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Descriptive sensory analysis in different classes of orange juice by a robust free-choice profile method

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Abstract

Free-choice profile (FCP), developed in the 1980s, is a sensory analysis method that can be carried out by untrained panels. The participants need only to be able to use a scale and be consumers of the product under evaluation. The data are analysed by sophisticated statistical methodologies like Generalized Procrustean Analysis (GPA) or STATIS. To facilitate a wider use of the free-choice profiling procedure, different authors have advocated simpler methods based on principal components analysis (PCA) of merged data sets. The purpose of this work was to apply another easy procedure to this type of data by means of a robust PCA. The most important characteristic of the proposed method is that quality responsible managers could use this methodology without any scale evaluation. Only the free terms generated by the assessors are necessary to apply the script, thus avoiding the error associated with scale utilization by inexpert assessors. Also, it is possible to use the application with missing data and with differences in the assessors' attendance at sessions. An example was performed to generate the descriptors from different orange juice types. The results were compared with the STATIS method and with the PCA on the merged data sets. The samples evaluated were fresh orange juices with differences in storage days and pasteurized, concentrated and orange nectar drinks from different brands. Eighteen assessors with a low-level training program were used in a six-session free-choice profile framework. The results proved that this script could be of use in marketing decisions and product quality program development.

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1. Introduction

A sensory quality programme requires the selection and training of tasting panel members. Next, the reference descriptors have to be determined and, finally, the panel is calibrated with those reference descriptors. However, the free-choice profile (FCP) method, developed in 1983, can be employed without training the assessors because they themselves freely generate the descriptors. Different authors have successfully reported this methodology: in cheeses [1,2], in dairy desserts [3], in orange-based drinks [4], in coffee [5], in boiled ham [6] and in fresh products [7], to mention a few examples. According to Muñoz and Civille [8], the descriptors of a product are the reference information that the members of a sensory panel mentally retain and share when carrying out tasting exercises.

The frequencies obtained in a sensory analysis are usually studied by means of a principal components analysis (PCA) although other multivariate analysis techniques are also used. In the free-choice profile procedure, exploratory tools for three-way data analysis like the Generalized Procrustean Analysis (GPA) [9] or STATIS [10–12] are often applied. Principal components analysis on merged data sets (PCAMDS) can also be performed following the schema proposed by Kunert and Qannari [13], who point out the easiness of its use.

The aim of this work was the generation and choice of a set of descriptors by a group of semi-trained assessors for its use in the sensorial differentiation of fresh and packaged orange juices, using a robust algorithm designed to increase the strength of the models set up. The results were compared with the STATIS procedure and with the PCA on merged data sets.

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1.1. RAPCA

The principal components analysis is sensitive to the presence of outliers. For that reason, robust versions resistant to the presence of these data have been developed. The RAPCA method aims to maximize robust spread measure in order to obtain consecutive robust directions, the so-called robust principal components that serve as a new coordinate system. Details about RAPCA can be found in Hubert et al. [14]. The RAPCA algorithm has been implemented in MATLAB code and included in the LIBRA toolbox for robust data analysis [15].

1.2. STATIS

The goal of STATIS is to analyse several sets of variables collected on the same observations. In a first step, the association matrices for each data set are determined. Considering different assessors, for each assessor table, X_k with I rows for the juices evaluated and J columns for the attributes employed in each juice, W_k ($I \times I$) is calculated:

 $W_{\rm k} = X_{\rm k} Q_{\rm k} X_{\rm k}^{\rm T},$

where $Q_k (J \times J)$ is used to compensate differences in the number of attributes in each table by using the diagonal elements equal to J_k^{-1} and X_k^{T} is the transpose matrix of X_k .

The similarity between two matrices W_i is calculated by the so-called RV coefficient and it is defined in the following way

$$RV(W_{k}, W_{k'}) = \operatorname{trace}(W_{k}DW_{k'}D) \times (\operatorname{trace}(W_{k}DW_{k}D)\operatorname{trace}(W_{k'}DW_{k'}D))^{-0.5}$$

where $D(I \times I)$ is a matrix with the diagonal elements equal to I^{-1} .

The closer to 1 RV(W_k , $W_{k'}$) is, the more similar the two matrices are. The weights are obtained from the PCA of the RV matrix by scaling the elements of the first eigenvector so that their sum is equal to one. The assessors who agree with most of the panel obtain larger weights. Finally, a true consensus is achieved by means of the weighted sum of the association matrices

$$W=\sum a_{\mathbf{k}}W_{\mathbf{k}},$$

where a_k is the vector of weights.

The matrix *W* is named *compromise* matrix, because it gives the best consensus of the matrices representing each study. The singular value decomposition of *W* gives the principal components, also called *eigenvectors* or *loadings*, of *W*. The subsequent projection of *W* on these eigenvectors or loadings gives a set of *scores* that can be represented to offer information on the similarity between objects.

1.3. PCAMDS

The PCA on merged data sets advocated by Kunert and Qannari is an unfolded PCA on weighted matrices. The weights are determined by the expression

$$a_i = T^{0.5} t_i^{-0.5}$$

where t_i is the sum of the variances of the attributes in each data matrix X_i and T is the average of t_i in all the data tables.

2. Experimental

The sensorial capacity of the assessors was previously verified by carrying out tests to detect incapabilities, to check their sensorial keenness and to determine their aptitude for description. The 18 tasters (7 women and 11 men) received training in the principles of sensory analyses. Fourteen samples in duplicate of orange juice from six firms and seven samples of fresh juice (cv. Valencia) stored under different refrigeration conditions (Table 1) were evaluated. This was done in six sessions, in which between 12 and 16 tasters took part. At each session, approximately 50 mL per juice was evaluated, at temperatures of between 15 and 17 $^{\circ}$ C.

In the sensorial assessment of each sample, the participants generated their freely perceived descriptors. It was decided not to include intensity scales, thus simplifying the method and preventing the introduction of a possible source of error due to an inexpert use of these scales. When the rating sessions were over, a first selection of descriptors was made with semantic criteria, eliminating hedonic terms and synonyms, so that 73 descriptors remained in the following sensory properties: odour, flavour, texture and aftertaste.

The data were analysed with the application of a robust principal component analysis (RAPCA). Taking a hyper matrix with three axes (tasters–descriptors–juices), three sets of values were obtained: matrix A with the descriptors used by each taster, matrix B with the descriptors employed in each of the juices evaluated and matrix C with the juices evaluated by each taster. The tasters did not attend all the sessions. As a result, the frequencies obtained in matrices A-C were weighted according to the number of juices evaluated by each taster, to the number of tasters who evaluated each juice and to the number of descriptors employed by each taster, respectively.

In the following figure, the obtainment of the matrices A-C for their analysis is summarized (Fig. 1).

Matrix *A* (tasters–descriptors) and matrix *C* (tasters–juices) were standardized by dividing by the standard deviation for matrices with *absent* values and centred by subtracting the median value from each descriptor. Then a RAPCA was applied on both matrices. To detect the extreme tasters, the robust distance was represented opposite the orthogonal distance (OD). The cut-off value on the horizontal axis was $(\chi^2)_{k,0.975}^{0.5}$, where the degrees of freedom *k* are the number of robust PCs in the model and 0.975 is the significance level; the squared Mahalanobis distances, calculated in the space of normally distributed scores, follow approximately the Chi squared distribution [11]. If any outlier taster were to be deleted according to the robust distance, then the matrix *B* could be rebuilt without the frequencies from that taster.

Table 1
Samples of commercial and fresh juices (B: brand)

Туре	Package	В	Code	Description	
Juice based on concentrate	Tetra	1	t1	Enriched with vitamins C and E	
	Bloc	2	b2	With vitamin C, <1.5 g of sugar	
	Glass	3	c3	Orange, grape and tangerine with pulp (4%)	
Nectar	Bloc	4	b4	Made of concentrates with sweeteners and 55% fruit	
	Glass	5	c5	Made from concentrate. Minimum 55% of orange, sugar, pulp (5%)	
	Pet	4	p4	Made from concentrate with sweeteners and 45% fruit	
Pasteurized orange juice	Pak	2	pk2s	Without pulp	
	Pak	2	pk2c	With pulp	
	Pak	3	pk3c	With pulp	
	Tetra	6	t6s	Without pulp	
	Tetra	6	t6c	With pulp	
	Pet	6	p6c	With pulp	
	Pet	6	p6s	Without pulp	
	Pet	6	рба	With 50 g L^{-1} of sugar and pulp	
Fresh orange juice	Pet	_	0	Fresh juice from orange with 1 day of storage	
	Pet	-	2	Fresh juice from orange with 67 days of storage (Refrigerator 1)	
	Pet	_	5	Fresh juice from orange with 110 days of storage (Refrigerator 1)	
	Pet	-	7	Fresh juice from orange with 153 days of storage (Refrigerator 1)	
	Pet	-	2	Fresh juice from orange with 67 days of storage (Refrigerator 2)	
	Pet	_	5	Fresh juice from orange with 110 days of storage (Refrigerator 2)	
	Pet	-	7	Fresh juice from orange with 153 days of storage (Refrigerator 2)	

Matrix *B* (juices–descriptors) was analysed unstandardized because no scales were applied in the evaluation of the samples. The frequencies obtained in both replications for each juice were averaged. Next, the matrix *B* was centered by subtracting the median value from each descriptor. Then, a robust analysis of principal components (RAPCA) was made to select the characteristic descriptors of each juice. The total contribution of each of the original variables (descriptors) in the robust PCA model is called *communality*; this indicates how well the original variables are accounted for by the retained principal components. It was calculated as the sum of the squared loadings from the retained principal components, as follows:

 $h_j = \sum s_{ij}^2$



Fig. 1. Obtainment of tables of frequencies A, B and C.

where h_j is the communality of the *j*th variable and s_{ij} is the loading for the *i*th principal component and the *j*th variable.

The robust PCA was applied independently for the descriptors of *odour*, *flavour* and of *texture* and *aftertaste* in all the samples (commercial and fresh juices) and without including the fresh juice samples. Finally, biplots were obtained showing the juices and their associated descriptors. To improve the visualisation of the descriptors on the biplots, the *loadings* were scaled by multiplying by two. Also, a rotation was made of the components obtained by the algorithm *Varimax* [16] to complement descriptors interpretation. The STATIS method and PCA on merged data sets were carried out with the same data and the results were compared according to the so-called index of quality [12] of the compromise, which is given by the percentage of variance explained by the first eigenvector.

3. Results

3.1. Analysis of tasters

The tasters with the highest robust distance values were calculated by means of successive robust PCA models with one, two, three and four robust PCs made on matrix A (tasters–descriptors) and matrix C (tasters–juices) to obtain a better insight into outlying assessors. According to matrix A, taster 13 showed high distance values for models with one, two, three, and four robust PCs, while tasters 4 and 16 only showed them for models with two and three robust PCs. According to matrix C, tasters 9 and 13 showed the highest distance values. It was decided not to eliminate any taster.



Fig. 2. Tasters according to their robust and orthogonal distance on matrix A (a, b, c, d) and C (e, f, g, h).

Fig. 2 shows the group of taster participants according to their robust and orthogonal distance to the models of 1, 2, 3 and 4 robust principal components on matrix A (a, b, c, d) and C (e, f, g, h).

3.2. Analysis and selection of descriptors by means of RPCA

The following figure shows the results of the analysis made for the categories defined of odour, flavour and of texture and aftertaste in commercial samples (Fig. 3a–c) and including the fresh juices (Fig. 3d–f). The coordinates of the descriptors weighted their importance in each axis or component and were related to juices located in similar coordinates. Both components explained 72% of the original variability for the odour descriptors in commercial juices (Fig. 3a) and 68.3% in all the juices (Fig. 3d). In the case of flavour descriptors, the variability percentage was of 61.2% (Fig. 3b) and 43.5% (Fig. 3e), respectively, and with texture and aftertaste descriptors, the variability explained was of 48.6% (Fig. 3c) and 53.4% (Fig. 3f).

The nectars b4, p4, and c5 were clearly differentiated from other types of juice by the strong presence of the odour descriptors *fruity*, *floral* and *artificial* (Fig. 3a). The concentrated juices t1 (packaged in *tetra*) and c3 were related to the odour descriptors *fermented*, *sweet* and *over-ripe*. Both juices (c3, t1) were near the other concentrated juice b2, which was more related to the descriptors *caramel*, *syrup* and *artificial*. The pasteurized juices of brand 6 (t6s, t6c, p6c, p6s, p6a) had greater frequencies of the odour descriptor *cooked* than those of brand 2 (pk2s, pk2c). In turn, the frequencies of the descriptor *cooked* were greater in those juices packaged in tetra than those packaged in *pet*. A greater presence of the *cooked* odour in juice with pulp of the brand 2 (pk2c) with respect to the pulpless juice of the same brand was noticed. Other odour descriptors were *burned*, and *cake*. The pasteurized juice of brand 3 (pk3c) had a lesser *cooked* odour and was related to a greater extent with the odour descriptor *citric*.

In incorporating the samples of fresh juice (Fig. 3d), two groups were formed on both sides of the first component: one determined by the odour descriptor *cooked*, encompassing both the pasteurized and the concentrated juices, and another group with the fresh juices determined by the odour descriptors *fresh* and *fruity*. The descriptors with the greatest discriminating power in the model were the odours *cooked*, *fresh* and *fruity*. In this figure, the nectars stood out for their similarity to the fresh juices. The odour descriptor *fruity* was greater in nectars packaged in *PET* and glass (p4, c5). The concentrated juices showed a weaker intensity of the odour descriptor *cooked* than the pasteurized juices.

The pasteurized juices of brand 6 (t6c, t6s, p6s, p6c) had a strong *cooked* flavour and they also had a higher correlation with the flavour *sour*. In turn, the pasteurized juices of brand 3 packaged in *elo pak* (pk3) and of brand 2 (pk2c) showed a lesser *cooked* flavour and had a *fruity* and *sweet* (pk2c) or *fruity* and *sour* (pk3) flavour. The nectars correlated with the flavours *sweet* (p4) and *fruity* (b4, c5), which was strongest in the glass packaging of brand 5. The pasteurized juice with added sugar packaged in *PET* (p6a) showed a greater relation with the *sweet* flavour and less so with the *cooked* flavour. The concentrated juices of brands 1 and 3 (t1, c3) and the pasteurized pulpless juice of brand 2 (pk2s) were differentiated by presenting flavours like



Fig. 3. Descriptors and juices on the plane formed by the two first principal components.

artificial, bitter and *burned.* However, the concentrated juice of brand 2 (b2) displayed a higher correlation with the flavour descriptor *sour* and *cooked.*

On including fresh juices (Fig. 3e), the descriptors of the greatest importance for differentiating the new type were the flavours *watery*, *fresh and resinous*. The differences can be observed between the flavour descriptors obtained by fresh juices from refrigerator 1 (*sour* and *watery* flavours) and those from 2 (*fresh*, *resinous*, and *over-ripe*). Similarly, the pasteurized and concentrated juices (t1, c3) were located close to the flavour descriptors *sweet*, *bitter*, and *cooked*. The three nectars and the concentrated juice b2 were differentiated from the pasteurized juices by presenting a greater intensity in the flavour descriptor *watery*.

A positive correlation was noted between the aftertaste descriptors *burned* and the texture descriptors *dense* and *astringent* (Fig. 3c) forming a group with most of the pasteurized juices with and without pulp, except for the pasteurized juice of brand 3 (pk3c), and the sweetened juice of brand 6 (p6a), which showed a *resinous* aftertaste and *smooth* and *spicy* texture. The concentrated juices (c3, t1) correlated with the aftertaste descriptors *bitter* and *sweet* and *hot* texture except the concentrated juice of

brand 2 (b2), which was related to the aftertaste *sweet* and *sour* and *watery* texture. On the contrary, the nectars (c5, b4) had a *bitter*, *sour*, and *watery* texture, but not a *burned* or *cooked* aftertaste.

The inclusion of fresh juice samples in the texture and aftertaste model determined the appearance of new descriptors like *fruity* and *resinous* aftertaste (Fig. 3f). The results showed two groups defined and differentiated by the first axis of variability, which was related to the texture descriptor *light* and aftertaste descriptor *fruity* in fresh juices and texture descriptors *astringent* and *dense* and aftertaste descriptor *bitter* in the remaining juices. A weaker intensity of the aftertaste descriptor *sour* was noted in the samples with the longest conservation time and in the samples from refrigerator 2.

The following table shows the results of RAPCA for odour, flavour and texture and aftertaste descriptors ordered by their communality value (h) in both cases, with only commercial juices and with all the juices. Some descriptors correlated more with the third or fourth component according to their *loadings* (L). To demonstrate the discriminant character of these descriptors, the samples can be represented on the plane formed by these components, thus obtaining a complementary image of

Table 2 (Continued)

Table 2

1

Loadings (L1 and L4) and communality associated with each odour, flavour, and texture and aftertaste descriptors in commercial juices and including fresh juices

	L1	L2	L3	L4	h
Attributes and load	dings with hi	gher comuna	lity value (h)	in the	
RAPCA models	with comme	rcial juices			
Odour					
Fruity	-0.01	-0.71	0.23	-0.25	0.62
Cooked	0.52	0.21	-0.03	0.35	0.44
Artificial	-0.49	0.16	-0.23	0.06	0.32
Burned	0.29	-0.15	-0.24	0.35	0.28
Citric	-0.1	-0.38	-0.29	0.13	0.26
Rancid	0.03	0.04	-0.28	-0.39	0.23
Floral	-0.35	0.04	0.11	0.28	0.22
Over-ripe	0.25	0.23	0.16	-0.27	0.22
Sweet	0.12	0.15	0.42	0.01	0.21
Syrup	-0.08	0.02	0.34	0.27	0.20
Sweetener	-0.14	0.04	0.36	0.18	0.18
Cake	0.12	-0.15	-0.16	0.31	0.16
Fermented	0.01	0.12	-0.33	-0.09	0.13
Citrus oil	0.02	-0.27	0.11	0.16	0.11
Caramel	-0.24	0.12	-0.05	0.17	0.10
Flavour					
Bitter	-0.27	-0.32	-0.74	-0.14	0.75
Sweet	-0.50	0.41	0.21	-0.52	0.73
Citric	0.36	0.52	-0.22	-0.07	0.46
Waterv	-0.20	-0.03	0.23	0.49	0.34
Cooked	0.33	-0.34	0.08	-0.25	0.29
Fruity	-0.06	0.45	-0.27	0.07	0.28
Sour	0.40	0.11	0.20	-0.04	0.22
Burned	-0.07	-0.23	0.17	-0.34	0.20
Artificial	-0.24	-0.06	0.15	0.34	0.20
Texture					
Smooth	-0.03	-0.12	-0.66	-0.04	0.45
Hot	-0.06	0.20	0.06	-0.56	0.36
Dense	0.47	0.23	-0.13	0.01	0.30
Astringent	0.30	0.40	0.06	-0.23	0.30
Watery	-0.28	-0.03	-0.11	-0.45	0.29
Resinous	0.09	-0.08	0.34	0.01	0.13
Aftertaste					
Bitter	-0.46	0.70	-0.10	0.29	0.80
Citric	0.29	0.02	-0.35	0.07	0.21
Sweet	-0.37	-0.01	0.00	0.25	0.20
Spicy	0.09	-0.11	-0.10	0.36	0.16
Burned	0.20	0.19	0.22	0.17	0.15
Sour	-0.20	-0.30	0.02	0.01	0.13
Cooked	0.22	0.03	-0.03	0.23	0.10
000.00	· · · · · ·	0.00	0.00	··	

Attributes and *loadings* with higher comunality value (*h*) in the RAPCA models with *commercial and fresh juices*

Odour					
Fruity	0.74	0.32	-0.23	0.09	0.71
Cooked	-0.53	0.64	-0.01	-0.05	0.69
Citric	-0.07	0.09	-0.40	-0.54	0.46
Fresh	0.23	0.06	0.31	-0.50	0.40
Floral	-0.05	-0.36	-0.00	-0.40	0.30
Artificial	-0.17	-0.30	-0.41	0.00	0.29
Over-ripe	0.02	-0.09	0.40	0.16	0.20
Burned	-0.11	0.07	0.32	0.12	0.14
Rancid	-0.03	-0.08	-0.30	0.16	0.12
Fermented	-0.11	-0.25	0.00	0.19	0.11
Flavour					
Sweet	-0.34	-0.26	0.37	-0.49	0.56
Cooked	-0.35	-0.24	-0.58	0.15	0.54

L1 L2 L3 L4 h Citric 0.17 -0.17-0.33-0.570.49 0.24 0.47 Sour -0.32-0.060.39 Watery -0.230.50 0.20 0.11 0.36 0.38 Burned -0.240.20 0.29 0.33 Fruity 0.04 -0.400.22 0.16 0.16 0.24 Bitter -0.32-0.220.11 0.22 Resinous 0.33 -0.250.01 0.15 0.20 0.02 Fresh 0.34 -0.250.08 0.18 Cake -0.08-0.06-0.06-0.370.15 Over-ripe -0.07-0.28-0.060.18 0.12 Texture -0.430.08 0.40 0.19 0.39 Dense Astringent -0.36 -0.390.31 -0.060.39 Smooth 0.09 0.13 -0.050.45 0.23 Light 0.33 0.15 0.04 -0.210.18 0.09 -0.16-0.220.22 Watery 0.13 Aftertaste Bitter -0.470.04 -0.57-0.220.60 Sour 0.14 -0.60-0.040.35 0.51-0.310.35 Citric 0.48 0.14 0.47 Sweet -0.15-0.12-0.410.11 0.22 -0.04Fruity 0.32 0.14 0.080.13 Burned -0.14-0.150.23 -0.130.11 Artificial -0.09-0.090.01 -0.300.11

the models. Only descriptors with a communality higher than 0.10 are shown in the following table and in the previous figures (Table 2).

To facilitate the interpretation of the eigenvectors, the application of the *Varimax* rotation procedure would be necessary. This will often make the eigenvectors more interpretable by maximizing the variance within each vector. Fig. 4 shows the results when the *Varimax* rotation procedure is applied.

The figures after the *Varimax* rotation (see Fig. 4b and d) procedure showed a similar configuration in both cases. The nectars (b4, p4, c5) exhibited few differences in odour descriptors. The rest of the juices except pk3c and pk2s showed *cooked* and *over-ripe* descriptors of a certain intensity. In the case of flavour descriptors, the juices c5, p4, pk3c showed stronger *fruity*, *sweet*, *citric* and *watery* descriptors than pk2c, p6a and p4 juices. The juices pk2s, c3 and t1 were *bitter* and the remaining juices displayed a *cooked* and *sour* flavour.

3.3. Analysis by means of PCA on merged data sets

The following figure shows the results when a PCA was carried out on the matrix formed by merging the data sets associated with the assessors into a matrix, whose columns are formed by all the attributes of all the assessors. The different data sets were column centered, subtracting the median of the corresponding column from each entry of each data set (Fig. 5).

This method compared well with the previous one with RAPCA. The relative position of the juices was very similar



Fig. 4. Descriptors and juices before and after the application of the Varimax rotation procedure.

to that obtained with RAPCA. But the percentage of variance explained in all the planes was lower: 34.1% for odour in commercial juices, 29.6% for odour in all the juices, 26.6% for flavour in commercial juices, 25% for flavour in all the juices and 15.6% and 21.3% for texture and aftertaste in commercial and all the juices, respectively.

The scaling factors defined by Kunert and Qannari were not applied in the previous analysis. The reason was that, in their sample evaluation, the assessors did not use scoring. According to Kunert and Qannari, the scaling factor compensates for the differences in the range of scoring between assessors in the use of intensity scales. The inverse value of the expression proposed by Kunert and Qannari was the one employed since, only in this way, did the factors upweight the good tasters. In the following figure, the scaling factors obtained by the different assessors are shown. If they are compared to the evaluations made with RAPCA, these results are very similar given that lower values were obtained by tasters 9 and 13 (Fig. 6).

3.4. Analysis by means of STATIS

Fig. 7 shows the results with the STATIS method. The PCA of the RV matrix reflects the similarity between tasters. The compromise matrix was centred on the median. The results with commercial juices (see Fig. 7a–c) compared fairly well with previous ones. Assessors 9 and 13 were those showing a

greater difference from the mean covariance and, therefore, their weights were smaller, with commercial juices (see Fig. 7d-f) and with all the juices (Fig. 7j-l). The first and second components after the PCA of the compromise with commercial juices explained 35.2% for variables of odour, 27.1% for variables of flavour and 27.8% for variables of texture and aftertaste (see Fig. 7g-i). When all the juices, commercial and fresh, were included, the first and second component explained 29.6% for odour descriptors, 26.2% for flavour descriptors and 22% for texture and aftertaste descriptors (see Fig. 7m-o). In both cases, the juices were clustered in a similar way to that in previous analyses. Nectars p4, b4 and c5 formed a cluster in all the characteristic descriptors with commercial juices (see Fig. 7g-i) and so the concentrated juices t1 and c3 were also similarly clustered. The pasteurized juices also gave similar results to the ones obtained with RAPCA. When all the juices were included, fresh juices formed their own cluster just on the right of the graphics (see Fig. 7m-o) the same as with the robust PCA method.

4. Discussion

The sensorial differences between orange juice types were remarkable, and were of the greatest importance when comparing processed juices to fresh juices. The processes used in the manufacture of orange juice (extraction, filtering, debitter-



Fig. 5. Descriptors and juices on the plane formed by the two first principal components after PCAMDS.

ing, concentrate, deodorization, pasteurisation, packaging) and its storage conditions notably modify the sensorial properties of the freshly squeezed product. Thus, the different types of juices (nectars, pasteurized, frozen, concentrates, fresh) are associated with certain odour, flavour or aftertaste and texture descrip-



tors. For instance, the descriptors odour–flavour–aftertaste of *cooked* were noted in pasteurized juices and juices made with concentrates. Other descriptors associated with thermally treated juices are vanilla, caramel and burned flavour [17].

Nectars are products resulting from adding ingredients like water, sugar or honey to juice, to fruit purée, or to a blend of both. Thus, the obtainment of sensorial profiles, similar to that of natural orange juice, is facilitated. For that reason, in nectars and fresh juices, odour–flavour–aftertaste descriptors *fruity*, *floral*, and other similar ones appeared. However, the descriptor *fresh* was most related to fresh juices probably due to the numerous volatile aromatic compounds present naturally in the freshly squeezed product.

On the other hand, thermally treated juices may contain defects due to their possible pollution from acidophilus or thermophilus microorganisms, which could have survived the heat treatment. One example of this type of microorganism is bacteria of the genus *Leuconostoc*, which alter the juice by producing *diacetyl* and which has been associated with butter and rancid aromas and tastes. Another descriptor generated was a *medicinal* odour, which, according to Wisotzkey [18], could be related to contamination by bacteria of the genus *Allyciclobacillus*.



Fig. 7. Results of STATIS for the centered data set: (a) PCA of the RV matrix: PC1–PC2 plot for assessors accounting for odour descriptors; (b) PCA of the RV matrix: PC1–PC2 plot for assessors accounting for flavour descriptors; (c) PCA of the RV matrix: PC1–PC2 plot for assessors accounting for texture and aftertaste descriptors; (d) bar plot of weights for assessors for variables of odour; (e) bar plot of weights for assessors for variables of flavour; (f) bar plot of weights for assessors for variables of odour; (e) bar plot of weights for assessors for variables of flavour; (f) bar plot of weights for assessors for variables of commercial juices for variables of odour; (h) PC1–PC2 plot of the compromise of commercial juices for variables of flavour; (j) bar plot of weights for assessors for variables of flavour; (i) PC1–PC2 plot of the compromise of commercial juices for variables of exture and aftertaste; (j) bar plot of weights for assessors for variables of flavour; (i) PC1–PC2 plot of the compromise of commercial juices for variables of exture and aftertaste; (j) bar plot of weights for assessors for variables of odour; (h) PC1–PC2 plot of the compromise of commercial juices for variables of flavour; (i) bar plot of weights for assessors for variables of flavour; (i) PC1–PC2 plot of the compromise of commercial and fresh juices; (h) bar plot of weights for assessors for variables of flavour; (i) PC1–PC2 plot of the compromise of commercial and fresh juices for variables of odour; (n) PC1–PC2 plot of the compromise of commercial and fresh juices for variables of texture and afterstate in all the juices; (m) PC1–PC2 plot of the compromise of commercial and fresh juices for variables of texture and afterstate.

5. Conclusions

In general, the results showed a great coherence between the products rated and the descriptors generated, thus greatly validating the methodology followed. The RAPCA analysis improved the visualization of the samples and their interrelations. Its usefulness lies in being easy to use and in the great variability it represents, so that the quality of the obtained compromise is higher than that commonly found in this type of study.

The algorithm used with robust PCA may be of interest in the obtaining of perception maps linked to the products. It can be

used with untrained tasters, although a short training programme in the concepts and practices of sensory analysis is advised. It can also be applied with the partial absences of tasters or with groups which have heterogeneous sensorial abilities. Its practical use is important as it combines two aims of interest in sensory analysis: the generation of a set of non redundant descriptors and the obtainment of results in a short period of time, making them useful in enterprise decision-making and in the development of new products. This tool made it possible to select a set of descriptors, ordered from greater to lesser importance, to discriminate or differentiate between types of orange juice available on the market.

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References

- A. Rétiveau, D.H. Chambers, E. Esteve, Food Qual. Preference 16 (2005) 517–527.
- [2] M.A. Drake, S.C. McIngvale, P.D. Gerard, K.R. Cadwallader, G.V. Civille, J. Food Sci. 66 (2001) 1422.
- [3] L. González-Tomás, E. Costell, J. Sensory Stud. 2 (2006) 22-33.
- [4] M. Lachnit, M. Busch-Stockfisch, J. Kunert, T. Krahl, Food Qual. Preference 14 (2002) 257–263.
- [5] C. Narain, A. Paterson, E. Reid, Food Qual. Preference 15 (2003) 31-41.

- [6] C.M. Delahunty, A.Mc. Cord, E.E. O'Neill, P.A. Morrissey, Food Qual. Preference 8 (5–6) (1997) 381–388.
- [7] S.V. Kirkmeyer, B.J. Tepper, Chem. Senses 28 (2003) 527-536.
- [8] A.M. Muñoz, G.V. Civille, J. Sensory Stud. 13 (1998) 57–75.
- [9] J.C. Gower, Psychometrika 40 (1975) 33-51.
- [10] C. Lavit, Y. Escofier, R. Sabatier, P. Traissac, Comput. Stat. Data Anal. 8 (1994) 97–119.
- [11] I. Stanimirova, B. Walczak, D.L. Massart, V. Simeonov, C.A. Saby, E. Di Crescenzo, Chemom. Intell. Lab. Syst. 73 (2004) 219–233.
- [12] H. Abdi, D. Valentin, in: N.J. Salkind (Ed.), Encyclopedia of Measurement and Statistics, Sage, Thousand Oaks, CA, 2007, pp. 955–962.
- [13] J. Kunert, E.M. Qannari, J. Sensory Stud. 14 (1999) 197-208.
- [14] M. Hubert, P.J. Rousseeuw, K. Vanden Braden, Technometrics 47 (2005) 64–79.
- [15] S. Verboven, M. Hubert, Chemom. Intell. Lab. Syst. 75 (2005) 127-136.
- [16] M.Á. Carreira-Perpiñán, in: Technical Report CS-96-09, Department of Computer Science, University of Sheffield, 1996.
- [17] D.A. Kimball, in: Procesado de cítricos, Ed. Acribia, Zaragoza, 2001, pp. 312, 328.
- [18] J.D. Wisotzkey, P. Jurtshuk, G.E. Fox, G. Deinhard, K. Poralla, Int. J. Systemat. Bacteriol. 42 (1992) 263–269.