

# Experimental design, sensorial and principal components analysis: Three complementary tools for cocktail optimization

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Ten cocktails containing rum, coca cola<sup>®</sup>, and lemon juice were formulated according to a mixture design, and were hedonistically rated on a nonstructured scale by a panel of 46 testers. Averaged scores have been correctly fitted by a quadratic polynomial and the optimum composition of the cocktail has been located thanks to the isoresponse curves. The principal components analysis of the results led to a first axis that separates subjects based on their rum/lemon preferences, whereas the two following axes, the third in particular, distinguish the subjects who appreciate cocktails with high ratio of coca cola<sup>®</sup> from those who dislike them.

Formulation was considered as the art, and now as the science, that consists in mixing different kinds of ingredients, to obtain an usable product. Every time an industrialist contemplates marketing a new product for the consumer, he has to optimize the ratio performance/cost. In such areas as pharmacy, detergency, lubrication, paints or adhesives, the required performances can be achieved by imposing technical criteria that will be measured by physico-chemical methods and application tests depicting the real conditions of use. On the other hand, in hedonistic sectors such as cosmetology, perfumery or food processing, the

evaluation of each formulated product is more difficult, since technical tests have to be completed by sensorial analysis realized by a trained panel. Thanks to these assessment criteria, the methodology of experimental designs can be employed to obtain the best composition. However, one can ask, whether it is better to market a single product that would be acceptable by all the consumers rather than several formulations fitting closely the diversity of tastes of the consumers.

In order to illustrate the use of three complementary tools, experimental design, sensorial and principal components analysis, we present in this paper, a strategy for the optimization of a cocktail (Cuba-libre) made from coca cola<sup>®</sup>, lemon juice and white rum [1].

## Material and methods

### Preparation and sensorial analysis of cocktails

The starting ingredients, stored at 4 °C, were white rum "rhum blanc agricole, Old Nick<sup>®</sup>", coca cola<sup>®</sup> and freshly squeezed yellow lemon juice. The ten cocktails were prepared according to the experimental design presented in table I, and the total amount of each formulation was calculated to provide a serving size of 10 mL. Mixtures were kept in a refrigerator and then poured into opaque goblets

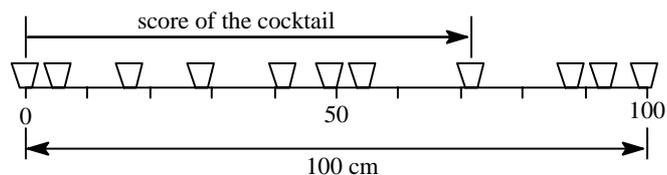


Figure 1. Hedonic rating of the 11 cocktails on a nonstructured scale.

under the bottom of which the number of the corresponding cocktail was written.

After tasting a given cocktail, subjects were asked to place the goblet on a 100 cm graduate scale (Fig. 1), putting the goblet of the least and most appreciated cocktails at 0 and 100 respectively. The other goblets were placed between them depending on the appreciation of the tester and their distances from zero were considered as the score of the cocktail. The series of scores of a given tester were retained if he was able to evaluate two identical cocktails with a difference of rating inferior or equal to 30.

### Matrix and experimental design

A cocktail must be optimized according to a mixture design [2,3], since the sum of the proportions of the ingredients is unity:

$$\% \text{ coca-cola}^{\circledR} + \% \text{ rum} + \% \text{ lemon} = 100\%.$$

Previous studies have shown that each ingredient must be present in the final formulation to get the original flavour [4]. For this reason, the minimal percentages of both coca cola and lemon were started at 5%. On the other hand, the fraction of coca cola<sup>®</sup> was always higher than 60% to avoid the saturation of the taste buds of subjects, with too acidic or alcoholic flavours. Finally, the constrained mixture space was defined by:

$$5\% \leq \text{lemon} \leq 35\%, 5\% \leq \text{rum} \leq 35\% \text{ and } 60\% \leq \text{coca cola}^{\circledR} \leq 90\%.$$

These constraints reduce our mixture space to the white equilateral triangle localized inside the complete ternary diagram shown in figure 2. Each vertex corresponds to a "pseudo-components" i.e. a mixture of the three pure components. To study this region, we have prepared the ten cocktails 1 to 10 according to the proportions indicated in table I.

If  $Z_1, Z_2, Z_3$  are the volumic fractions of coca cola<sup>®</sup>, lemon juice and rum respectively, previous constraints on each proportion of component can be also written:

$$60\% \leq Z_1 \leq 90\%, 5\% \leq Z_2 \leq 35\% \text{ and } 5\% \leq Z_3 \leq 35\% \text{ with } Z_1 + Z_2 + Z_3 = 100\%.$$

Normalized coordinates ( $X_1, X_2, X_3$ ) of each pseudo-components 1, 2 and 3 are constrained to lie in the range  $0 \leq X_i \leq 1$  and the sum of the  $X_i$  equals 1. They are related to the volume fractions  $Z_i$  according to the following system:

$$Z_1 = 90 X_1 + 60 X_2 + 60 X_3$$

$$Z_2 = 5 X_1 + 35 X_2 + 5 X_3$$

$$Z_3 = 5 X_1 + 5 X_2 + 35 X_3.$$

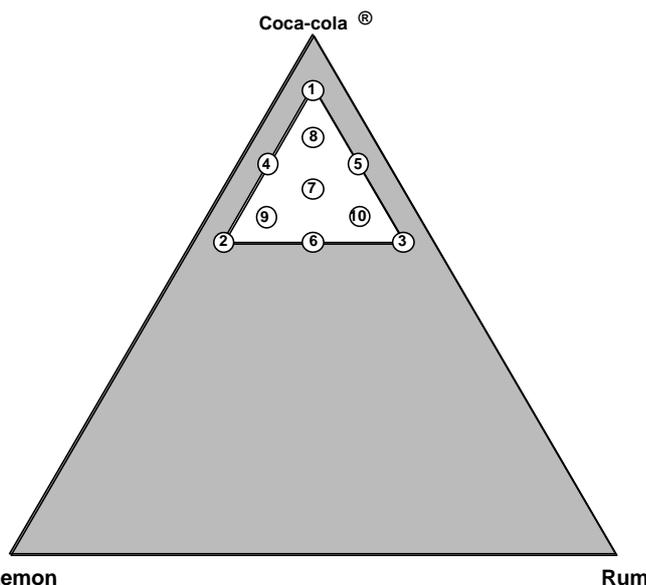


Figure 2. Experimental region defined by the constraints ( $5\% \leq \text{lemon} \leq 35\%$ ,  $5\% \leq \text{rum} \leq 35\%$  and  $60\% \leq \text{coca cola}^{\circledR} \leq 90\%$ ) and localization of the tested cocktails.

## Results

46 untrained subjects (21 women and 25 men, aged between 22 and 24) were asked to rate the ten cocktails (Tab. I) using a 100-points hedonic scale according to conditions recommended in sensorial analysis [5]. The results are presented in table II. To assess the reliability of each subject i.e. his ability to give similar notes to the same product [6], he was presented with two identical cocktails among the nine other cocktails during the blind test. These duplicated cocktails, and the difference between their scores ( $\Delta$ ) have been listed in the two last columns. This test led us to eliminate subjects 40 to 46 for the calculation of the mean score of each cocktail because they were considered insufficiently reliable ( $\Delta > 30$ ). However the standard deviations have been calculated both from the reliable subjects ( $\sigma = 10$ ) and from all the panel ( $\sigma = 18$ ).

## Discussion

### Axial matrix

The influence of each pseudo-component 1, 2 and 3 on a mixture containing the two others in equal amount can be studied by the ten points lying on the three medians of the axial matrix. To simplify the analysis, we have shown (Fig. 3) the variation of the mean scores versus the volume fraction of each ingredient (coca cola<sup>®</sup>, lemon and rum) instead of the pseudo-components 1, 2 and 3. This representation is quite correct for the axis corresponding to pseudo-component 1 (points 6, 7, 8, 1) which is colinear to the median "coca cola<sup>®</sup>". In fact, moving along this axis from point 6 to point 1, increases the proportion of coca cola<sup>®</sup>, while the ratio rum/lemon is held to a constant value

Table I. Matrix and experimental design used for cocktail optimization.  $Y_{exp}$ ,  $Y_{calc}$  and  $\Delta$  are the mean scores given by the panel, the scores calculated from the quadratic polynomial model and the differences between these scores, respectively.

N° Cocktail	Matrix			Experimental design			$Y_{exp}$	$Y_{calc}$ quadratic model	$\Delta$
	$X_1$	$X_2$	$X_3$	% coca	% lemon	% rum			
1	1	0	0	90	5	5	55	57	-2
2	0	1	0	60	35	5	14	10	4
3	0	0	1	60	5	35	42	44	-2
4	1/2	1/2	0	75	20	5	45	45	0
5	1/2	0	1/2	75	5	20	49	55	-6
6	0	1/2	1/2	60	20	20	52	52	0
7	1/3	1/3	1/3	70	15	15	54	55	-1
8	2/3	1/6	1/6	80	10	10	65	57	8
9	1/6	2/3	1/6	65	25	10	30	40	-10
10	1/6	1/6	2/3	65	10	25	62	54	8

of 1. This is no more true for the two other segments (5, 7, 9, 2) and (4, 7, 10, 3) which were parallel but not colinear to the medians "lemon" and "rum". These three graphs show that the lemon is the prevalent factor and the first one points out that its percent must not exceed 15% in the cocktail. The two last graph exhibit weak maxima for the proportion of rum (15 to 25%) and of coca cola® ( $\approx$  80%).

Mean scores reported in table II can be analyzed using the methodology of isoresponse curves, which is complementary to the previous method. The Scheffe algorithm [7,8] can be applied to points 1 to 10 of the experimental design, in order to obtain a representative mathematical model, able to predict the score for any point within the experimental region. The process is used in a sequential way, by testing more and more complicated models, i.e. polynomials of higher and higher degrees. Some experimental points are selected to calculate the coefficients of the postulated model. Then, this model is validated or rejected by comparing the predicted scores for the non-selected points with the experimental values. The current model was considered to give adequate prediction of  $Y_{exp}$  when the polynomial fitting fall within a maximum difference ( $\Delta_{max}$ ) of 12. This arbitrary value was obtained from the following formula:

$$\Delta_{max} = \Delta_{moy} + u \cdot \sigma / (n)^{0.5}$$

where  $\Delta_{moy}$  (10),  $u$  (1.64),  $\sigma$  (10) and  $n$  (39) represent the mean of differences for the duplicated cocktail, the Student

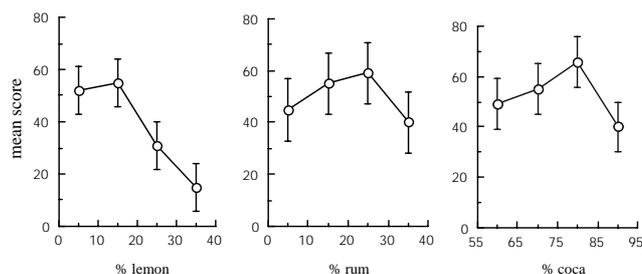


Figure 3. Evolution of the mean scores of cocktails versus the volume fractions of lemon, rum and coca-cola®.

factor for 95% confidence interval, the standard deviation of the differences and the number of reliable testers respectively. Hence, if the differences between calculated and experimental values do not exceed  $\Delta_{max}$ , the coefficients of the model are refined by taking into account all the experimental data using the least squares method and NEMROD software [9]. If the model is rejected, the same strategy is applied to a polynomial with a higher degree.

In order to simplify the equations (see below), we used the notation  $Y_i$  to represent the mean score for the cocktail n°  $i$ . The first mathematical model to test is a simple linear model which assumes that the response  $Y$  is strictly proportional to the ratio of each pseudocomponent 1, 2 and 3.

$$Y = b_1 \cdot X_1 + b_2 \cdot X_2 + b_3 \cdot X_3.$$

The three experimental responses obtained for each vertex 1, 2, and 3 allow us to determine directly the coefficients  $b_i$  ( $b_i = Y_i$ ). Hence, the following polynomial is obtained:

$$Y = 55 \cdot X_1 + 14 \cdot X_2 + 42 \cdot X_3.$$

Its validity is controlled with the test points 4 to 10 (Tab. III). This first degree model is of poor quality since most of the test points exhibit differences with the measured values much higher than 12. It points out that the effect of each component on the response  $Y$  is not only additive, but there are probably interactions between them. Therefore, a quadratic polynomial must be examined:

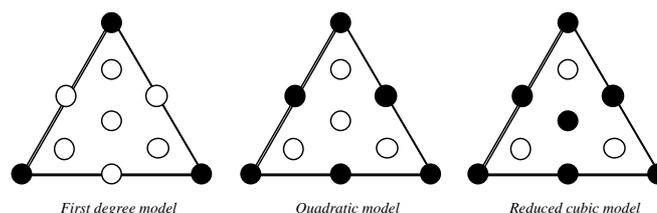


Figure 4. Points of the ternary diagram used to calculate (black dots) and to validate (white dots) the first degree, quadratic and reduced cubic models.

Table II. Hedonic scores of the ten cocktails given by a panel of 46 untrained subjects including 25 men (M) and 21 women (W).

tester		cocktail number										duplicated	$\Delta$
		1	2	3	4	5	6	7	8	9	10	cocktail	
1	W	60	0	100	10	10	80	40	50	0	70	8	10
2	W	47	15	55	0	55	100	37	90	77	65	2	0
3	W	100	0	50	50	30	60	60	70	10	55	8	10
4	W	0	0	20	10	50	80	50	100	10	70	10	10
5	W	50	0	20	60	100	20	80	30	10	60	9	20
6	W	100	33	61	44	100	0	94	86	22	78	8	5
7	W	80	0	100	20	70	20	35	60	10	50	7	10
8	W	10	0	90	60	40	70	40	30	20	100	7	20
9	W	20	0	30	50	90	50	50	100	10	70	7	20
10	W	40	0	0	10	70	50	75	100	20	30	7	30
11	W	100	10	0	80	40	30	65	90	50	20	7	10
12	W	100	30	0	40	10	50	25	80	60	20	7	10
13	W	10	0	20	50	70	80	100	30	50	90	7	0
14	W	14	36	100	0	57	71	43	0	0	93	7	30
15	W	70	70	0	100	20	30	60	50	100	10	7	0
16	W	60	30	0	100	10	20	85	70	90	0	7	30
17	W	20	10	40	80	0	100	40	50	10	90	5	30
18	M	100	20	0	40	10	10	80	50	20	60	2	10
19	M	0	0	100	0	60	90	30	20	0	80	8	10
20	M	100	0	20	40	50	80	50	60	10	30	1	10
21	M	100	0	60	40	40	70	10	80	20	70	10	0
22	M	80	0	20	90	60	30	50	100	40	40	6	0
23	M	10	0	30	20	10	70	30	60	10	100	6	10
24	M	60	0	10	30	50	100	40	80	30	90	3	10
25	M	70	0	50	80	30	100	30	90	40	50	3	10
26	M	30	0	10	20	60	70	60	90	0	100	3	0
27	M	71	0	77	41	100	18	6	60	24	47	8	10
28	M	22	0	11	56	67	100	22	56	0	89	8	20
29	M	60	0	100	20	70	40	35	50	10	80	7	10
30	M	50	15	100	40	80	25	55	70	0	80	7	10
31	M	56	31	88	75	44	0	69	69	19	100	7	20
32	M	20	0	90	10	80	30	45	60	80	100	7	10
33	M	50	90	20	60	80	10	95	40	70	0	7	10
34	M	50	60	0	90	20	30	80	100	70	10	7	0
35	M	90	70	10	100	20	30	45	60	80	0	7	10
36	M	60	30	10	0	20	30	89	60	20	90	7	20
37	M	30	0	10	100	60	50	90	40	0	20	7	0
38	M	100	0	40	20	70	30	90	80	40	70	7	0
39	M	60	0	80	5	10	100	30	70	20	100	4	30
40	W	20	30	0	100	60	20	80	40	10	50	1	50
41	W	70	0	30	60	40	90	10	10	80	100	9	80
42	W	26	0	75	13	75	51	66	100	23	38	7	33
43	W	100	0	90	30	30	10	50	20	0	60	7	40
44	M	80	10	30	20	0	100	10	90	0	30	7	50
45	M	100	25	0	13	63	75	65	100	44	50	7	35
46	M	20	90	80	60	0	50	100	30	70	10	7	60
Mean (Y)		55	14	42	45	49	52	54	65	30	62		10
Standard deviation ( $\sigma$ )		32	23	37	32	28	31	25	24	28	31		10 (18)

$$Y = b_1 \cdot X_1 + b_2 \cdot X_2 + b_3 \cdot X_3 + b_{12} \cdot X_1 \cdot X_2 + b_{13} \cdot X_1 \cdot X_3 + b_{23} \cdot X_2 \cdot X_3.$$

It is easy to prove, using the vertex points, that  $b_1$ ,  $b_2$  and  $b_3$  remain unchanged. The determination of the interaction coefficients  $b_{12}$ ,  $b_{13}$  and  $b_{23}$  is realized with the three mid-points of each edge. Thus, applying this model to point 4 ( $X_1 = X_2 = 0.5$ ;  $X_3 = 0$ ) give:

$$Y_4 = (b_1 + b_2) / 2 + b_{12} / 4$$

$$\text{i.e. } b_{12} = 4 \cdot Y_4 - 2 \cdot (Y_1 + Y_2) = 42$$

in the same way  $b_{13} = 2$  and  $b_{23} = 96$  were obtained; thus, the quadratic model can be expressed as:

$$Y = 55 \cdot X_1 + 14 \cdot X_2 + 42 \cdot X_3 + 42 \cdot X_1 \cdot X_2 + 2 \cdot X_1 \cdot X_3 + 96 \cdot X_2 \cdot X_3.$$

Points 7, 8, 9 and 10, which are used to verify the model fitting, prove that this model is much better than the first degree polynomial (Tab. III). Differences  $\Delta$  are smaller than the maximal accepted discrepancy ( $\Delta \leq 12$ ) and positive and negative differences show a balanced distribution of experimental values around calculated values. Since this model is now validate, the coefficients are refined by the least squares method using all the experiences 1 to 10 (Eq. 1).

$$Y = 57 \cdot X_1 + 10 \cdot X_2 + 44 \cdot X_3 + 45 \cdot X_1 \cdot X_2 + 16 \cdot X_1 \cdot X_3 + 98 \cdot X_2 \cdot X_3. \quad (1)$$

Calculated values from equation (1) are listed in table I. As expected the model is satisfactory since none of the differences exceeds the upper value of 12. However, since this last value is somewhat arbitrary, it is possible that a more complicated model would exhibit a better predicting ability. Therefore, the reduced cubic model has been determined from experimental points 1 to 7.

$$Y = 55 \cdot X_1 + 14 \cdot X_2 + 42 \cdot X_3 + 42 \cdot X_1 \cdot X_2 + 2 \cdot X_1 \cdot X_3 + 96 \cdot X_2 \cdot X_3 + 39 \cdot X_1 \cdot X_2 \cdot X_3$$

$$\text{where } 39 = 27 \cdot Y_{123} - 12 \cdot (Y_{12} + Y_{13} + Y_{23}) + 3 \cdot (Y_1 + Y_2 + Y_3).$$

This last model does not give better results than the quadratic polynomial (Tab. III).

At last, we used least squares regression through all the data points ( $390 = 39 \times 10$ ) instead of the ten averages. The coefficients of the quadratic model are identical to those obtained by the standard methodology of experimental design (Eq. (1)). The values of the confidence intervals of the model parameters are 9 for  $b_i$  and 42 for  $b_{ij}$  while the confidence interval of the response are equal to 16.

Predicted responses calculated from equation (1) can be represented through isoresponse curves [10], obtained by maintaining  $Y_{\text{calc}}$  at a given value. Graphic representation in figure 5 shows that the preferred region is delimited by points 1, 5 and 8. The maximum calculated by derivation of equation (1), is ( $X_1 = 0.75$ ;  $X_2 = 0.07$ ;  $X_3 = 0.18$ ). To foresee the success of such a cocktail, we have examined the scores of the cocktail n° 8, which has the closest composition to this maximum. Table II shows that this mixture is highly appreciated by 67% of reliable testers (26 subjects) since they gave it a score superior to 60, while only 13% of the testers (subjects 5, 8, 13, 14 and 19) do not like it at all (score  $\leq 30$ ). This result confirms that it is possible to sat-

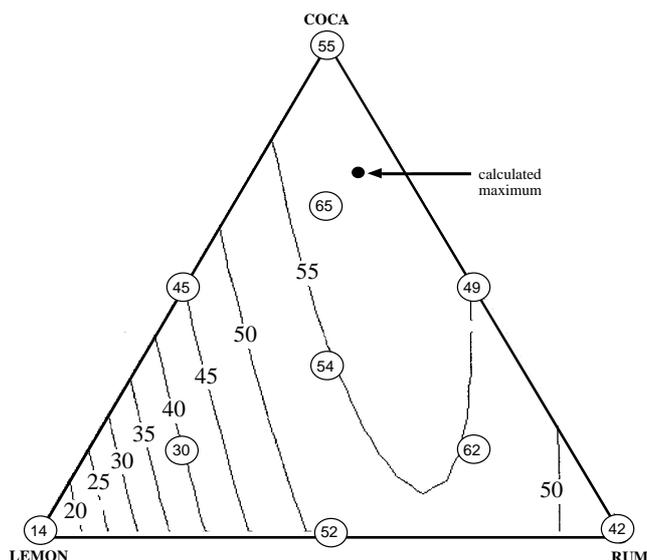


Figure 5. Isoresponse curves of the average score  $Y$  obtained from the quadratic model. Experimental score of the ten cocktails have been encircled.

Table III. Experimental and calculated scores from first degree, quadratic and reduced cubic model.  $\Delta$  is the difference  $Y_{\text{exp}} - Y_{\text{calc}}$ .

Cocktail N°	$Y_{\text{exp}}$	First degree model		Quadratic model		Reduced cubic model	
		$Y_{\text{calc}}$	$\Delta$	$Y_{\text{calc}}$	$\Delta$	$Y_{\text{calc}}$	$\Delta$
1	55	55	0	55	0	55	0
2	14	14	0	14	0	14	0
3	42	42	0	42	0	42	0
4	45	34	21	45	0	45	0
5	49	48	1	49	0	49	0
6	52	28	24	52	0	52	0
7	54	37	17	52	2	54	0
8	65	46	19	54	11	54	11
9	30	25	5	41	-11	42	-12
10	62	39	23	52	10	52	10

isfy most of the potential consumers, with such an average cocktail.

However, the methodology of experimental design could not point out the preference of each tester for sweetened (coca cola®), acid (lemon) and alcoholic (rum) flavours whereas principal components analysis is well adapted to undertake such a study.

### Principal components analysis (PCA)

A rough examination of the results reported in table II leads to the conclusion that the mean scores obtained by the 10 cocktails exhibit a smooth variation from the lemon rich cocktail 2 to the preferred cocktail 8. However, the

regularity resulting from the calculation of a mean value of many individual scores hides considerable variations between the scores given by each subject. For example, six testers gave to cocktail 3 the higher score (100) while seven other subjects disliked it (score = 0). This discrepancy results in the individual difference of appreciation and not in the lack of reliability of the rating method used. Actually, the variability of the rating method may be estimated with the standard deviation calculated from all the duplicated cocktails ( $\sigma = 18$ ). It is always lower than any standard deviations to one of the ten cocktails ( $23 < \sigma < 37$ ). This last standard deviation value piles up two types of variability: those coming from the rating method and those resulting from the individual preferences.

Calculation of the mean scores conceals the inter-individual differences and outlines the best average formulation. However, rather than formulating one cocktail which will be appreciated by all subjects overall, it can be better to distinguish several classes of consumers in order to fit a cocktail to a given class. To assess the preferences of each subject, results of table II were analyzed by PCA [11,12]. The principles involved can be illustrated geometrically as follows: each subject of table II is characterized by the set of scores he gave to the ten cocktails (variables). Let each cocktail define a coordinate axis. Hence the ten different axes will define a 10-dimensional space. In this space each tester will be described by a point for which the coordinates on the different axes are equal to the rating of the cocktail. PCA constitutes a projection of this swarm of points down to a space of fewer dimensions. The projection is done in such a manner that the first component vector describes the direction through the swarm showing the largest variation. The second component vector describes the direction through the swarm showing the second largest variation, etc. The determination of this PC (eigen)vectors [13], which are linear combinations of the original variables (cocktails), results from calculations involving the 390 data of table II (39 subjects  $\times$  10 cocktails). For a given subject, the hedonic scores for all the cocktails were centred by subtracting the mean score in order to make calculation easier. Hence, the sum of the transformed scores was the same for all subjects, i.e. zero. Moreover, these last data were reduced to avoid the problem of the choice of the scale. Eigenvalues (Tab. IV) and vectors (Tab. V) of the transformed matrix, permit to obtain new axes that allows the localization of the 10 cocktails and 39 testers.

Table IV has to be examined in order to obtain the best compromise with regard to two conflicting aims: choosing a space of fewer dimension than the initial one and getting a high percent of information. This table shows that a three dimensional description describes 64% of the total information, while the best description in one dimension represents only 36%. This first axis of the analysis represents the weight of almost 4 initial variables (3.6), whereas, the second and the third axes, 1.5 and 1.3 respectively. The information contained in the next principal axes is less important than the one contained in each initial axis. Hence, they have been deleted and we have kept only the first three ones.

There are no hard and fast rules for selecting the best number of axes. However, more formal methods [14] can be followed to aid judgment. One useful tool is called a "scree plot" based on the plot of the eigenvalues as a function of the factor ordering. Another method is by retaining only

**Table IV. First five eigenvalues, percent and cumulated percent of the total variance obtained from centred and reduced data of table II.**

N° axis	Eigenvalue	% total variance	% cumulated
1	3.6	36	36
2	1.5	15	51
3	1.3	13	64
4	1.1	11	75
5	0.7	7	81

**Table V. Coordinates of the 10 cocktails on the three first eigenvectors and their squares.**

Cocktail N°	Vector 1		Vector 2		Vector 3	
	x	(x) <sup>2</sup>	x	(x) <sup>2</sup>	x	(x) <sup>2</sup>
1	0.27	0.07	0.10	0.01	0.47	0.22
2	0.37	0.14	-0.17	0.03	-0.38	0.14
3	-0.34	0.12	-0.24	0.06	-0.00	0.00
4	0.37	0.14	0.06	0.00	-0.15	0.02
5	-0.12	0.01	-0.55	0.30	0.37	0.14
6	-0.30	0.09	0.52	0.27	-0.23	0.05
7	0.27	0.07	-0.43	0.18	-0.04	0.00
8	0.15	0.02	0.34	0.12	0.62	0.38
9	0.38	0.14	0.09	0.01	-0.17	0.03
10	-0.44	0.19	-0.13	0.02	-0.06	0.00

those factors which have an eigenvalue greater than the average eigenvalue. A more statistically precise method for determining whether a factor explains a significant amount of variability is by performing test on successive residual matrices.

Table of the eigenvectors  $V$  gives explanations of the new axes *versus* initial variables (cocktails). Each axis is a combination of these variables, the contribution of which can be estimated by the square of the corresponding coefficient. For example in the axis 1, the variable 1 contributes for  $(0.27)^2 = 7\%$ , the variable 2 for 14%, ... and the variable 10 for 19%. In order to simplify the interpretation of axis 1, we keep only variables 2, 3, 4, 9 and 10 that describe 73% of the total information:

$$\text{Axis 1: } [0.37 (\text{cocktail 2}) + 0.37 (\text{cocktail 4}) + 0.38 (\text{cocktail 9}) - [0.34 (\text{cocktail 3}) + 0.44 (\text{cocktail 10})].$$

Localization of these cocktails in the ternary diagram (Fig. 1) points out the opposition between lemon-flavoured cocktails (2, 4, 9) and rum concentrated cocktails (3, 10).

In the same way, the second eigenvector defines the second axis:

$$\text{Axis 2: } [0.52 (\text{cocktail 6}) + 0.34 (\text{cocktail 8}) - [0.55 (\text{cocktail 5}) + 0.52 (\text{cocktail 7})].$$

Since these four cocktails have very similar composition, no immediate conclusion can be drawn from this second axis. A weak opposition between the mixtures rum-coca (6) and

rum-lemon (5) can be eventually found. Hence, this axis is not discriminating to classify the testers.

The third axis is mainly composed of variables 1 and 8 (60% of the information).

$$\text{Axis 3: } 0.47 (\text{cocktail 1}) + 0.62 (\text{cocktail 8}).$$

It is directed towards the two coca-rich cocktails.

In an attempt to visualize more information than that revealed by a single eigenvector, a bidimensional scale was also defined. Since the principal axes (1, 3) appear to be correctly related to the different flavours present in the ten formulations, we chose to locate the 10 cocktails and the 39 testers in the plane defined by these two axes.

Rather to use the biplot methodology [15,16] that would give an unclear graphic with both 10 variables and 39 observations on the same principal component axes 1 and 3, we preferred to separate the analysis of cocktails and testers.

It is noteworthy that the PC projection of the cocktails in the circle of correlation (Fig. 6) is topologically similar to the pseudoternary diagram of figure 2. Thus, the three types of extreme cocktails containing a high amount of coca (1, 8), lemon (2, 9) or rum (3, 10) stand well apart from each other while each binary mixture (cocktails 4, 5 and 6) is actually located between the projection of the constituent cocktails. This result clearly shows the ability of our panel to distinguish the various flavours of the presented cocktails. The closeness of the three groups of cocktails (1, 8), (3, 10), and (2, 4, 9) in figure 6 suggest that they could have been replaced by only three cocktails in order to simplify the sensorial analysis. In fact, these cocktails are relatively close together in the sphere of correlation determined by axes 1, 2 and 3.

The following step is the study of the projection of the 39 testers in the same plane. The distances between subjects that show a difference in their flavour patterns, are interpretable with the graphic of associated variables (Fig. 6). The quality of the representation of a point M according to a principal axis is measured by the square of the cosine of the angle between the considered axis and the segment that links this point to the barycentre of the swarm. Hence, we have encircled (with unbroken lines) all the subjects for which  $\cos^2$  was superior to 0.3 for axis 1 (36% of the total information). Since axis 3 contains less information (13%), we imposed a smaller restrictive value of 0.2 for the selection of the subjects (circled in dotted lines). On the other hand, we did not take into account the 13 complementary subjects (2, 3, 4, 5, 18, 20, 24, 25, 26, 30, 31, 36, 37) localized close to the zero point since they do not carry any significant information in this plane. In fact, they correspond to the subjects who prefer intermediate cocktails rather than the extreme ones. The numbers corresponding to women are bold italicized. So, it can be seen from figure 7, that the representative points for men and women are randomly distributed and it is not possible to draw any conclusion from the correlation between the sex of the subjects and the preference patterns.

Axis 1 allows the separation of the subjects based on their rum/lemon preferences. The most important group includes subjects who preferred rum-rich cocktails and do not like lemon-flavoured cocktails. For example, subjects (1, 8, 14, 19, 23, 28, 29, 39) localized in the circled region gave the

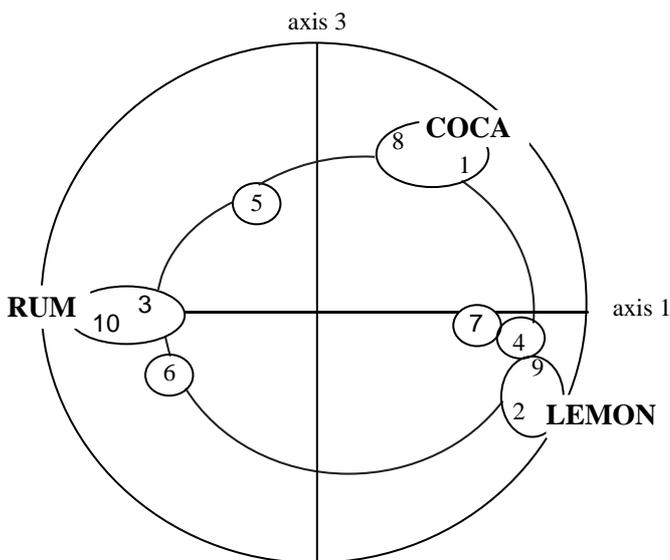


Figure 6. PC projection of the ten cocktails in the plane (1, 3).

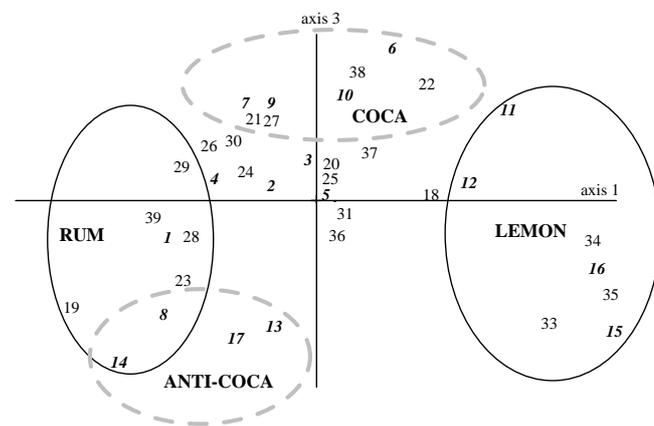


Figure 7. PC projection of testers in the plane (1, 3). For identification numbers, see table II, numbers corresponding to women are bold italicized. Circled subjects have their  $\cos^2$  superior to 0.3 on axis 1 (unbroken lines) and superior to 0.2 on axis 3 (dashed lines).

best rating (except 28) to the alcoholic cocktails (1 or 8) whereas they attributed at the same time, the zero score to one of the most lemon concentrated cocktails (2 or 9). The second class, on the right of axis 1, comprised the 7 subjects (11, 12, 15, 16, 33, 34, 35) who exhibit opposite preferences.

Axis 3 is mainly based on the opposition between coca-lovers and coca-haters. Thus, most of the circled testers lying at the top of this axis (6, 7, 9, 10, 21, 22, 27, 38) have chosen their preferred cocktail among 1 or 8. On the contrary the circled testers (8, 13, 14, 17) in the bottom, dislike these cocktails since the sum of the corresponding scores (except 17) do not exceed the value of 50.

According to this PCA results, we can now give an explanation to the dislike ( $0 \leq \text{score} \leq 30$ ) of cocktail 8 (which is nearest point to the optimum formulation), by 13% of the

testers (5, 8, 13, 14 and 19). In fact, figure 7 clearly indicates that subjects (8, 13, 14) consider that this cocktail contains too much coca cola®, they do not appreciate. Moreover, subjects 8, 14 and 19 shows that they would prefer a more alcoholic cocktail. The case of tester 5 is less clear since he is not located in a circled preference region, but his coordinate on axis 2, which opposites cocktails 6, 8 against 5, 7, is very high. This is fully confirmed by the scores assigned to these cocktails i.e. 20, 30, 100 and 80 respectively. However, it is likely that this peculiar set of scores is simply caused by an error during the sensorial evaluation of cocktails, since good scores (50, 60, 100, 80) were given for all the cocktails (1, 4, 5, 7) surrounding cocktail 8, whereas this last cocktail get a bad score of 30.

### Conclusion

This example shows that the optimization of a formulation may be readily achieved using mixture designs even when subjective data have to be handled. Principal component analysis proved to be a useful complementary method since it led to a preference pattern where four types of consumers could be clearly identified.

This strategy can be applied in all fields which involve a sensorial analysis to assess the value of a product. The taste was the evaluating method, but the four other senses could be involved for other formulations. The sense of smell to evaluate the ability of a detergent according to provide a sweet-smelling to clean washing, the eyesight to judge the glossy of hair after shampooing, the touch to evaluate the sensation of softness and the lack of sticking during application of a cosmetic cream, and at last, the sense of hearing

to point out the quality of a mascara thanks to the noise emitted when the brush is extracted from its tank.

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