpretation is important in model selection in exploratory analyses. Because of this interpretational aspect, the model with three common components was preferred for the yoghurt case, although the third common component was less stable than the two first.

**Cheese**

For the Cheese data, there was no clear differences between stability of common components from TDS and TCATA. The stability was high for the two first common components. In contrast to the Yoghurt case described above, no additional insight on differences between TDS and TCATA could be obtained by extracting additional common components. Hence, for this case the stability results confirmed the previous model selection.

**Bread**

For the Bread data the congruence coefficients indicated low stability of the components, reflecting a higher noise level and more variation between the replicates. However, Måge et al. (2019) demonstrated that PCA-GCA does not give false discoveries, i.e. extracting common components when there are none in the underlying model. Thus, the lack of consistency between replicates of bread evaluations may be related to a larger competition between texture and flavour attributes for bread than the other products as discussed above. Based on simulation studies Måge et al. (2019) reported that PCA-GCA performed well with respect to selecting the correct number of components. Problems could, however, occur for noisy data when common components dominate the blocks and there is little systematic distinct variation. This situation may be the case for the Bread data. The canonical correlations indicated a large number of common components, in particular when analysing data from complete evaluation period. Nevertheless, there was a gap in the explained variation between principal and common (canonical) components, which indicated unique variability for each data block. Distinct components were, however, more difficult to identify than for the other cases as the interpretation was the same for both blocks also when a large number of common components were extracted.

### 4.7 Future challenges and implications

In the present work, the temporal data were first compressed by PCA. Another alternative would have been to use correspondence analysis (CA) which has also been applied to study trajectories of temporal data (Castura et al. 2016). An anonymous reviewer suggested that the blocks of data can be analysed by CA, followed by decomposition into common and unique components via GCA. Such an approach could be considered a topic for further research.

Varela et al. (2018) discussed competition between modalities rather than attributes in TDS; i.e. that assessors must choose one attribute at a time which can only belong to one modality (flavour vs. texture). Textural attributes will more likely be chosen when food physics dominates the oral processing (beginning of the mastication or formation of the bolus at the end). Flavour attributes on the other hand are more likely to be chosen during the middle of the oral processing, when saliva release and wetting of the sample dominate the process. It is therefore interesting to see that it is mostly flavour attributes which contribute to better separation with TCATA than TDS. Better separation of samples with TCATA
than TDS was in particular observed for yoghurt and bread, and in both these examples the distinct components were related to flavour attributes; Sweet and Vanilla for yoghurt (Figure 6c) and Sweet and Salt for bread (Figure 10c). In the cheese study both texture and flavour attributes differed for the distinct components (Figure 8c and d), however, there were some differences in how some of the flavour attributes loaded on the common components (Figure 7c).

It is clear that difference between TDS and TCATA can vary during the evaluation period since the better sample separation observed for TCATA seems to be related to the second half of the evaluation period (this is when TDS trajectories tend to become more entangled). Further investigations should therefore to a larger extent focus more on different time intervals. Temporal data have been divided into intervals in for instance Dinnella et al. (2013) and by Nguyen et al. (2018). With similar strategies as those papers, the distinct-component analyses can be performed separately for each time interval. Such data analyses can be expected to shed more light on the relationship between textural and flavour attributes for different temporal methods and how these are perceived during the mastication process.

5 Conclusions

A trained panel analysed samples from three different product categories using TDS and TCATA. The data from the two methods were analysed using PCA-GCA which is a framework for extracting common and unique information, through sequential application of PCA, canonical correlation analysis and orthogonalization. This tool was useful for highlighting and visualising differences between TDS and TCATA although some difficulties in selecting model was experienced for the bread data. The stability of the solutions was investigating by comparing replicates. The results were sufficient for a proper interpretation.

By use of PCA-GCA a large degree of similarity in the multivariate structure between data from TDS and TCATA was observed for all three product categories in the study. TCATA discriminated samples better than TDS both when looking at common components, and also when components which have the highest similarity between the methods (the common parts) were extracted. Differences in sample separation were mostly related to flavour attributes, this suggests that TCATA provides better separation than TDS because there is less competition between modalities than in TDS. The results support previous findings and suggest that the opportunity to select more attributes in TCATA provides more structured (less variable) data. The unique information in TDS shows more fluctuations in perception dynamics (wiggly curves). More research is needed to understand if the small fluctuations in TDS are relevant to consumer acceptance. Further comparisons of TDS and TCATA should focus on different parts of the mastication process, use samples with subtle differences or link the data to consumer acceptance data.

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