Food Quality and Preference 109 (2023) 104893

Contents lists available at ScienceDirect

Food Quality and Preference

journal homepage: www.elsevier.com/locate/foodqual

Analyzing temporal dominance of sensations data with categorical functional data analysis

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ARTICLE INFO

Keywords:
Temporal dominance of sensations
Categorical functional data analysis
S PLSDA

ABSTRACT

Recently, an R package was developed for categorical functional data analysis (CFDA). This statistical approach extends the usual functional data analysis to temporal categorical data, and as such is particularly relevant for TDS data.

CFDA produces a PCA-like map of the sensory evaluations (subject × product) based on the sequences of sensations. Each axis represents leading temporal patterns and the coordinates of sensory evaluations on these axes depict their main temporal characteristics. Then, those coordinates can be used as inputs for further statistical analyses such as clustering of subjects or discriminant analysis of products, both based on temporal perception of the products.

Classical analysis of TDS data consists of a series of independent analyses of specific variables: number of citations, dominance rate, duration of dominance or transitions. CFDA presents the advantage of dealing with the entire TDS signal in the same analysis. This paper demonstrates the relevance of CFDA for the analysis of TDS data by using pedagogical data and a real TDS dataset.

1. Introduction

In the last years, Temporal Dominance of Sensations (TDS, Pineau et al., 2009) has been extensively used in sensory analysis. In TDS, subjects click on the dominant sensation they perceived over time, during the whole tasting of products. Most usual statistical analyses of TDS data rely on the calculation of (i) dominance rates (proportions of subjects having cited a given descriptor as dominant at a given timepoint), (ii) number of citations of the descriptors or (iii) dominance durations (elapsed times between the choice of a given descriptor as dominant and the choice of the next one). With the analyses based on (i), such as TDS curves (Pineau et al., 2009), the individual sequences are used to represent the evolution of the dominance rates at the panel level. Difference curves (computed by considering the difference of the dominance rates for each descriptor of two products or groups of products) can also be calculated. While TDS curves are almost systematically computed, the analysis of the number of citations is rarer but is based on non-parametric tests and Correspondence Analysis (CA as presented in Frost et al., 2018). Regarding (iii), the analysis of dominance durations can be investigated with univariate analyses such as Analyses Of Variances (ANOVAs) or multivariate analyses including Principal Component Analysis (PCA, Pearson, 1901) or Canonical Variate Analysis (CVA, Fisher, 1936; Peltier et al., 2015) as in Albert et al. (2012), Lesme et al. (2020) and Galmarini et al. (2017). PCA (or CVA) allows individual sequences to be represented on maps (with individual projections). However, the sequentiality of sensations is lost. An alternative analysis is usually referred to as PCA or CA of sensory trajectories (Lenfant et al., 2009). It consists in several steps: (i) decomposing the total sequence in successive timepoints (usually equally sized) into which either the citation rate or the dominance duration of each descriptor is determined, (ii) analyzing by CA or PCA the resulting table having productperiod pairs as observations (subjects were averaged) and descriptors as variables, (iii) joining the successive timepoints by product to represent trajectories. This output can also be adapted by calculating dominance durations by periods of time. Although this analysis allows the evolution of perceptions in each product to be observed, it considers a fixed correlation structure among the descriptors. However, when the temporality of taste is studied, the correlations between descriptors should be able to evolve along time. For example, imagine three chocolate candies: Ch0, Ch1 (Ch0 + coconut

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https://doi.org/10.1016/j.foodqual.2023.104893
Received 16 December 2022; Received in revised form 17 May 2023; Accepted 17 May 2023
Available online 20 May 2023

heart + coconut and chocolate coating) and Ch2 (Ch0 + chocolate heart + coconut and chocolate coating). In the beginning of the tasting, chocolate should be highly correlated to coconut (Ch1 and Ch2 have the same coating including both sensations), while at the end of the tasting, chocolate would be inversely correlated to coconut (The heart of Ch1 is coconut contrarily to the one of Ch2 that is chocolate). The role of temporal methods is specifically to highlight such correlations evolving with time. PCA of trajectories is not able to catch them which is a major flaw for anyone being interested in the temporal evolution of the products. Furthermore, PCA of trajectories consists in maximizing the variance of the product*period points. Consequently, the variability of these points does not differentiate between product variability and period variability.

Castura & Li (2016) decomposed TDS sequences into short sequences – monads, dyads, triads and tetrads – in order to provide a new way of looking at TDS data, with emphasis on transitions of one dominant attribute to another. This approach considers the sequentiality of descriptors but not the duration of each descriptor. Later, stochastic semi-Markov processes were used as an alternative to these usual statistical analyses (Lecuelle et al., 2018; Cardot et al., 2019; Kurata et al., 2022). This probabilistic way to model TDS data offers the opportunity to apply usual likelihood methods for product comparison and consumer segmentation by perception. However, these methods assume that the probability of choosing a given descriptor as dominant only depends of the previous dominant one and does not change over time. Note that, in Lecuelle et al. (2018), semi-Markov chains are applied on sequences split in time periods with specific durations, with one model per time period. This model can only vary with periods, not evolve continuously with time. Another approach for considering temporality in the statistical analysis was introduced by Okamoto et al. (2020). They considered a method coupling resampling of the dominance rates and non-negative factorization which allows the temporality to be considered at the panel level. Consequently, this method does not allow to detect clusters of subjects or outliers.

Therefore, analyzing TDS data in all their complexity (sequentiality and durations) remains challenging, and, until now, no statistical analysis has fully exploited both the temporality of the signal of TDS sequences and individual responses.

Deville & Saporta (1979), Deville (1982) and Saporta (1981) introduced a method that considers the whole temporality of the data: the so-called (in French) “analyse harmonique qualitative”, renamed later as “Categorical Functional Data Analysis” (CFDA, Preda et al., 2021). This method is an extension of functional analysis (FDA, Hsing & Eubank, 2015; Ramsay & Silverman, 2005) previously used in sensory analysis for modeling time intensity data (Bi & Kuesten, 2013; Kuesten & Bi, 2018). While FDA is dedicated to temporal quantitative variables, CFDA is dedicated to temporal qualitative variables and allows TDS data to be analyzed. Saporta (1996) presented it as a natural extension of Correspondence Analysis. Later, Preda et al. (2021) made available an R package for an easy computation of CFDA. Note that other R packages such as TraMineR (Gabadinho et al., 2011) provide also functions to perform descriptive analysis of temporal qualitative variables, where distance functions between sequences are defined to perform clustering analysis.

The objective of the paper is to demonstrate that Categorical Functional Data Analysis allows TDS data to be statistically analyzed by considering both subject variability and temporality (without restricting temporality to durations or transitions). In this purpose, several analyses using CFDA outputs are presented, illustrated on pedagogical examples and then applied to a real TDS dataset.

2. Material and methods

2.1. Elements of theory about CFDA adapted for TDS data

2.1.1. Notations

This paper does not aim to exhaustively present the mathematical background of CFDA but this section summarizes the general ideas. For further details, the reader interested in mathematical details can refer to Deville (1982), Preda et al. (2021). Other accessible presentations of CFDA are available in Saporta (1996), Saporta (1985) and Saporta (1981). Readers that would not be interested in the technical details can skip this part and go directly to 2.2.

The notations are similar to those of Deville (1982). Here, each CFDA technical term is linked to its related TDS sensory term in italics. Let X be a continuous-time stochastic process $X = \{X_t, t\in[0,T]\}$ *(TDS evaluation)* such that all $t\in[0,T]$, X_t is a categorical random variable taking values in a set of D states (*descriptors*) $S = \{s_1, \ldots, s_D\}$. Without loss of generality, we can consider that T = 1 in the rest of the paper *(corresponding to the so-called “time-standardization” in TDS)*. The sample paths of X are called here categorical functional data generated by the stochastic process X.

2.1.2. CFDA as optimal encoding of the TDS descriptors

Finding an encoding of the descriptors means that a numerical value is attributed to each descriptor of the qualitative variable, giving a new quantitative variable.

Deville (1982) presented CFDA as the temporal optimal encoding of qualitative variables. Considering X_t taking values in $S = \{s_1, \ldots, s_D\}$, for every $t\in[0,1]$, the idea is to find a numeric encoding of its descriptors, such that the correlations between these encodings of the TDS sequences are maximal under identifiability constraints (zero expectation and unit variance). These encodings are varying with time.

Such an encoding amounts to finding D functions of time α_{s_d} (with $d = 1, \ldots, D$). In practice, these functions cannot be directly obtained but are approximated by their projections (denoted α_{s_d}) onto a finite basis of functions $(\psi_1, \ldots, \psi_p)$, chosen by the user (p being the number of chosen functions in the basis). We would like to highlight.

Restricted to the subspace spanned by this finite basis of functions, the optimization problem was shown to be solved by matrix diagonalization tools (Deville, 1982). Here, each individual (line) corresponds to a product*subject (also *replicate if any) TDS sequence. As in usual PCA, the individuals can be projected in a basis of eigenvectors. The individual coordinates on the k^{th} eigenvector is called the k^{th} CFDA component. The obtained eigenvectors are called harmonics and contains the d optimal encodings α_{s_d} of the TDS descriptors (varying with time).

To summarize, the outputs are comparable to those of PCA. They include (i) the cumulative scree-plot of eigenvalues, (ii) the coordinates of the individuals in the obtained basis, (iii) the optimal encodings (that are related to the loadings represented as harmonics).

2.1.3. CFDA as an extension of correspondence analysis

Saporta (1996) considered CFDA as an extension of Correspondence Analysis. In the simple case where the period [0, 1] can be divided into two sub-periods (period 1 and period 2) of equal duration where only one descriptor would be measured for each sub-period, the data could be analyzed with Correspondence Analysis considering the two variables “X in period 1” and “X in period 2” taking their values in S. This case can be extended to three or more periods using Multiple Correspondence Analysis (MCA) instead of Correspondence Analysis. The general case can be obtained by considering a potentially infinite number of periods: this is CFDA.

2.1.4. Choice of parameters required in CFDA

As presented in 2.1.2., running CFDA implies choosing a basis of functions $(\psi_1, \ldots, \psi_p)$ to expand the temporal components related to each

descriptor.

In this paper, the basis of functions is made of B-splines (Thévenaz et al., 2000). B-splines functions are polynomial segments joined end-to-end at argument values called knots. The segments have specifiable smoothness across these knots. B-spline basis functions have the advantages of very fast computation and great flexibility. Once the knots are defined, the degree of the polynomial has to be chosen. A high degree of polynomial implies smoother curves (as represented in Fig. 1) but requires more coefficients to be estimated (and consequently more observations).

In this paper, we consider B-splines with eight equidistant knots and degree zero for toy dataset (as they have a low number of evaluations) and degree two for the real dataset (as they have a high number of evaluations). Fig. 1 shows the rectangular non-overlapping basis functions for degree zero and smooth overlapping curved basis functions for degree 2. The choice of the number of knots was determined from the data, as it allows a sufficient screening of the time period and does not lead to overfitting.

2.2. Using CFDA in practice for analyzing TDS data: presentation

2.2.1. Time standardization

As specified in 2.1.1., CFDA requires that all evaluations have the same beginning times (0) and same ending times (1). For this purpose, each TDS sequence was left–right standardized (first, each evaluation was translated to start at a zero time, then the time of each transition from a descriptor to another was divided by the total duration of the evaluation). Thus, after this pretreatment, the time of the first citation is 0 and the time of the end of the perception is 1. After time standardization, TDS data are categorical functional data by construction and can be analyzed using CFDA tools.

2.2.2. Exploratory analysis: analyzing CFDA results on a first pedagogical example

CFDA can be run on the standardized TDS data in order to visualize the main sources of variability in the data. Therefore, the individual coordinates (subject*product) can be plotted on a map, where points can be colored according to the product, to visually assess potential product discrimination. This “individual map” allows potential outliers or clusters to be detected but also allows products to be naturally discriminated (if they are the main source of variation in the data). The evolution of optimal encoding of each descriptor is also plotted giving the so-called “Harmonic 1” (“Harmonic 2” for the second component of CFDA, respectively). Thus, a harmonic consists of D curves. For a simplification purpose, only the first two-dimensional map was presented here with the first two harmonics, but further maps and harmonics could also be represented by selecting more components of CFDA (exactly as in PCA). These four outputs (cumulated eigenvalues, individual map and the two harmonics) allow all the TDS sequences to be summarized and to retrieve original product, subject (and potentially replicate) information.

A first example (toy dataset 1, with sequences presented in Fig. 2a) was used for explaining CFDA and to illustrate the differences compared to PCA of product durations. In this fictive dataset, two products (P1 and P2) were each evaluated by three subjects (S1, S2, S3). The first product P1 was described as B, then A and finally C by all subjects. The second product was described as A, then B and finally C, also by all subjects.

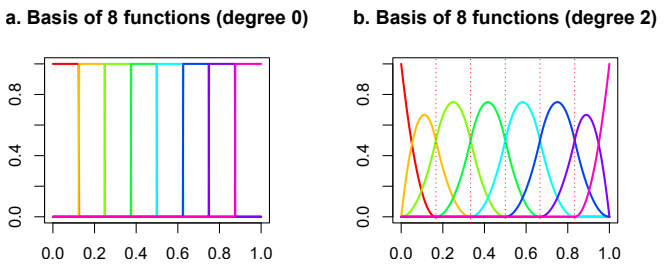

Fig. 1. Chosen bases of functions for toy datasets(a) and real dataset (b). Each color and line type correspond to a function of the basis. Vertical dotted lines correspond to the chosen breaks.

Fig. 2 shows the results of CFDA on toy dataset 1. Regarding the individual map (Fig. 2b), products were well discriminated on the first axis (P2 had negative scores while P1 had positive scores). The positive part of harmonic 1 shows that a positive score on the first axis (as P1 scores) comes from selecting B as dominant, then A (Fig. 2c). Similarly, the negative part of harmonic 1 shows that a negative score on the first axis comes from selecting A as dominant then B. C appeared only at the end of the tasting and does not allow to separate products or subjects. Regarding the second axis, P1S3 and P2S3 have positive scores and the harmonic 2 indicates that positive scores comes from selecting A as dominant in the period [0.25–0.375] of the tasting (Fig. 2d). Similarly, P1S2 and P2S2 have negative scores on the second axis and the harmonic 2 indicates that negative scores come from selecting B as dominant in the period [0.25–0.375] of the tasting. Finally, the cumulative eigenvalues were plotted, indicating the quantity of information accounting by successive axes. In the example (Fig. 2e), the cumulative eigenvalue graph shows that only two components are required to describe the whole data (with the first one representing more than 75% of variability). Note that the number of possible components in CFDA is theoretically high: number of descriptors*number of bases (here 3*8 = 24). The software automatically removed the last eigenvalues.

All the conclusions obtained from CFDA are consistent with the raw data represented in Fig. 2a. As expected, CFDA captures the main source of variability in the data. Note that performing a PCA of durations on this dataset considering all the evaluations as individuals (n = 6) would not discriminate P1 from P2. Indeed, the mean proportions of durations were identical for P1 and P2, and consequently the points corresponding to P1 and P2 would be confounded.

2.2.3. Exploratory analysis: analyzing CFDA results on a second pedagogical example

The analysis of a second dataset (toy dataset 2, with sequences presented in Fig. 3a) aims to show how a discriminant technique based on the CFDA individual scores is able to separate products. This fictive dataset represents 3 products (P1, P2, P3) tasted by 3 subjects (S1, S2, S3). S1, S2 and S3 were different during the whole tasting except for the middle section. The products were perceived differently during a small proportion of time in the middle of the sequence.

Fig. 3 illustrates the results of CFDA on toy dataset 2. The first axis discriminates subjects S1 and S3 while the second axis discriminates S2 from S1 and S3 (Fig. 3b). The points corresponding to the three products have identical coordinates in the first two axes and the product discrimination is consequently not captured by this analysis.

The first harmonic (Fig. 3c) shows that positive scores come from selecting the F descriptor as dominant during the whole evaluation (middle excepted), which S1 did for all three products (in pink), while negative scores come from selecting the E descriptor as dominant (in dark blue) at the beginning and end of the evaluations, which S3 did for all three products. The C descriptor, represented in the middle of harmonic 1 is superimposed to A and B and is related to positive scores in [0.40–0.50] and to negative scores in [0.65–0.7]. It shows that the product information (A, B or C) began and finished earlier in S1 than in S3.

The second harmonic (Fig. 3d) shows that positive scores (as for S2) come from selecting D as dominant most of the time. This conclusion is consistent with the raw data represented in Fig. 3a. As expected, CFDA captures the main source of variability in the data, which here is the subject effect.

Fig. 3e. shows that two components are sufficient to explain 75% of the whole variability.

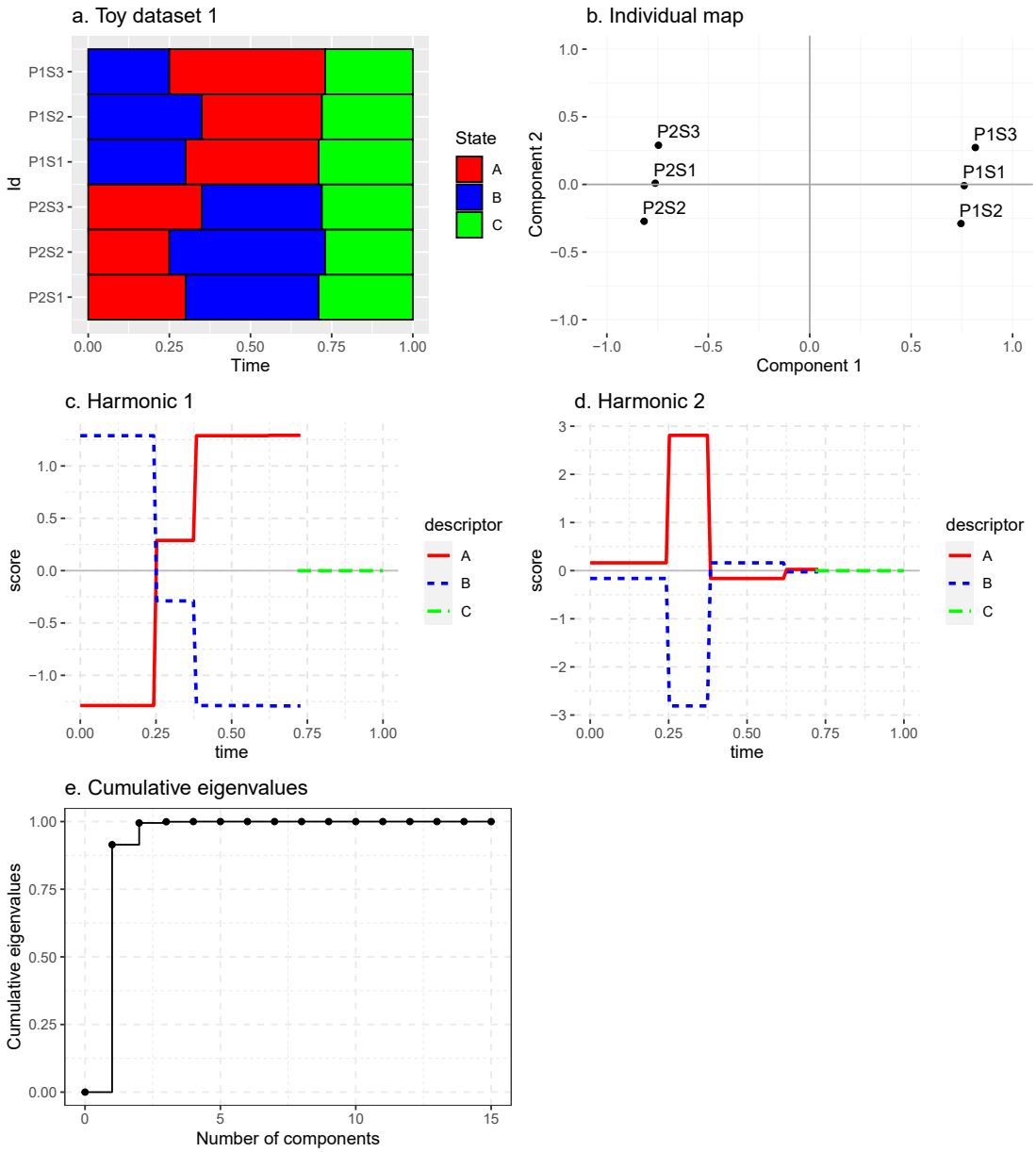

Fig. 2. Results of CFDA on toy dataset 1: (a) individual TDS sequences for toy dataset 1 (b) represents the individual scores on the map of the first two components, (c) and (d) are the representations of the first two harmonics, (e) cumulative eigenvalues.

2.2.4. Finding differences between products in TDS data using sPLSDA

Next, we wanted to explain the differences between products. To do this, we used CFDA coordinates as inputs of Partial Least Squares Discriminant Analysis (PLSDA, Pérez-Enciso and Tenenhaus, 2003) There is a risk of overfitting because CFDA results have fewer rows (number of evaluations) than variables (number of selected basis functions*number of descriptors = number of columns after running CFDA). Consequently, a solution could be to use algorithms integrating variable selection such as the sparse Partial Least Squares Discriminant Analysis (sPLSDA, Lê Cao et al., 2011). In this case, the number of CFDA components to be kept in sPLS-DA can be tuned using cross validation techniques (Rohart et al., 2017). This tuning function (available in MixOmics R package) used with its default parameters, returns the Balanced Error Rate (BER, percentage of observations that are not well-classified by the chosen model) according to the selected number of selected features (i.e. the number of selected CFDA components). The lower the BER, the better the model. Note that the number of sPLS-DA components can also be tuned by this function. Consequently, two parameters could be tuned: the number of components in the sPLSDA and the number of variables (CFDA components to be selected) for each sPLSDA component. However, in this paper, only the case with two sPLDSA components was considered: it allows us to build one single map.

Applying this method on dataset 2, only one CFDA component was selected for each of the two sPLSDA components as shown by the big orange diamond (Fig. 4a).

The first axis of sPLDA separated P2 (on the right) from P3 (on the left) (Fig. 4b). Positive scores on the first axis were highly correlated to the dominance of C between 0.4 and 0.75 while negative scores on the first axis were highly correlated to the dominance of A between 0.4 and 0.75 (Fig. 4c). The second axis separated P1 (top) from P2 and P3 (bottom). Positive scores on the second axis were highly correlated to the dominance of B between 0.4 and 0.75 (Fig. 4d). This interpretation was consistent with the raw data and the fact that the three products differ in the middle of tasting, P1 being perceived B, P2 being C and P3 being A. On the toy dataset 2, sPLSDA on CFDA scores returns exactly

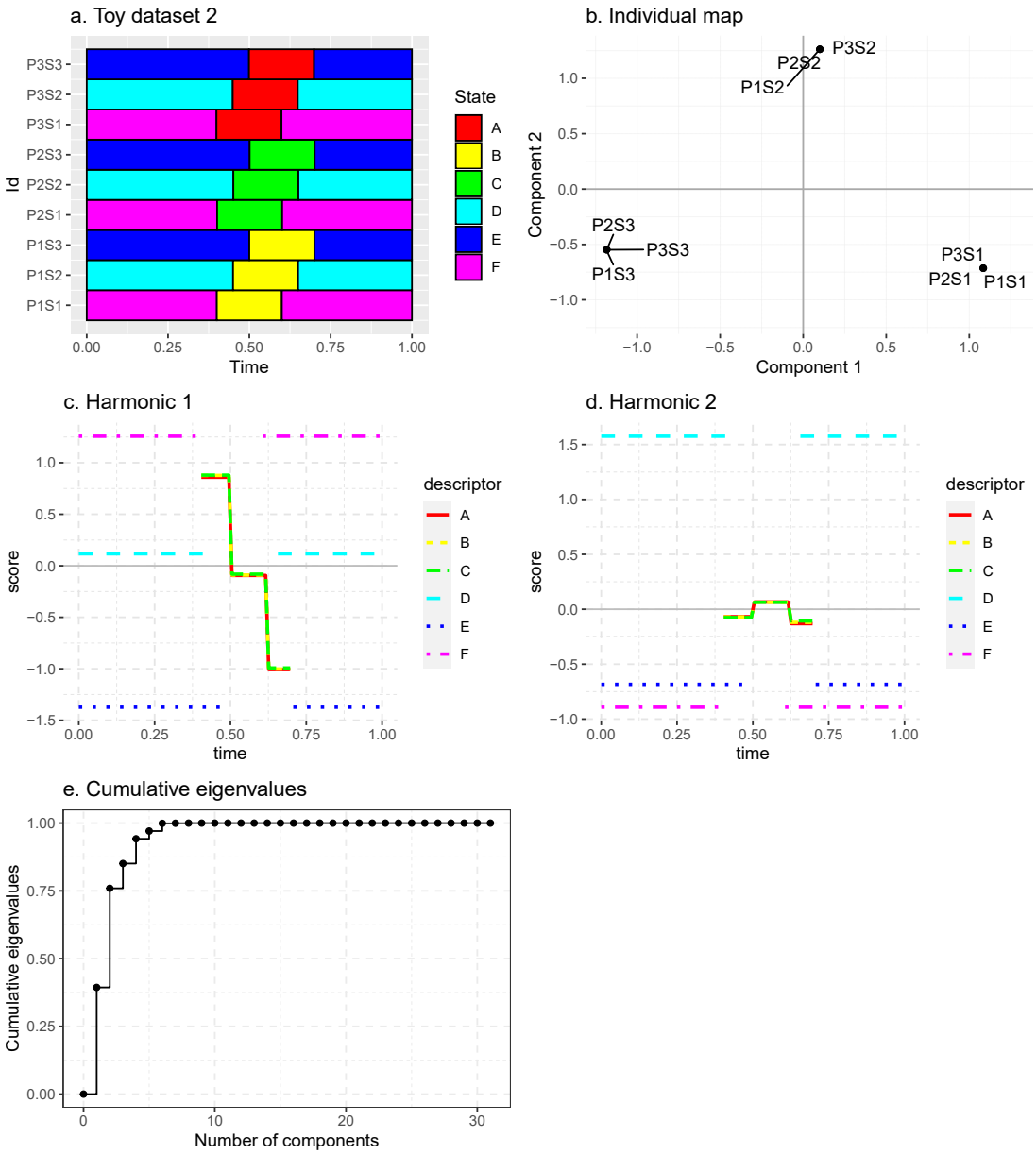

Fig. 3. Results of CFDA on toy dataset 2.: (a) individual TDS sequences for toy dataset 2, (b) represents the individual scores on the map of the first two components (c) and (d) are the representations of the first two harmonics, (e) cumulative eigenvalues.

the expected results: it finds exactly where and how the products are discriminated.

2.3. Application on a real TDS dataset

2.3.1. Presentation of the dataset

The dataset was collected in 2021 and was recently published in a data paper (Visalli et al., 2022). Seventy consumers evaluated four crisps (C1, C2, C3 and C4) at home using TDS. They were previously invited to a collective briefing at lab where the temporal method was explained, the descriptors were presented and a demonstration of the task was done by the panel leader. The descriptors were *Bland, Crackly_Hard, Crispy, Fat, Melting, Potato, Roasted, Salty* and *Sticky_Pasty ("None" was not included such that the subject is forced to choose a sensory descriptor)*.

The given instructions (reminded on the screen before tasting) were: "You will put a crisp in mouth, while simultaneously pressing the 'In mouth' button. A list of buttons will be displayed on the screen. Throughout the tasting, as soon as you perceive a dominant sensation, you will have to press the button corresponding to this sensation. Some sensations may never be selected, others may be selected multiple times during the tasting. You will continue to indicate the sensations perceived after swallowing the crisp. When you no longer perceive anything, you will click on 'I no longer perceive sensations' button.".

2.3.2. TDS curves and PCA

First, TDS curves and PCA of product durations were conducted on this dataset for illustrating the dataset. Building TDS curves was obvious at it is systematically used for TDS data. PCA of durations was also chosen because it aims to show the differences between products with a factorial map, exactly as CFDA paired with sPLSDA. However, PCA of durations does not consider the temporality: comparing PCA of durations to CFDA paired with sPLSDA is consequently of interest.

2.3.3. CFDA on the real TDS dataset for a multivariate exploratory analysis

CFDA was conducted and the individual map (two first dimensions) and the first two harmonics were plotted to observe the main sources of

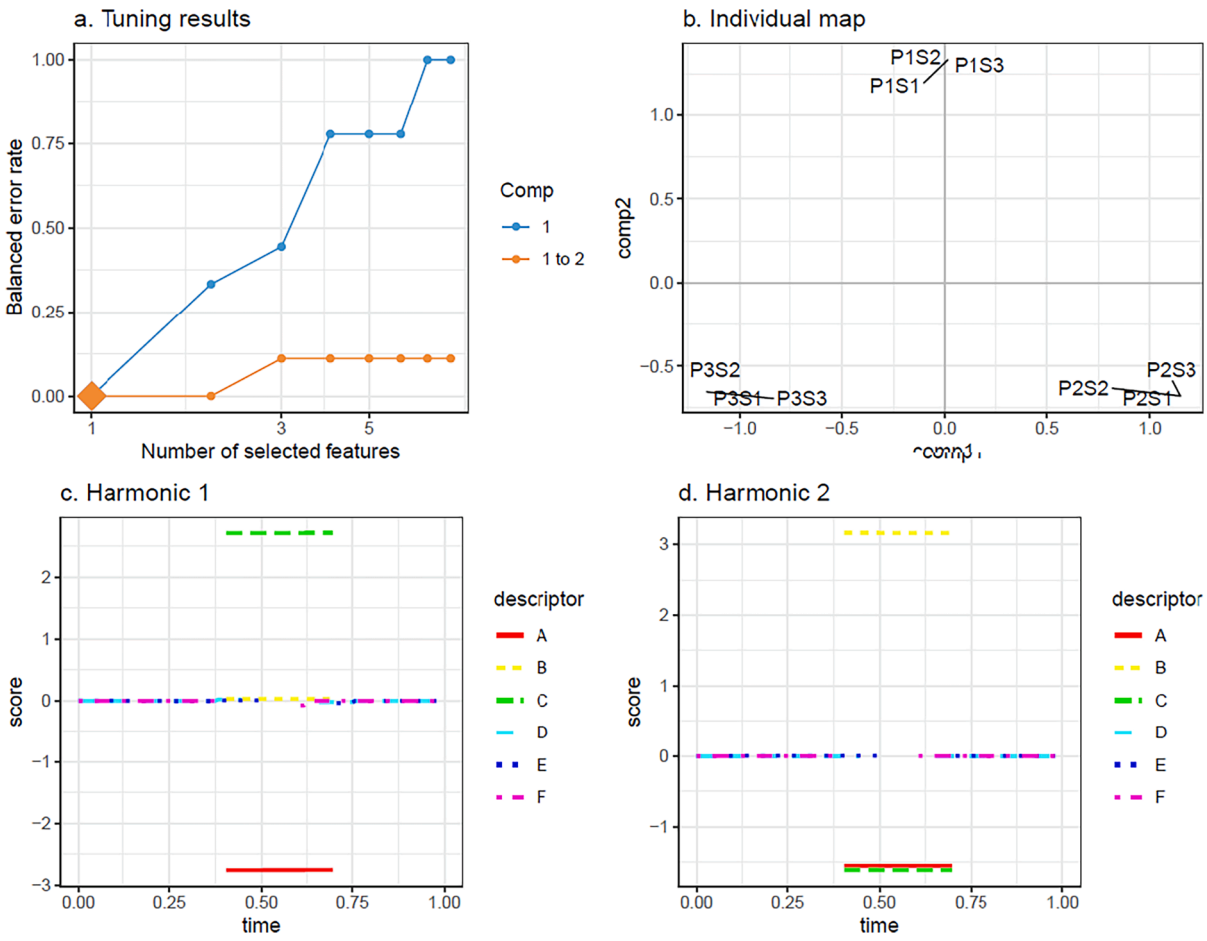

Fig. 4. Results of sPLSDA (a) represents the tuning results for the number of selected features (b) represents the individual map (c) and (d) are the representations of the first two harmonics.

variability in the experiment. As each harmonic is constituted here of nine descriptor curves (one for each descriptor), this output can be difficult to read. Thus, the cumulative probability of each descriptor at each given time (all products combined) was also plotted as a supplementary indication. This is an alternative to TDS curves that represents the cumulated probability, which is a natural choice as dominance rates sum to one at every time. To see if CFDA analyses make sense, the raw data were represented as barplots (each bar representing an evaluation over [0, 1] where the color at a given time gives the dominant descriptor for this evaluation).

2.3.4. *sPLSDA on the CFDA scores to analyze product discrimination*

As in the analysis of toy dataset 2 analysis, sPLSDA was conducted to detect how the sensations of different products differ along time.

In order to compare the product discrimination between static (PCA of durations) and dynamic (CDFA) method, the F statistics of the one-way MANOVA with product effect were computed on the first two sPLSDA components. Hotelling T^2 tests were also computed for each pair of products. MANOVA and the Hotelling T^2 test were also conducted on PCA of durations by using the projection of the individual durations on the same map as the product means. If temporality is relevant to discriminate products, CFDA should be more discriminant than PCA of durations. P-values and T^2 values were consequently reported for CFDA and PCA of durations.

Note that running Hotelling T^2 test on first two components only aims to replace the subjective interpretation of product discrimination on the represented map (first two dimensions). If the objective of this test was to detect discrimination between products, a first step would consist to select an appropriate number of components to work on (exactly as in PCA).

2.3.5. *Using CFDA scores for clustering subjects*

CFDA outputs can also be used as inputs for clustering subjects according to the dynamic of their sensations. The first step is to run CFDA on the data with the TDS sequences to be clustered, then a clustering algorithm on the obtained individual CFDA coordinates for the first two or more dimensions. To illustrate clustering on CFDA outputs, we focused our study on a single product (we have chosen to represent C3 where the obtained groups were the most obvious). For this purpose, hierarchical cluster analysis was computed with Ward's clustering criterion (Murtagh et. al., 2014) on the first two components of CFDA results.

2.3.6. *Computational aspects*

CFDA was computed with the cfda package (Preda et al., 2021) and most of the analyses of this paper are based on it. The package MixOmics (Gonzalez et al., 2012) was used to estimate the number of variables to keep in sPLSDA and to calculate and plot sPLSDA. Additional R functions – specific to the product*subject structure of TDS data – and the code required to reproduce the results are available on github (https://www.github.com/ChemoSens/ExternalCode/CFDA-TDS/).

3. Results

3.1. TDS curves and PCA of durations

Fig. 5a represents the TDS curves of the four products. Regarding C1, the dominant descriptor was frequently chosen as *Crackly_Hard* or *Crispy*, then *Salty* and *Potato*. C2 and C3 had similar profiles to C1. C4 was cited more often *Crispy*, then *Bland*.

Fig. 5b represents the PCA individual map of the mean durations. Evaluations were projected as supplementary data and colored relatively to the products. The first axis visually separated C4 from the other products. C4 seems to have scores positively correlated with *Bland* and *Sticky_Pasty*, and negatively correlated with *Salty*. The second axis opposes *Fat* and *Crackly_Hard* to *Crispy*, *Potato* and *Melting* and shows no visual product discrimination.

3.2. CFDA

Running CFDA on the dataset of crisps gave the results presented in Fig. 6. The first axis splits C4 from the other products (Fig. 6b). Harmonic 1 (Fig. 6c) shows that a positive score on the first axis comes from selecting *Bland* during the whole tasting, *Sticky_Pasty* as dominant at the beginning, and *Cracky Hard* at the end of tasting while a negative score comes from selecting *Salty* as dominant during the whole tasting. The second axis did not seem to separate products but shows individual variability. Harmonic 2 (Fig. 6d) shows that this variability was due to *Crackly_Hard* (positive scores on the second axis of the map come from selecting *Crackly_Hard* as dominant), especially in the end of the tasting. High positive scores on the first and second axis come from selecting *Crackly_Hard* at the end of the tasting (which was an unexpected behavior). Fig. 6e represents the probability for each descriptor to be dominant at each time point. It shows that *Bland, Salty* and *Potato* had high probabilities while those of *Crackly_Hard* at the end of the tasting and of *Sticky_Pasty* were small (and was consequently cited by only a few subjects). Fig. 6f shows the data of the evaluations with scores higher than 0.5 on the first and second axis (15 evaluations in the up-right square) were indeed mainly *Crackly_Hard* at the end of the tasting, and constituted indeed a group of evaluations with a different behavior.

3.3. sPLSDA

Fig. 7a. shows the results of sPLSDA tuning: it shows that the best-balanced error rate was obtained for two sPLSDA components and five selected features (CFDA components). Regarding the sPLSDA results (Fig. 7b), the first axis discriminated C4 (positive scores) from the other products. *Bland* was selected as more dominant in C4 along all the tasting while *Salty* was selected as more dominant in the other products (Fig. 7c), which was congruent with the results observed in Fig. 5. The second axis (Fig. 7d) discriminated C3 (negative scores) from C2 (positive scores). Regarding the main cited descriptors along the whole tasting (*Potato, Salty* and *Bland,* see Fig. 6e): *Potato* was more selected as dominant in C2 than in C3. Specific behaviors were also observed: *Sticky_Pasty* was selected as dominant in the beginning of C2 while *Fat, Roasted, Crackly_Hard* or *Bland* were selected as dominant for C3. The results presented in TDS curves on Fig. 5 confirmed these interpretations: these descriptors were indeed clicked for few evaluations in C3 (and not cited for the other products).

The MANOVA indicating the discrimination on map of the first two dimensions returned F = 38.25 for sPLSDA and F = 26.02 for PCA of durations, quantifying a better discrimination in sPLSDA map of the first two dimensions than in PCA of durations (degrees of freedom: 3 and 550). Regarding the results of Hotelling's T^2, all pairs of products were more discriminated in sPLSDA than in PCA of product mean durations while projecting individual evaluations as supplementary individuals (Table 1). One pair of products (C1-C2) were significant in sPLSDA but unsignificant in PCA of mean durations.

3.4. Clustering on CFDA scores

Fig. 8 (a, b, c) shows the results of CFDA for the data of C3 with three groups. These three groups were not well balanced: Group 1 contained most of the subjects (52), while group 2 and 3 contained 7 and 11

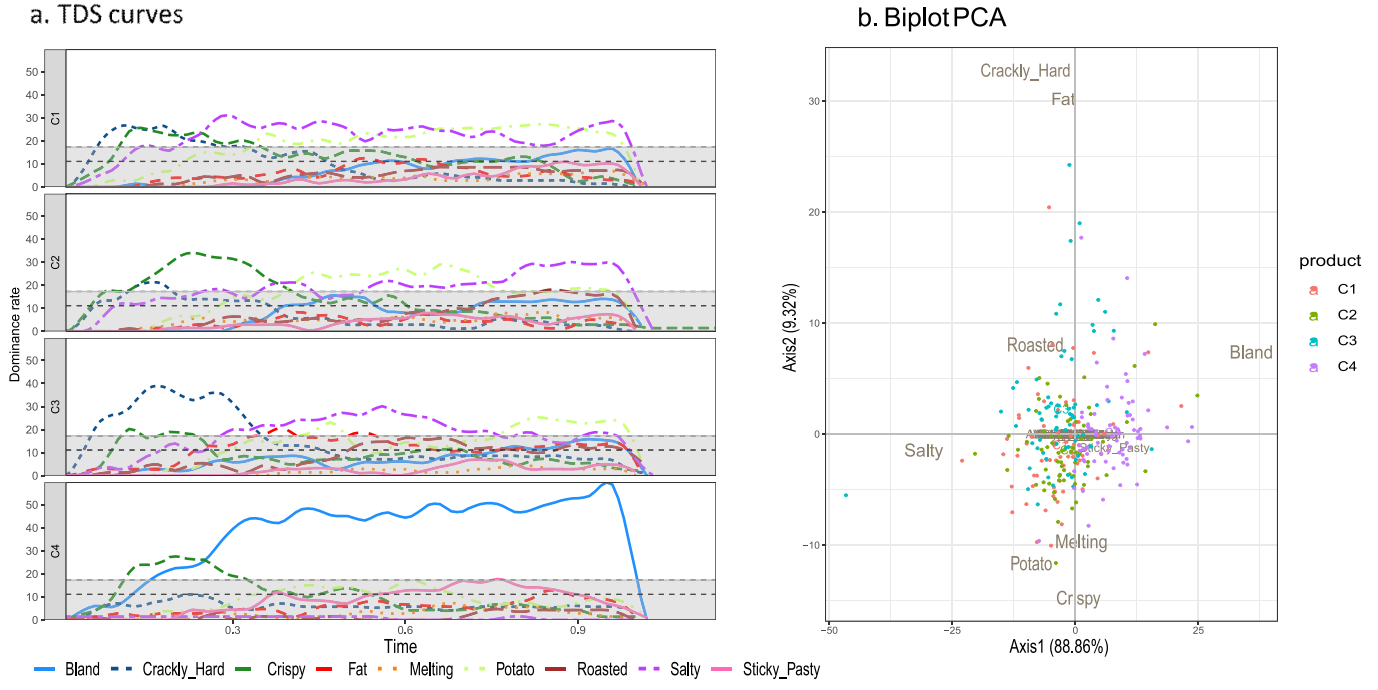

Fig. 5. (a) Standardized TDS curves of the four crisps. The dotted line represents the chance line and TDS dominance rates are significant (p = 0.05) above the grey zone (b) Covariance PCA results (biplot of PCA of dominance durations).

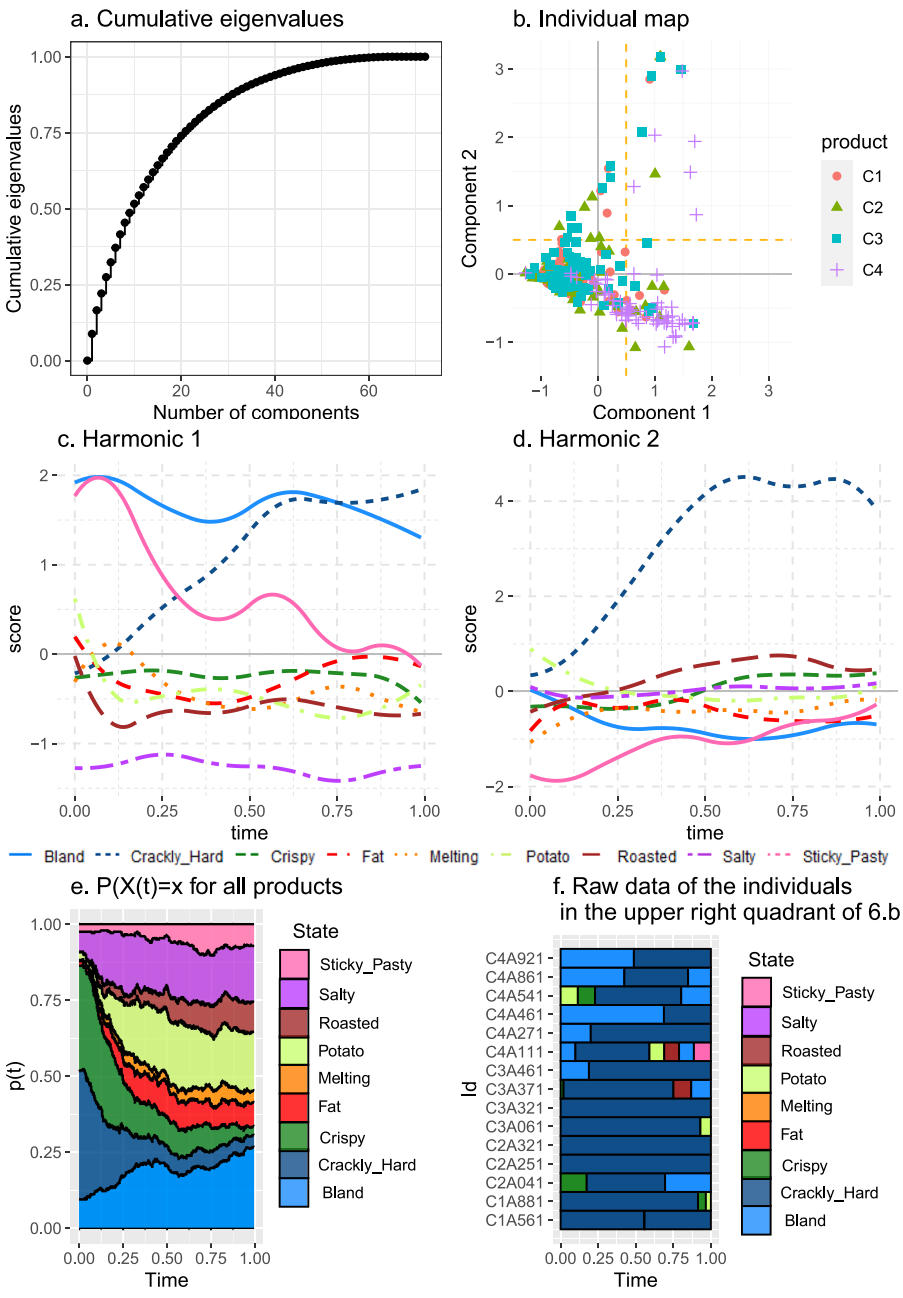

Fig. 6. Results of CFDA on a real dataset on crisps. (a) plots the cumulative eigenvalues (b) represents the individual scores on the map of the first two components. The yellow lines represent the 0.5 limits used for 6f., (c) and (d) represents the first two harmonics (e) represents the probability of a descriptor to be cited (all products confounded) and (f) represents the raw data of the individuals whose CFDA coordinates in the map of the first two components were higher than 0.5 (in the upper right quadrant of 6b. defined by the yellow lines). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

subjects, respectively (note that the number of subjects is quite low for clustering, but this aims to illustrate the possibilities of the method on larger datasets).

The first axis discriminates group 1 (with negative scores) from group 2 and 3 (positive scores) (Fig. 8a). Harmonic 1 (Fig. 8b) shows that positive scores indicate a strong probability for *Bland* to be dominant during the whole tasting and for *Crackly_Hard* to be dominant after 0.25. while negative ones were correlated to almost all other descriptors.

The second axis discriminates group 2 (positive scores) from group 3 (negative scores). Harmonic 2 (Fig. 8c) shows that positive scores were related to *Crackly_Hard* from 0.25 while negative scores were related to *Bland*. This suggests that group 2 contained the subjects that had selected *Crackly_Hard* as dominant after 0.25, while group 3 contained the subjects that had selected *Bland* as dominant during a large part of the tasting. It is was confirmed by Fig. 8d, 8e, and 8f. Group 1 contains the rest of the subjects (not clicking *Bland* or *Crackly_Hard* after 0.25).

4. Discussion

4.1. Discussing the real dataset results

CFDA results allowed for representing the diversity of the individual (product*subjects) patterns during the experiment. In this study, the main source of variability was the discrimination between C4 and the other products (Fig. 6b). The second source of variability was the use of *Crackly/Hard* at the end of the tasting (Fig. 6b, d). This pattern, having temporal specificities, is impossible to catch by working only with durations and is particularly relevant in our study. Indeed, clicking on *Crackly/Hard* at the end of the tasting raises the question about the quality of the data of these fifteen evaluations and how these subjects have understood the instructions. The CFDA outputs are consequently relevant for a multivariate exploratory analysis of TDS data and allows outliers or groups of subjects to be detected.

Regarding the sPLSDA on CFDA scores (Fig. 7) and PCA on the

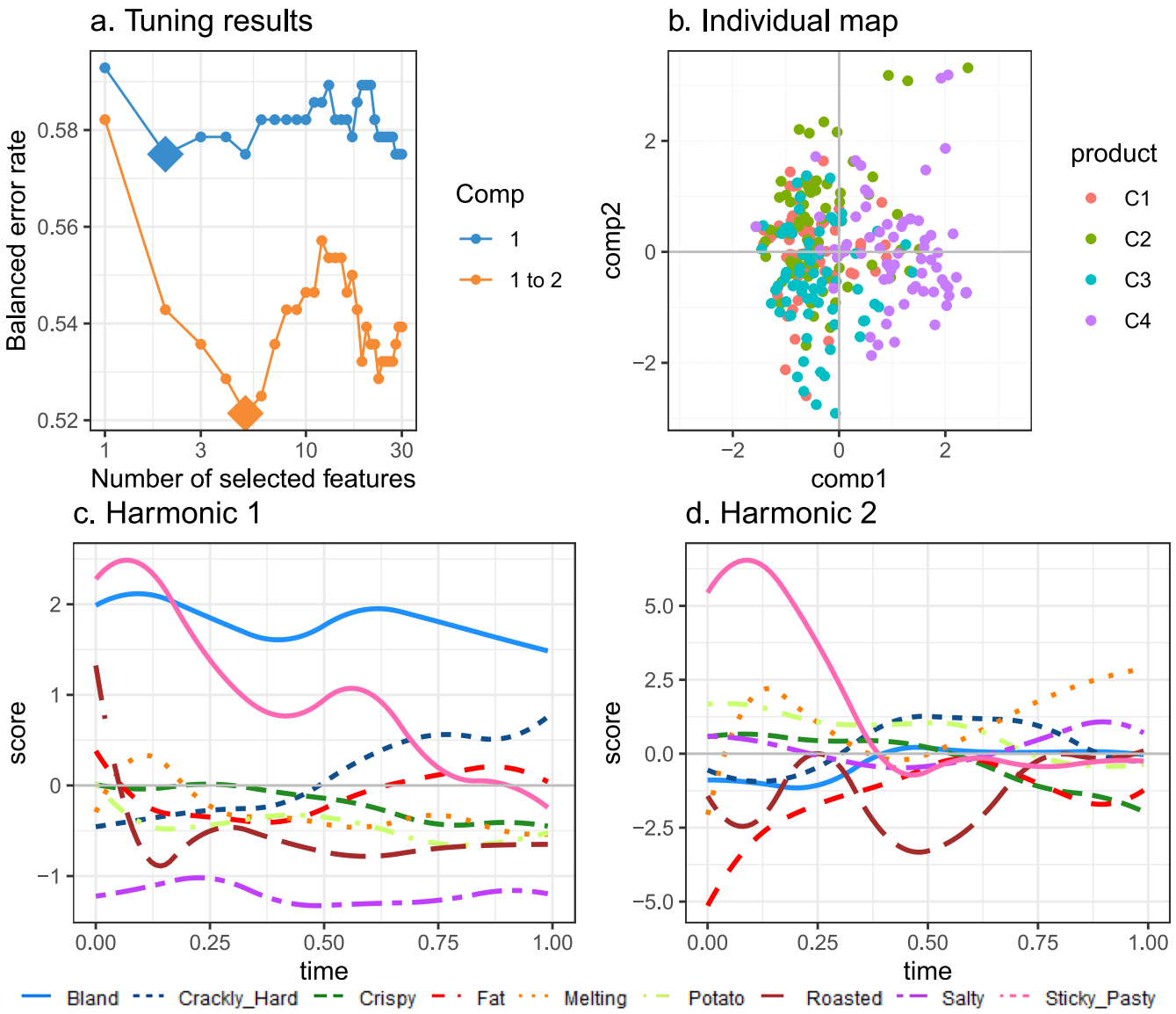

Fig. 7. sPLS results on real dataset: (a) Balanced error rate of sPLSDA model according to the number of selected features (CFDA components) and the number of components in the sPLSDA model (sPLSDA components), (b) individual map, (c) first harmonic, (d) second harmonic.

Table 1
Hotelling T^2 test p-values (and test statistics) on the map of PCA of mean durations and map of sPLSDA on CFDA scores (on the first two dimensions).

Product Pair	PCA	sPLSDA on CFDA
C1-C2	0.227 ($T^2 = 1.50$)	0.0181 ($T^2 = 4.13$)
C1-C3	0.001 ($T^2 = 6.92$)	<0.001 ($T^2 = 8.68$)
C1-C4	<0.001 ($T^2 = 52.54$)	<0.001 ($T^2 = 71.02$)
C2-C3	<0.001 ($T^2 = 13.28$)	<0.001 ($T^2 = 19.39$)
C2-C4	<0.001 ($T^2 = 38.43$)	<0.001 ($T^2 = 61.72$)
C3-C4	<0.001 ($T^2 = 54.79$)	<0.001 ($T^2 = 68.75$)

product mean durations (Fig. 5b), the main conclusions were similar (product C4 was found different from the others as it was found *Bland* during the tasting). However, CFDA allows to go further and to identify individual patterns specific to some product: C3 was shown to be different from C2 because *Fat, Roasted, Crackly_Hard* or *Bland* were dominant at the beginning of the tasting, while for C2 *Sticky_Pasty, Potato* and *Crispy* were dominant. Even if these descriptors were not dominant for the whole panel, they were shown to be more relevant to identify the differences between C3 and C2 in the sPLSDA. This type of information is available neither in difference curves, nor in PCA of durations.

Regarding the clustering results on C3, three groups were highlighted. Group 2 was found to select *Crackly_Hard* at the end of the tasting and could be made up of people having not understood and/or having rushed the task. Group 3 found the crisps mainly *Bland,* especially in the end of the tasting. These two types of behaviors from a minority of subjects were visible neither in TDS curves based on a panel consensus, nor in PCA of durations where the notion of "end of the tasting" does not exist. The subject clustering on CFDA scores was consequently relevant and could be related to liking scores in further works. For example, sPLS could be conducted in order to explain liking results with CFDA scores.

4.2. *Relevance of CFDA for TDS data analysis*

CFDA and its derived results presented in this paper allows for taking the temporality into account in the statistical analysis (including visualization of the raw data and outlier detection, visualization of the product effect and clustering of subjects). It offers a unified framework

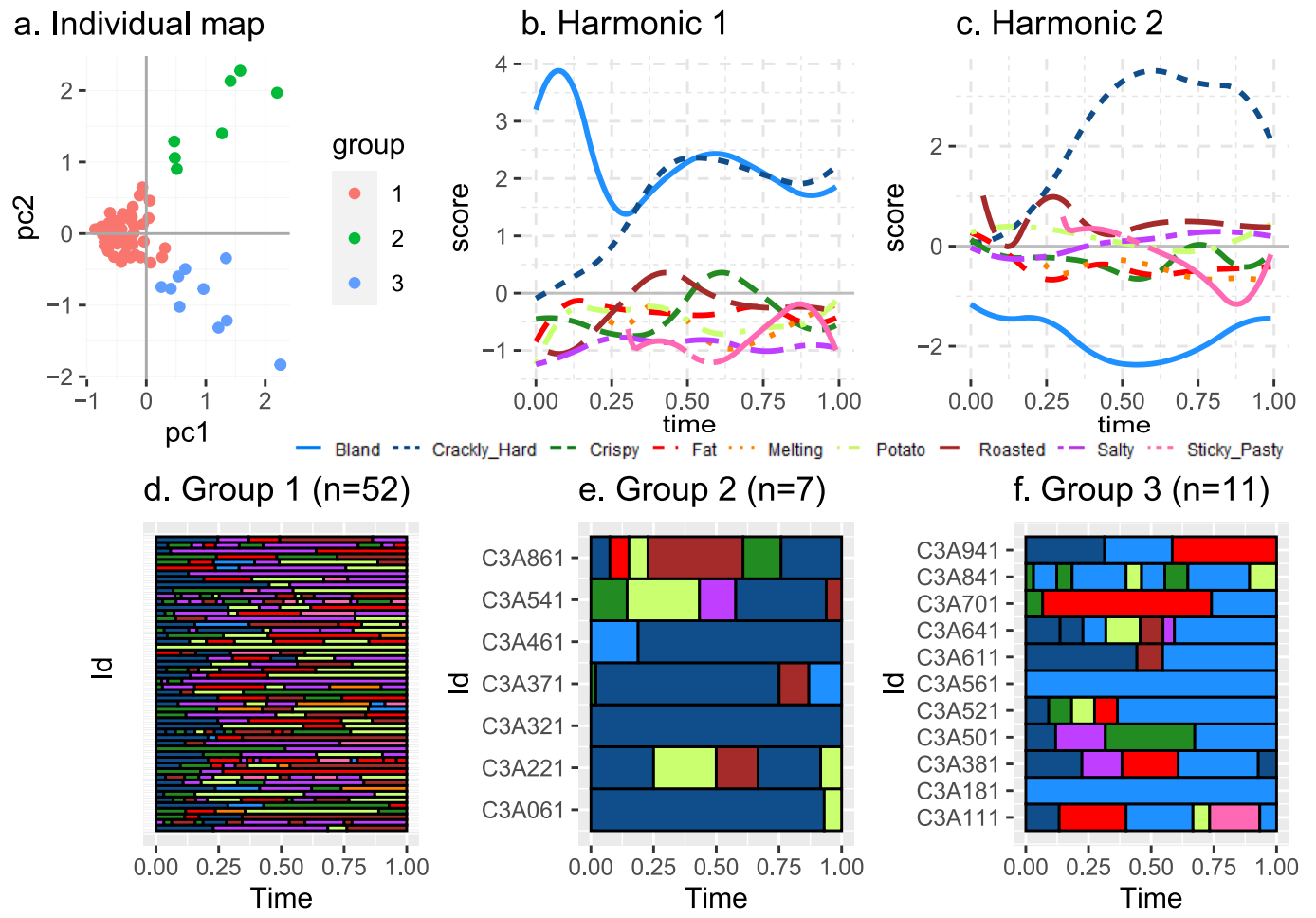

Fig. 8. Results of clustering the TDS sequences of C3 products. (a), (b) and (c) are the results of CFDA. In (a) the individual points are colored accordingly to the result of the clustering where 3 groups (G1, G2 and G3) were identified. (d), (e) and (f) shows the raw data in G1, G2 and G3.

for statistical TDS data analysis based neither on durations nor dominance rates but on exhaustive information, namely the TDS sequences. It should be remembered that, until now, the temporality of TDS data was not fully considered for statistical analysis. Indeed, PCA or CVA were applied only on durations or citations. The only mapping analysis taking temporality into account is the PCA of trajectories that can only show fixed (not temporal) correlations between descriptors. Thus, the conclusions obtained with conventional analyses (separating durations and sequences) may be too restrictive. Consequently, CFDA appears as a very promising approach to analyze TDS data.

4.3. Methodological discussion

4.3.1. CFDA: Choice of parameters and further applications

Perspectives of this work naturally include research on the effects of the choice of different tuning parameters on the obtained CFDA results. Several parameters have to be set before running CFDA: (i) the parameters defining the basis of functions used for projecting the optimal encoding: type (B-splines, here), breakpoints (equidistant, here), number (8, here) and polynomial degree (zero in simulated data, two in real data here), (ii) time standardization of the data, (iii) number of CFDA components to be considered (that was tuned here with sPLSDA). The optimization of the choice of these parameters is still to be studied in order to obtain correct default parameters (for TDS data) that would make the method more accessible for sensory scientists.

The parameters related to the basis of functions could have been different and optimized. For example, the number of eight equidistant knots was arbitrarily chosen (in practice, eight was supposed to be a good compromise between time resolution and overfitting) but other choices could have been made. If the time resolution is more important in specific periods (the beginning of the tasting, for example), the knots could be distributed unevenly (more frequent in the beginning of the tasting). They could also be established directly from the data, by looking to the number of total citations along time and making period durations inversely proportional to the number of citations within these periods. The choice of the spline parameters is well documented (Eilers & Marx, 1996) but is still to be studied with the special case of TDS data. Machine learning could also be used to optimize the choice of the basis (Basna et al., 2022).

The choice of standardizing the data can also be discussed. Regarding CFDA, the fact that all sequences should have the same stop time is mandatory. An alternative to the standardization presented in this paper could also be considered: not standardizing the data but adding a descriptor “no perception” for the evaluations lasting less than the maximum duration (option included in https://www.github.com/ChemoSens/ExternalCode/CFDA-TDS/). The differences between the results obtained with usual standardization and with this alternative could be studied.

As the real duration of the tasting is the only unused information in CFDA, it could also be relevant to add it in the different outputs (as gradient color or point size in the individual maps for example). In this case, if the differences of perception between evaluations were mainly

due to the total durations of perception, it would be possible to directly see them on the map. Thus, this output would summarize all the data collected during TDS (standardized sequences + total duration of tasting).

In this papier, only the first two CFDA dimensions were investigated, but further maps with more axes can also be computed for deeper investigations (especially when the first two axes explain little variance, as was the case with the real dataset). As with usual PCA of durations for example, the first two CFDA axes could discriminate four of seven products, and the three last products can be discriminated only on further dimensions. The number of dimensions to be included should also be discussed and further works should help to determine it. A first natural approach could be to use the elbow criteria (based on CFDA eigenvalues) but alternatives should also be considered.

4.3.2. Using sPLSDA on CFDA data for product discrimination: Limits and perspectives

The sPLS-DA on the CFDA results allows products to be characterized, taking the temporality into account. However, in order to have an easier interpretation, not all the CFDA components are required. In practice, we recommend to automatically remove the eigenvectors corresponding to too low eigenvalues with the help of the cumulative eigenvalues plot, then to tune the sparsity parameters and number of components by choosing a model with "good" performances and a small number of components for an easier interpretation. To discriminate the products alternatives to sPLSDA could also be considered such as Linear Discriminant Analysis (LDA) or CVA on CFDA scores (Peltier et al., 2015). These methods would maximize the discrimination of the products (instead of the inter-product variance) in a fixed model for discriminant analysis (Rencher, 2005) or in a mixed model for CVA. MANOVA on CFDA scores could also allow more sophisticated models to be used for assessing discrimination (Rencher, 2005).

5. Conclusions

Categorical Functional Data Analysis is a statistical analysis that is, by construction, totally adapted to TDS data. It was shown to be relevant in pedagogical examples and a real TDS dataset and offers many tools, taking properly the temporality of the data into account, such as detection of outliers or clustering of subjects. Furthermore, CFDA results can be used as input to other methods, for example to sPLSDA to study product discrimination.

CRediT authorship contribution statement

Caroline Peltier: Conceptualization, Methodology, Software, Formal analysis, Writing – original draft, Visualization. **Michel Visalli:** Conceptualization, Methodology, Writing – review & editing. **Pascal Schlich:** Conceptualization, Methodology, Writing – review & editing. **Hervé Cardot:** Conceptualization, Methodology, 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.

Data availability

The data used is in a published data paper. The R code is available on github.

Acknowledgments

We would like to thank here the reviewers for their comments that helped us to considerably improve the paper.

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