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6 **Generalized pair-wise correlation and method comparison: impact assessment**
7 **for JAR attributes on overall liking**

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3

1 **Abstract**

2 In product development using JAR (just-about-right) scales, it is important to identify precisely,
3 which direction of a given attribute affects hedonic scores the most. The Generalized Pairwise
4 Correlation Method (GPCM) is a non-parametric one and it is useful to rank JAR variables
5 according to their impact on liking. This is done using appropriate statistical tests: the
6 McNemar's, the Chi-square, the Conditional Fisher's and the Williams' *t*-test. As GPCM requires
7 one-directional variables, JAR data needs to be transformed based on the dummy variable
8 approach. GPCM gives those attributes in that order, which should be increased/decreased to gain
9 higher consumer liking scores. An order can be created according to the impact on liking, which
10 order determines the development of product attributes, as well. The non-parametric tests
11 incorporated in the method are able to identify smaller differences than other statistical methods.
12 As a result, GPCM identifies more significant product attributes; hence, it can help product
13 development processes even if other methods cannot.

14

15 **Keywords:** Generalized Pairwise Correlation, just-about-right data analysis, Penalty Analysis,
16 product optimization, feature selection, software

17

1 **1. Introduction**

2 Just-About-Right (JAR) scales are bipolar scales used to measure the level of an attribute relative
3 to a sensory assessor's ideal level, having a midpoint labeled "just about right" or "just right". A
4 scale is bipolar when the end anchors are semantic opposites; for example, "not nearly sweet
5 enough" to "much too sweet," and there is an implied or anchored neutral mid-point (ASTM
6 E253; ASTM E456). A discussion about the meaning of the JAR levels was published by Gacula
7 *et al.* in 2007.

8 Figure 1

9 The number of categories used in the JAR scales usually varies between three and nine. Figure 1
10 shows a JAR scale consisting of five categories. In consumer research and sensory sciences, JAR
11 scales are typically measured along with hedonic scores: the relationship between the JAR
12 variable and the hedonic score is used for either optimization or further development of products.
13 JAR scales have been used to optimize salsas (Popper & Gibes, 2004), raisin jams (Rababah *et*
14 *al.*, 2012), probiotic Petit Suisse Cheese (Esmerino *et al.*, 2013), mixed juices from Amazon
15 fruits (Freitas & Mattietto, 2013), mango nectar (Cadena & Bolini, 2012), cooked steaks (Chan *et*
16 *al.*, 2013), Bulgogi (Korean traditional barbecued beef) (Hong *et al.*, 2011) and juice blends
17 (Lawless *et al.*, 2013), just to name a few. Despite frequent usage, there are several unsolved
18 issues regarding the JAR scales: (i) consumers must understand the attributes in question; (ii) the
19 endpoints must be true opposites (Lawless & Heymann, 2010); (iii) there is no conclusive
20 evidence that the use of JAR scales predicts optimal products (Epler *et al.*, 1998). Earthy *et al.*
21 (1997) and Popper *et al.* (2004) showed that JAR questions present in the questionnaire have an
22 effect on overall liking and some authors do not recommend the use of JAR scales (Stone &
23 Sidel, 2004). On the other hand, others report that JAR methods perform well during product

1 development as we mentioned above; (iv) it is not known how much of products should be
2 adjusted to reach optimal JAR likeness. Lesniasuskas and Carr concluded that JAR data analysis
3 should answer three questions (Popper & Gibes, 2004):

4 (1) Are some products more JAR than others?

5 (2) If the product is not JAR, in which direction should it be advanced?

6 (3) How much is the acceptance affected when a product is not JAR?

7 Several methods have been introduced to evaluate JAR data: Penalty Analysis (ASTM MNL63),
8 Multivariate Adaptive Regression Splines (MARS) (Xiong & Meullenet, 2004), Partial Least
9 Squares Regression (PLS-R) with dummy variables (Xiong & Meullenet, 2006), Canonical
10 Variate Analysis (CVA) (Popper & Gibes, 2004) and Thurstonian Ideal Point (TIP) modeling
11 (Goerlitz & Delwiche, 2004).

12 Penalty Analysis appears to be the most commonly used method to analyze JAR data. Penalty
13 Analysis consists of three main steps in case of a five point JAR scale. Firstly, the JAR values are
14 amalgamated into three groups. Categories 1 and 2, category 3, and category 4 and 5 give the
15 three new levels: "not enough", "JAR", and "too much". Then, the mean overall liking (rating) is
16 calculated for each group. The penalties (or mean drops) are calculated as the differences
17 between the means of the two non-JAR categories and the mean of the JAR category. These
18 values are plotted *versus* the percentage giving each response in a so-called mean drop plot.

19 Several papers dealing with the improvement of the method have been published in the past few
20 years. Plaehn and Horne (2008) introduced a regression-based approach for testing the
21 significance of JAR variable penalties. Plaehn (2013) created a Penalty Allocation Map (PAM) to
22 improve the estimation of the "penalties". Pagès *et al.* (2014) used Multiple Correspondence
23 Analysis (MCA) to visualize the uncertainty in penalties. The main aim of analyzing JAR data is

1 to identify the strengths/weaknesses of a given product and to determine, which attributes should
2 be increased or decreased in future product formulations.

3 Most of the above mentioned methods are able to reach this goal, but for product developers it
4 would be very useful to identify precisely, which direction (not enough or too much) of a given
5 attribute affects the hedonic scores the most. Feature selection methodologies (methods applied to
6 define a subset of relevant variables in model construction) would answer this question after
7 proper data pretreatment.

8 A nonparametric approach for feature selection was introduced by Rajkó and Héberger, named
9 Pairwise Correlation Method (PCM), which can discriminate between two features (Rajkó &
10 Héberger, 2001). Let us assume that a dependent feature (Y) contains the hedonic scores and that
11 two independent features (JAR variables, X_1 and X_2) have been measured. PCM makes a
12 distinction between the two features. This idea was later generalized (Generalized Pairwise
13 Correlation Method, GPCM) up to several hundred features (Héberger & Rajkó, 2002a, 2002b).

14 The present paper introduces this new technique, which uses a different set of information present
15 in the data than usual. The aim of this study is to investigate the usefulness of GPCM to identify
16 the main factors influencing the hedonic scores. The outcome helps to create proper regression
17 models for predicting hedonic scores or building preference maps.

18

19 **2. Materials and Methods**

20 **2.1 Data analysis**

21 **2.1.1. Coding of the JAR data**

22 The bipolar Just-About-Right (JAR) scales cannot be evaluated using linear approaches, as the
23 optimal point is located above the points next to it (Figure 2). The JAR data set consists of ratings

1 from the consumers. These ratings are not normally distributed and furthermore the scale has two
2 directions. In the case of a general five point JAR scale, the midpoint (rating 3) belongs to the
3 term “just about right”, rating 1 belongs to the term “the attribute is too weak” and rating 5
4 belongs to the term “the attribute is too strong”. Therefore, two linear relations would be suitable
5 by just cutting the JAR scale in the middle in two parts. In creating a one directional scale, loss of
6 information is inevitable because the number of consumers, who rated the product as JAR, cannot
7 be calculated.

8 Figure 2

9 The bipolar scale can be transformed into a unipolar one by applying the dummy variable
10 approach introduced by Xiong and Meullenet (2006). This transformation has to be performed
11 before running Generalized Pairwise Correlation Method (GPCM). A possible creation of one
12 directional scales is shown in Table 1.

13 Table 1

14 2.1.2 Pairwise Correlation Method (PCM)

15 PCM is a non-parametric method, developed for the discrimination of features. It has the
16 advantage of non-parametric statistics so the assumption of normality is not required. Let us
17 define three vectors as a dependent variable (Y or consumer’s liking) and two independent
18 variables (X_1 and X_2 or JAR attributes). Both of the X_1 and X_2 features have positive
19 correlations with the Y feature. The task is to choose for the response feature (Y) the superior one
20 from the coequal predictor features X_1 and X_2 . Consider all the possible element pairs for Y_i vs.
21 X_{1i} and X_{2i} as well as Y_j vs. X_{1j} and X_{2j} (running coordinates are i and j 1, 2, ... N) (see Figure
22 3). Four basic events can be counted *i.e.* A , B , C , and D . The frequencies of the events A , B , C ,
23

1 and D (k_A , k_B , k_C and k_D , respectively) are counted and ordered (see Table 2). Event A means that
2 both $X1$ and $X2$ strengthen the changes in Y . Event B means that $X1$ strengthens but $X2$ weakens,
3 while event C means that $X2$ strengthens but $X1$ weakens the same changes. Event D means that
4 both $X1$ and $X2$ weaken the changes in Y (Figure 3) (Rajkó & Héberger, 2001).

5 Table 2

6 Figure 3

7 The frequencies for the four possible events are arranged in a 2×2 contingency table. If both
8 differences ($\Delta X1$ and $\Delta X2$) are positive (or both are negative), the distinction cannot be made
9 between $X1$ and $X2$. If the frequency value for opposite signs of $\Delta X1$ is significantly greater, then
10 $X1$ is termed as superior, otherwise $X2$. Whether the frequency value is significantly greater (or
11 not) can be determined by the next statistical tests: the McNemar's, the Chi-square and the
12 Conditional Fisher's tests as non-parametric statistical ones. For the sake of comparison, the
13 Williams' t -test as a parametric test was also included.

14 The program calculates the critical sum and the limit (theoretical) probability at which the
15 frequencies in B and C boxes can still be considered as significant. An example shows a case of
16 clear superiority of a feature: Table 3 contains the comparison of Color+ and Carbonation+ where
17 Carbonation+ overrides Color+ i.e. (wins) unambiguously.

18 Table 3

19 In its generalized form (GPCM), all possible independent feature pairs are compared and a
20 number of "superiority" is determined. The number of "superiority" is termed as the number of
21 wins, i.e. how many times a given X feature was "superior" to the other X features. The number
22 of "inferiority" is termed as the number of losses; i.e. how many times an X feature was inferior
23 to the other X features. The number of wins is simply summed for all possible comparisons of

1 feature pairs. Three ranking methods (a) simple ranking according to the number of wins, (b)
2 ranking according to the differences in wins and losses and (c) probability weighted ranking
3 according to the differences in wins and losses were elaborated in the Generalized Pairwise
4 Correlation method (Héberger & Rajkó, 2002a).

5 It has to be mentioned that GPCM might be sensitive to outliers in Y direction (dependent
6 variable) either on the plot of $X1$ variable or in the plot of the $X2$ variable. Such outliers of Y
7 influence the frequencies of events B or C . If a Y outlier is present in both plots of $X1$ and $X2$,
8 then, the frequency of event D is influenced and would not be evaluated further. Random
9 fluctuations do not affect the results of GPCM. The method uses systematic information; hence
10 outliers have to be removed before analysis. Let us notice that logical operations require more
11 calculation time than arithmetical operations, hence the high number of observations increase
12 computation time, but this is not mandatory.

13

14 **2.1.3 Generalization of PCM based on simple ranking**

15 Only the number of wins is counted in the case of simple ranking; *i.e.* the features are ranked
16 according to the number of wins. The features, which did not win at all, are excluded
17 automatically. A percentage (*e.g.* 95 %) of the total number of wins indicates the number of
18 variables, which have to be selected (Héberger & Rajkó, 2002a).

19

20 **2.1.4 Generalization of PCM based on ranking according to differences**

21 PCM has to be carried out pairwise for all possible (different) feature pairs as above. In case of
22 this GPCM ranking, the features are ranked according to the number of wins minus the number of
23 losses. A percentage value (*e.g.* 95 %) in the number of wins minus number of losses indicates

1 the number of features which have to be selected. Features, which did not win at all and those for
2 which the number of wins is less than or equal to the number of losses are not selected to be
3 significant features. However, the numbers of wins minus losses are suitable to rank all of the
4 features (just the zero and negative values should not be excluded). This ordering method is the
5 second most sensitive but data characteristics can also influence the number of significant
6 differences.

7

8 **2.1.5 Generalization of PCM based on ranking according to probability-weighted** 9 **differences**

10 PCM has to be done for all possible different pairs as in the previous sections. Wins and losses
11 are counted as above, but they are weighted with the calculated confidence level (=1-calculated
12 error level) based on any test statistics. In this way the features are ranked according to the sum
13 of the weighted differences. Subtracting the error levels, the numbers of wins and losses will not
14 be integer numbers (Héberger & Rajkó, 2002a). This type of ranking produces the most sensitive
15 one, it takes into account whether the wins were overwhelming or not.

16 GPCM data analysis was done using a Microsoft Excel VBA spreadsheet application:

17 <http://aki.ttk.mta.hu/gpcm>

18 Spearman's rank correlation, Multiple Linear Regression (MLR), Partial Least Squares
19 Regression (PLS-R) and Penalty Analysis was done using XL-Stat Sensory solution (Addinsoft,
20 28 West 27th Street, Suite 503, New York, NY 10001, USA).

21

22 **2.2 JAR experiment**

23 **2.2.1 Materials**

1 In our study, flavored mineral water samples were evaluated by consumers. The tested samples
2 were prototypes with the mango-passion fruit aroma.

3 **2.2.2 Sample preparation**

4 The preparation of the samples (stored at 10 °C) was conducted using the same standardized
5 parameters (refrigerator, sample quantity, material and brand of the glasses, etc.). Samples were
6 poured into plastic glasses. The recommendations of Kilcast were followed during the sample
7 presentation, so the quantities of samples (180 cm³/person) were prepared by one person using a
8 measuring cup to achieve better homogeneity (Kilcast, 2010). Samples were labeled, according to
9 the international practice using 3-digit random numbers and a balanced block design was applied
10 (ISO 6658:2005). The samples were presented to the assessors in plastic glasses (200 cm³) at a
11 typical consumption temperature (15 °C), which was strictly monitored to maintain
12 commensurable conditions. Between the evaluations of the products, assessors used a very
13 neutral non-carbonated mineral water as taste neutralizer (Sipos *et al.*, 2012). Evaluations were
14 performed under artificial daylight-type illumination, temperature control (between 22 and 24 °C)
15 and air circulation.

16 **2.2.3 Consumer test**

17 Næs *et al.* suggests a minimum of 60 consumers for these kinds of tests (Næs *et al.*, 2010); hence
18 117 consumers were recruited from the Corvinus University of Budapest, Hungary. Consumers
19 were selected according to relevant market figures: 60 % / 40 % males/females aged between 18
20 and 30 years, regular carbonated soft drink (CSD) consumers, as they consumed CSD products
21 more than 2-3 times a week. Consumers were instructed prior to the evaluation to ensure the
22 reliability of the results and asked to evaluate overall liking on a 9-point hedonic scale (1 =
23 “dislike extremely”, 9 = “like extremely”). The attributes of color intensity, odor intensity, fruit

1 flavor, carbonation, sweet taste, sour taste, bitter taste and aftertaste intensity were evaluated
2 using a five point “Just About Right” scale (Figure 1). In this study, the data set of the most
3 preferred product will be presented.

4

5 **3. Results**

6 Table 4 lists the most important product attributes. Based on the ordering methods, simple
7 ordering has resulted in the most sensory attributes (out of the 16) as significant. The non-
8 parametric tests (Conditional exact Fisher’s test (CondExact), McNemars, ChiSquare) show
9 significant effects on the liking in case of at least ten attributes.

10

Table 4

11 The last column in Table 4 illustrates the marginal efficiency of a parametric test: only three
12 attributes were significant, of which the first two were identical to the results given by the non-
13 parametric tests. Simple ordering method has produced the largest number of significant
14 variables, because this is the least strict method. In contrast, difference ordering and significance
15 ordering have more and stricter conditions (see Sections 2.1.3-2.15).

16 The difference ordering method, which takes into account the number of losses, has a similar
17 result as that of the significance ordering. The main difference to the simple ordering is the
18 number of significant attributes, which were reduced to 2-5 depending on the applied test.

19 Significance ordering is the most strict and least sensitive ordering method. The ranks of the
20 attributes do not change except in the case of the McNemar’s test. In this case the too weak sweet
21 taste is on the fourth rank, but in the case of simple ordering this attribute goes to the fifth rank
22 (Table 4). As it is worth to consider the consensus of ordering methods, the three most important
23 attributes were FruitFlav-, Aftertaste+ and Bittertaste+, in decreasing order.

1 Based on these results, the main direction of product development should be increasing the fruit
2 flavor. However, reduced aftertaste and bitter taste intensity would also increase the liking of
3 consumers.

4 A new visualization tool summarizes the results of the three ordering methods and three
5 statistical tests (Figure 4). The first rank is given to the attribute which has the highest influence
6 on consumer's liking (FruitFlav-). The second rank is given to the second most influential
7 (Aftertaste+), and the third is to the third most influential (Bittertaste+) and so on. Horizontal
8 lines represent the consensus; crossing lines represent the lack of consensus between the tests and
9 ordering methods. Connection of the points is done to enhance interpretability of the plot. It is
10 easier to compare the ordering methods, if they are grouped next to each other on the x -axis.

11  Figure 4

12 Another new, Penalty Analysis-like visualization gives the percentage of the consumers *vs.* the
13 ranks given by the GPCM method using bubble plot (Figure 5).

14  Figure 5

1 The plot is divided into four subspaces using two lines. The horizontal line represents 20 % of the
2 consumers, while the vertical line represents the border of the significant attributes. The size of
3 the bubbles defines the rank of the attributes. The upper left subspace contains the significant and
4 important (> 20 % of consumers' rates) attributes. These attributes should be emphasized during
5 product development. The bottom left subspace contains the significant but not important
6 (< 20 % of consumers' rates) attributes. The upper right quadrant shows the non-significant but
7 important attributes. These attributes have little effect on consumers liking but more than 20 % of
8 the consumers rated as true. The bottom right subspace contains the non-significant and not
9 important attributes. The bigger the size of a bubble, the higher its impact on liking.

10 The rank of the attributes is based on their impact on consumers liking (x coordinate and the size
11 of the bubble), while the y coordinate gives the percentage of the consumers. For example, in the
12 case of color, 30 % of the consumers said that it is not intensive enough (Color-), but it has no
13 significant effect on liking (its rank is 16). In contrast, 5 % of the consumers rated the color as too
14 intensive (Color+), but for these consumers this had significant effect on their liking.

15 To validate the results of GPCM, the following methods were used: Spearman's rank correlation,
16 Multiple Linear Regression (MLR) (ASTM MNL63), Partial Least Squares Regression (PLS-R)
17 (Xiong & Meullenet, 2006) and Penalty Analysis (ASTM MNL63).

18 GPCM does not require high correlations between the independent and dependent variables. Due
19 to the non-parametric nature of JAR variables, the relationships between the attributes and liking
20 were defined using Spearman's rank correlation coefficients (Table 5).

21 Table 5

22 Out of the 16 investigated variables, eight had significant correlation with the dependent variable
23 ($\alpha=0.05$): FruitFlav-, Aftertaste+, Sweettaste-, Bittertaste+, Odor-, SourTaste-, Carbonation+ and

1 Sourtaste+, respectively. The Spearman's rank correlation coefficients support and validate the
2 results of GPCM. The rank of the attributes created by both methods is identical, c.f. Table 4.
3 Using MLR, out of the 16 attributes, seven had significant positive or negative effect on overall
4 liking: FruitFlav- (positive effect), Aftertaste+ (negative effect), Carbonation+ (negative effect),
5 FruitFlav+ (negative effect), Aftertaste- (positive effect), Carbonation- (positive effect),
6 Sourtaste+ (negative effect). Thus, these attributes should be addressed. The sign (positive or
7 negative) suggests how to reformulate the product. If the sign is positive, more is better (up to a
8 certain point). Likewise, if the sign is negative, less is better. FruitFlav+ and Aftertaste+ proved
9 to be the first two most important attribute based on the *t*-values. Table 6 shows the results of
10 MLR; the attributes are sorted according to their *t*-value.

11 Table 6

12 PLS-R was also used to identify variables, which have significant effect on liking. Compared
13 with MLR, our PLS-R model had a slightly lower R^2 (0.480 vs. 0.508), and RMSE value (1.347
14 vs. 1.360). MLR had lower intercept (7.837), while our PLS-R model gave a value of 7.673,
15 which can be interpreted as the estimated mean of overall liking for the product if all JAR
16 attributes are JAR. Table 7 displays the Variable Importance for the Projection (VIP) values for
17 each explanatory feature that measure the importance of each feature. This allows the quick
18 identification of those explanatory features that contribute the most to the model.

19 Table 7

20 The VIP results of our PLS-R model showed that FruitFlav- (positive effect), Aftertaste+
21 (negative effect), Sweettaste- (positive effect), Odor- (positive effect), Bittertaste+ (negative
22 effect), Sourtaste- (positive effect), Carbonation+ (negative effect) and Carbonation- (positive
23 effect) have significant effect on liking.

1 On the VIP chart (Figure 6) (one bar per component), a border line is plotted to identify the VIPs,
2 which are greater than 0.8. These thresholds, suggested by Wold (1995), allow identifying the
3 features which are moderately ($0.8 < \text{VIP} < 1$) or highly influential ($\text{VIP} > 1$).

4 Figure 6

5 Penalty Analysis identified the following attributes as significant ones (sorting is based on the
6 mean drop values): FruitFlav-, Aftertaste+, Sweettaste-, Sweettaste+, Carbonation+, Sourtaste-,
7 Carbonation-, Aftertaste-, Odor-. According to the mean drop plot (Figure 7), FruitFlav- seems to
8 be the most important but the importance of Aftertaste+ and Sweettaste- is not highlighted as
9 much as GPCM does.

10 In Penalty Analysis, the generally applied one sample *t*-test is used to compare the JAR and the
11 two other endpoints and the test requires normally distributed variables. The results of Shapiro-
12 Wilk's tests show, which variables do not fulfill the criteria of normality. In Table 8, Shapiro-
13 Wilk's test *p*-values in bold indicate the non-violation of normality. As Table 8 indicates, the *t*-
14 test was used several times on not normally distributed data.

15 Table 8

16 Figure 7

17 Table 9

18 It can be seen in Table 9 that the sequence of the first two significant variables is identical in the
19 case of all JAR methods. The order of variables varies according to the differences of the applied
20 methods and criteria. The highest number of variables were found in the case of GPCM simple
21 ordering CondExact method and the strictest were GPCM difference ordering and significance
22 ordering methods. Though the rankings of the attributes were similar; some switches were found
23 in some cases.

1

2 **4. Discussion and Conclusions**

3 Generalized Pairwise Correlation Method (GPCM) proved to be suitable for analyzing the impact
4 of Just-About-Right (JAR) variables on liking. An order can be created according to the impact
5 on liking, in which order determines the development of product attributes as well. The non-
6 parametric tests incorporated in the method are able to identify small differences and they have
7 proved to be more sensitive than other statistical methods (*e.g.*: Williams' *t*-test). GPCM can
8 provide differences when other statistical tests cannot. GPCM identifies more significant product
9 attributes, so it can help the product development process.

10 One of the advantages of GPCM comes from its non-parametric nature. Hence, it is better suited
11 to JAR variables which generally do not follow normal distribution and have significant
12 correlations with each other. GPCM chooses relevant independent variables, which means higher
13 safety when interpreting the results. Moreover, it is based on well-known and well-proven
14 statistical criteria. GPCM requires one-directional scales, but they do not cause considerable loss
15 of information and they preserve the dominant information of JAR scales (Xiong & Meullenet,
16 2006).

17 However, the proposed GPCM method cannot be used for prediction in a way similarly to
18 Penalty Analysis. Besides, due to the characteristics of the method, the result is always an
19 ordered list of variables. It will provide a result even if the first variable has a very low impact on
20 the dependent variable. In contrast, GPCM is able to rank seemingly undistinguishable variables
21 as well.

22 A new visualization tool (line plot) summarizes the results of the three ordering methods and
23 three statistical tests. Of the three ranking methods, the simple ranking is the least conservative (it

1 selects more descriptors). The best method, which can utilize even small differences in statistical
2 tests, is the ranking according to probability-weighted differences. In our case study the ranks
3 given by difference and significance ordering were similar. Based on this, the suggested order of
4 product development should be the following: FruitFlav-, Aftertaste+, Bittertaste+, Sweettaste-,
5 Sourtaste+. Another new, easily interpretable visualization tool was proposed to show the
6 significant and important (> 20 % of consumers' rates) attributes in one single bubble plot.

7 Results of Spearman's rank correlations support and validate the results of GPCM. It is
8 noteworthy that in our case study both approaches led to similar conclusions even if the train of
9 thought is totally different. To validate a more precise method with accepted less precise ones
10 (GPCM with simple ordering and Spearman rho; non parametric tests and Williams *t* test) is
11 virtually impossible. Spearman rho shows that the results are in conformity (not in contradiction)
12 with the earlier, well-known methods. Again, the train of thought of GPCM is totally different
13 from the Spearman rho.

14 Multiple Linear Regression (MLR) has some model restrictions: *e.g.* number of cases \geq number
15 of variables, overfitting, signs of the regression coefficients cannot be interpreted in many cases,
16 and strong correlation between the variables reduces the prediction ability (Krishnamurthy *et al.*,
17 2007). In contrast, Partial Least Squares Regression (PLS-R) handles the strongly correlated
18 variables. Both PLS-R and MLR use the information present in the dependent variable, but PLS-
19 R uses the information present in *Y* (Næs *et al.*, 2010) in a better way.

20 The main advantage of GPCM, compared to Penalty Analysis, is that it applies three ordering
21 methods and four statistical tests to determine the sequence of variables having the greatest
22 impact on liking. Penalty Analysis does not take into account the correlation between variables

1 (JAR variables tend to have strong correlations) and cannot be used to predict liking data (Plaehn,
2 2013).

3 Using GPCM, MLR, PLS-R and Penalty Analysis, the two most important attributes, which have
4 high impact on liking, were determined unambiguously: FruitFlav- and Aftertaste+. The
5 specificity of MLR and PLS-R is that they have been developed primarily for prediction
6 purposes. But in the case of JAR data analysis the main aims are ranking and selecting attributes,
7 determining the sequence of the significant attributes but not the prediction.

8

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- 13

1 Table 1
 2 Scheme for using two dummy variables (Aftertaste+ and Aftertaste-) or one dummy variable
 3 (Aftertaste) to represent one JAR scale variable (X) on a 5-point JAR scale based on Xiong and
 4 Meullenet (2006). All the attributes are indicated based on this table.

Original JAR values (5 point JAR scale)	Aftertaste	Aftertaste+	Aftertaste-
1 – much too weak	-2	-2	0
2 – somewhat too weak	-1	-1	0
3 – just about right	0	0	0
4 – somewhat too strong	1	0	1
5 – much too strong	2	0	2

5

6 Table 2

7 Frequencies obtained by applying GPCM

	$\Delta X_1 > 0$	$\Delta X_1 < 0$
$\Delta X_2 > 0$	$k_A =$	$k_C =$
$\Delta X_2 < 0$	$k_B =$	$k_D =$

8

9 Table 3

10 Comparison of Color+ and Carbonation+ features based on Conditional Fisher's exact test, The
 11 contingency table contains frequencies:

	Delta(Color+)>0	Delta(Color+)<0
Delta(Carbonation+)<0	$k_D = 58$	$k_B = 9$
Delta(Carbonation+)>0	$k_C = 64$	$k_A = 89$

12 Naturally, the equal Y values do not carry any information, they were ignored; critical value = 30,
 13 Predefined error limit $\alpha(\text{user}) = 0.05$, Theoretical (threshold) $\alpha = 0.0000$; Carbonation+ won, as
 14 nine is (much) less than 30. Delta means the difference in JAR attributes as described in 2.1.2
 15 part.

1 Table 4

2 Rank of the attributes of product mango-passion fruit (all GPCM methods and all applied tests)

	Attributes	CondExact	McNemars	ChiSquare	Williams' <i>t</i>
Simple ordering	<i>FruitFlav-</i>	1	1	1	1
	Aftertaste+	2	2	2	2
	Bittertaste+	3	3	3	NS
	<i>Sweettaste-</i>	4	5	5	3
	Sourtaste+	5	4	4	NS
	Carbonation+	6	6	6	NS
	<i>Odor-</i>	7	7	7	NS
	<i>Sourtaste-</i>	8	8	8	NS
	Sweettaste+	9	10	10	NS
	Color+	10	9	9	NS
	<i>Carbonation-</i>	11	NS	11	NS
	Odor+	NS	NS	12	NS
Difference ordering	<i>FruitFlav-</i>	1	1	1	1
	Aftertaste+	2	2	2	2
	Bittertaste+	3	3	3	NS
	<i>Sweettaste-</i>	4	NS	5	NS
	Sourtaste+	5	NS	4	NS
Significance ordering	<i>FruitFlav-</i>	1	1	1	1
	Aftertaste+	2	2	2	2
	Bittertaste+	3	3	3	NS
	<i>Sweettaste-</i>	4	4	5	NS
	Sourtaste+	5	NS	4	NS

3 Attributes in bold indicate the “too much” region, attributes in italic indicate the “too weak”

4 region of the JAR scale. NS stands for non significant.

5

- 1 Table 5
- 2 Spearman's rank correlation matrix of the evaluated attributes. Attributes are ordered according
- 3 to their correlation coefficients.

Features ^a	Overall liking ^b
<i>FruitFlav-</i>	0.477
Aftertaste+	-0.342
<i>Sweettaste-</i>	0.315
Bittertaste+	-0.305
<i>Odor-</i>	0.227
<i>Sourttaste-</i>	0.224
Carbonation+	-0.213
Sourttaste+	-0.188
<i>Carbonation-</i>	0.155
Sweettaste+	-0.155
FruitFlav+	-0.082
<i>Aftertaste-</i>	0.074
Odor+	0.07
Color+	0.065
<i>Bittertaste-</i>	-0.012
<i>Color-</i>	0.001

4 ^a Attributes in bold indicate the “too much” region, attributes in italic indicate the “too weak”

5 region of the JAR scale.

6 ^b Values in bold are significantly different from 0 at an error level $\alpha=0.05$ (XL-Stat).

7

1 Table 6

2 Significant model parameters of Multiple Linear Regression. (Insignificant variables are not
3 shown. Attributes are sorted based on their t -values.

Source	Value	Standard error	t	Pr > t	Lower bound (95 %)	Upper bound (95 %)
Intercept	7.837	0.236	33.201	< 0.0001	7.369	8.305
FruitFlav-	1.554	0.228	6.823	< 0.0001	1.103	2.006
Aftertaste+	-1.041	0.237	-4.393	< 0.0001	-1.511	-0.571
Carbonation+	-0.751	0.274	-2.738	0.007	-1.294	-0.207
FruitFlav+	-0.926	0.347	-2.67	0.009	-1.614	-0.239
Aftertaste-	0.614	0.253	2.426	0.017	0.112	1.116
Carbonation-	0.571	0.263	2.174	0.032	0.051	1.092
Sourtaste+	-0.885	0.436	-2.029	0.045	-1.75	-0.021

4 Root mean square error: 1.360 on 109 degrees of freedom, Multiple R-Squared: 0.508,

5 F-statistic: 16.073 on 7 and 109 degrees of freedom, the overall p -value is < 0.0001

6

7

1 Table 7

2 Results of the PLS-R model. Attributes are sorted based on their Variable Importance (VIP)
3 value. The upper bold line represents a VIP value of 1, while the lower bold line represents a VIP
4 value of 0.8.

Feature	VIP	Standard deviation	Lower bound (95 %)	Upper bound (95 %)	Standardized coefficients (Feature liking):
FruitFlav-	2.133	0.251	1.641	2.626	0.280
Aftertaste+	1.616	0.274	1.079	2.152	-0.212
Sweettaste-	1.359	0.191	0.984	1.734	0.178
Odor-	1.249	0.491	0.286	2.212	0.164
Bittertaste+	1.143	0.260	0.633	1.652	-0.150
Sourtaste-	0.974	0.407	0.177	1.772	0.128
Carbonation+	0.952	0.264	0.434	1.470	-0.125
Carbonation-	0.848	0.273	0.313	1.383	0.111
Sourtaste+	0.769	0.393	-0.001	1.538	-0.101
Sweettaste+	0.682	0.480	-0.259	1.622	-0.089
Aftertaste-	0.454	0.510	-0.545	1.454	0.060
FruitFlav+	0.390	0.589	-0.764	1.545	-0.051
Color+	0.282	0.262	-0.232	0.796	0.037
Odor+	0.187	0.474	-0.742	1.116	0.025
Bittertaste-	0.127	0.270	-0.402	0.655	-0.150
Color-	0.076	0.395	-0.698	0.850	0.010

5 The PLS-R model used one component.

6 Root mean square error: 1.347 on 115 degrees of freedom,

7 Multiple R-Squared: 0.482, $R_{val} = \sqrt{Q^2} = 0.610$,

8 Intercept=7.673, Observed mean=5.812, Predicted mean=5.812.

9

1 Table 8

2 Results of the Penalty Analysis. The last two columns of the table contain the results of a
 3 normality test to identify which features follow normal distributions.

Feature	Level	%	Mean (liking)	Mean drops	<i>t</i> -test <i>p</i> -value ^a	Shapiro-Wilk's <i>p</i> -value ^b
Color	Too weak	30.77 %	5.806	-0.032	0.933	0.00295
	JAR	64.10 %	5.773			0.00533
	Too strong	5.13 %	6.333	-0.56		0.55438
Odor	Too weak	32.48 %	5.263	0.787	0.033	0.26424
	JAR	51.28 %	6.05			0.01004
	Too strong	16.24 %	6.158	-0.108		0.55008
Fruit flavour	Too weak	51.28 %	5.033	2.146	< 0.0001	0.11198
	JAR	33.33 %	7.179			0.00549
	Too strong	15.38 %	5.444	1.735		0.09078
Carbonation	Too weak	21.37 %	5.24	1.039	0.025	0.1925
	JAR	58.12 %	6.279			0.00094
	Too strong	20.51 %	5.083	1.196	0.006	0.00175
Sweet taste	Too weak	31.62 %	4.973	1.657	< 0.0001	0.07956
	JAR	46.15 %	6.63			0.00078
	Too strong	22.22 %	5.308	1.322	0.001	0.16676
Sour taste	Too weak	39.32 %	5.261	1.18	0.001	0.04608
	JAR	50.43 %	6.441			0.0042
	Too strong	10.26 %	4.833	1.607		0.02516
Bitter taste	Too weak	24.79 %	5.655	0.58	0.127	0.00755
	JAR	58.12 %	6.235			0.00109
	Too strong	17.09 %	4.6	1.635		0.1307
Aftertaste	Too weak	25.64 %	5.6	0.977	0.009	0.44519
	JAR	44.44 %	6.577			0.0069
	Too strong	29.91 %	4.857	1.72	< 0.0001	0.00553

4 ^a Values in bold are significantly different from 0 at an error level $\alpha=0.05$ (XL-Stat).

5 ^b Values in bold indicate the non-violation of normality at an error level $\alpha=0.05$ (XL-Stat).

6

1 Table 9

2 Comparison of all methods.

	GPCM (simple ordering, CondExact)	GPCM (significance ordering, CondExact)	GPCM (difference ordering, CondExact)	Multiple Linear Regression	Partial Least Squares Regression	Penalty Analysis
1	FruitFlav-	FruitFlav-	FruitFlav-	FruitFlav-	FruitFlav-	FruitFlav-
2	Aftertaste+	Aftertaste+	Aftertaste+	Aftertaste+	Aftertaste+	Aftertaste+
3	Bittertaste+	Bittertaste+	Bittertaste+	Carbonation-	Sweettaste-	Sweettaste-
4	Sweettaste-	Sweettaste-	Sweettaste-	Sourttaste+	Odor-	Sweettaste+
5	Sourttaste+	Sourttaste+	Sourttaste+	FruitFlav+	Bittertaste+	Carbonation+
6	Carbonation+			Carbonation+	Sourttaste-	Sourttaste-
7	Odor-			Aftertaste-	Carbonation+	Carbonation-
8	Sourttaste-			-	Carbonation-	Aftertaste-
9	Sweettaste+			-	-	-
10	Color+			-	-	-
11	Carbonation-			-	-	-

3

1 Caption to figures

2 Figure 1

3 A general five category JAR scale ranging from much too weak to much too strong.

4 Figure 2

5 Effects of Fruit flavor, Aftertaste and Sweet taste on overall liking. The “rooftop” shape of the

6 bipolar JAR scales requires to create two one-directional variable.

7 Figure 3

8 Graphical representation of the four possible events as the basis of pair correlation method.

9 Frequencies of cases *C* and *B* (indicated as blue on the plot) are the basis of the method.

10 Figure 4

11 Line plot summarizing the results of the three ordering methods and the three statistical tests.

12 Crossing lines represent differences between methods and/or tests.

13 Figure 5

14 Bubble plot of the results of simple ordering and Conditional exact Fisher’s test. The vertical line

15 divides the significant and non-significant variables. The horizontal line represents 20 % of the

16 consumers. The size of bubbles defines the impact on liking.

17 Figure 6

18 Attributes sorted based on their variable importance. The two vertical interrupted lines indicate

19 the Variable Importance for the Projection (VIP) value of 1 and 0.8.

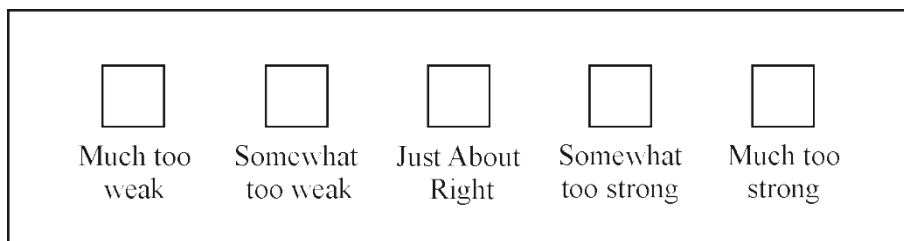
20 Figure 7

21 Mean drop plot of Penalty Analysis. Mean drops are plotted against the percentage of the

22 consumers. The vertical line represents 20 % of consumers.

23

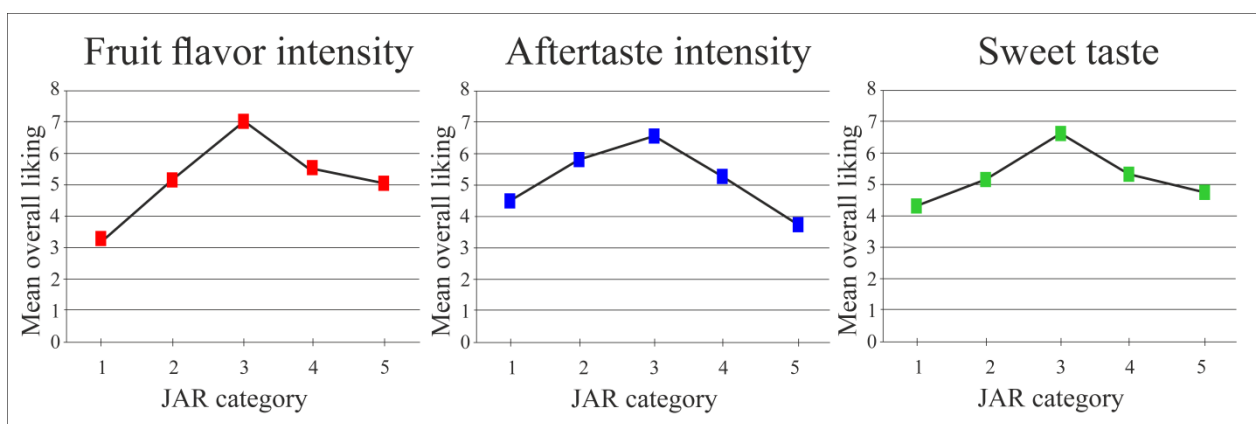
1 Figure 1



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3

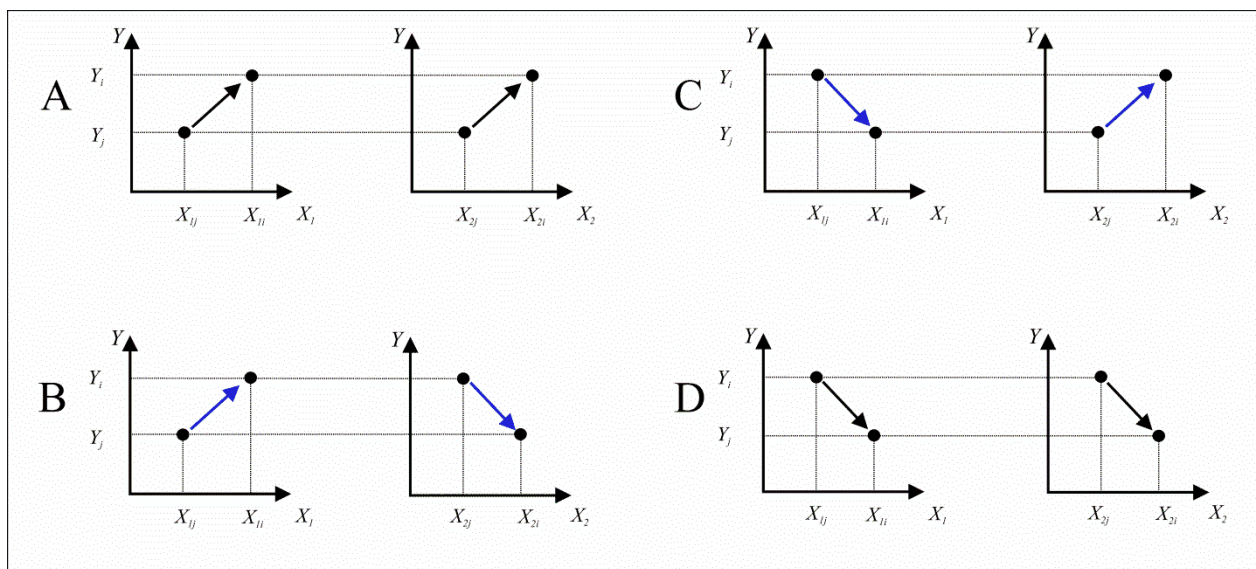
4 Figure 2



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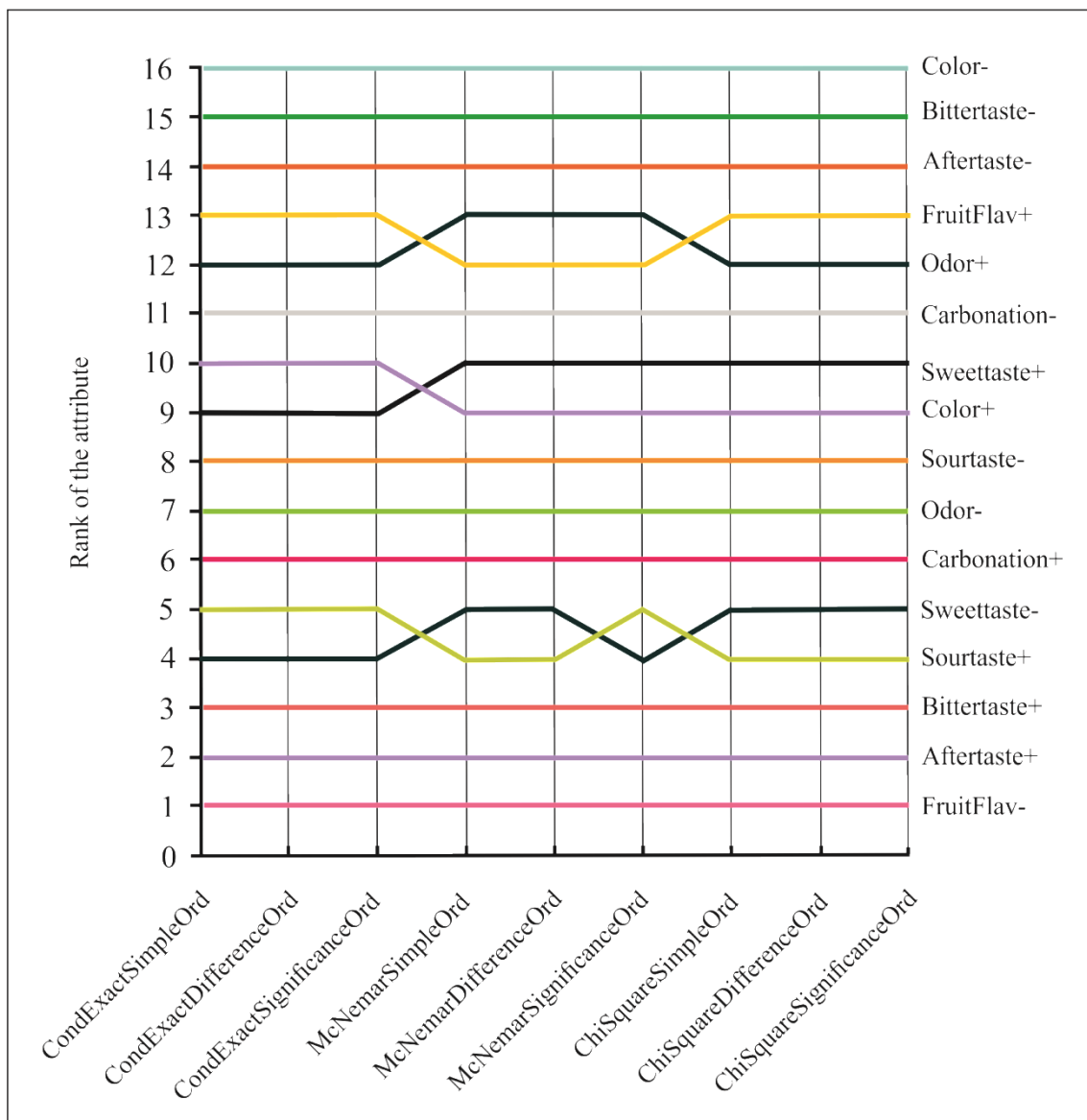
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7 Figure 3



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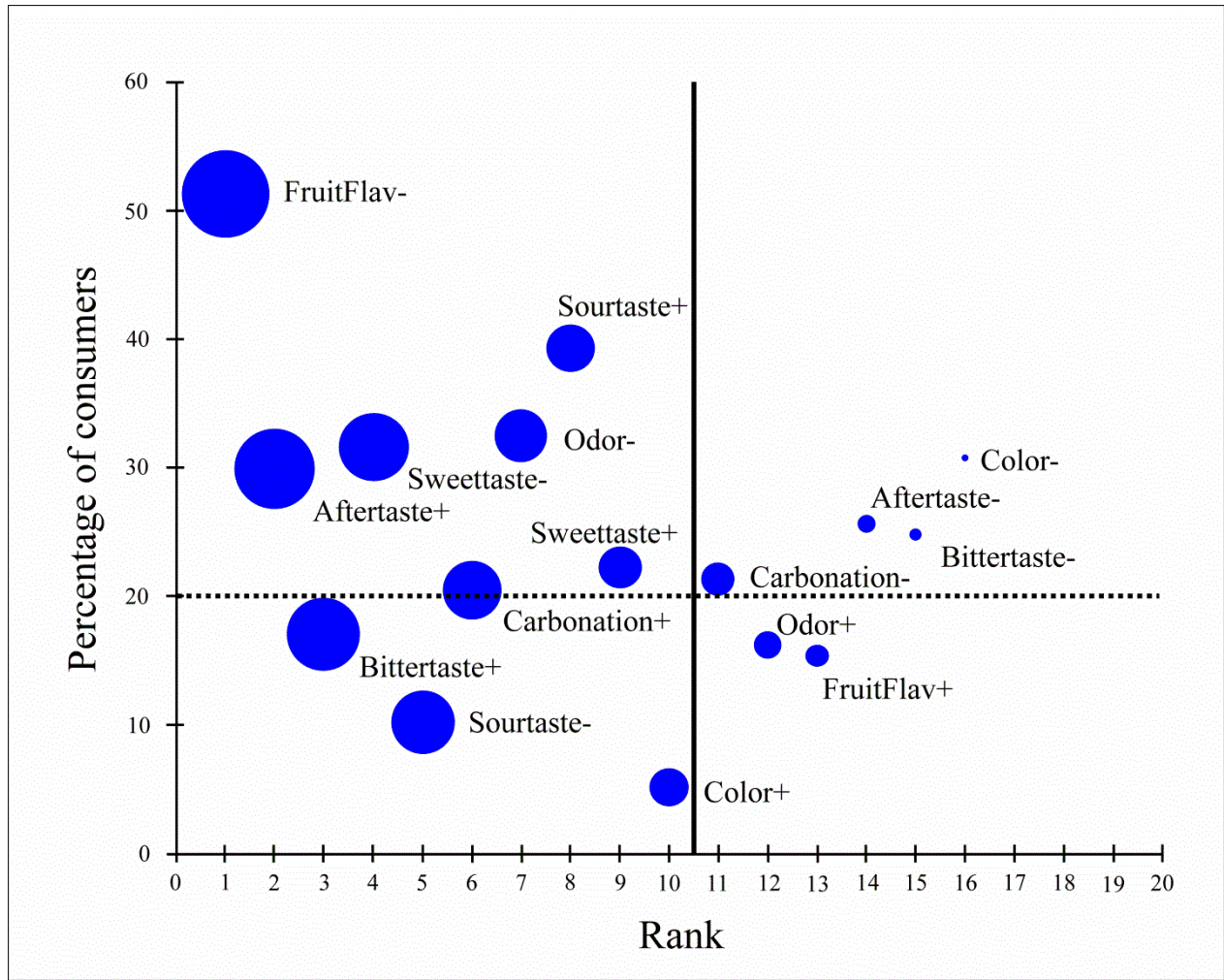
1 Figure 4



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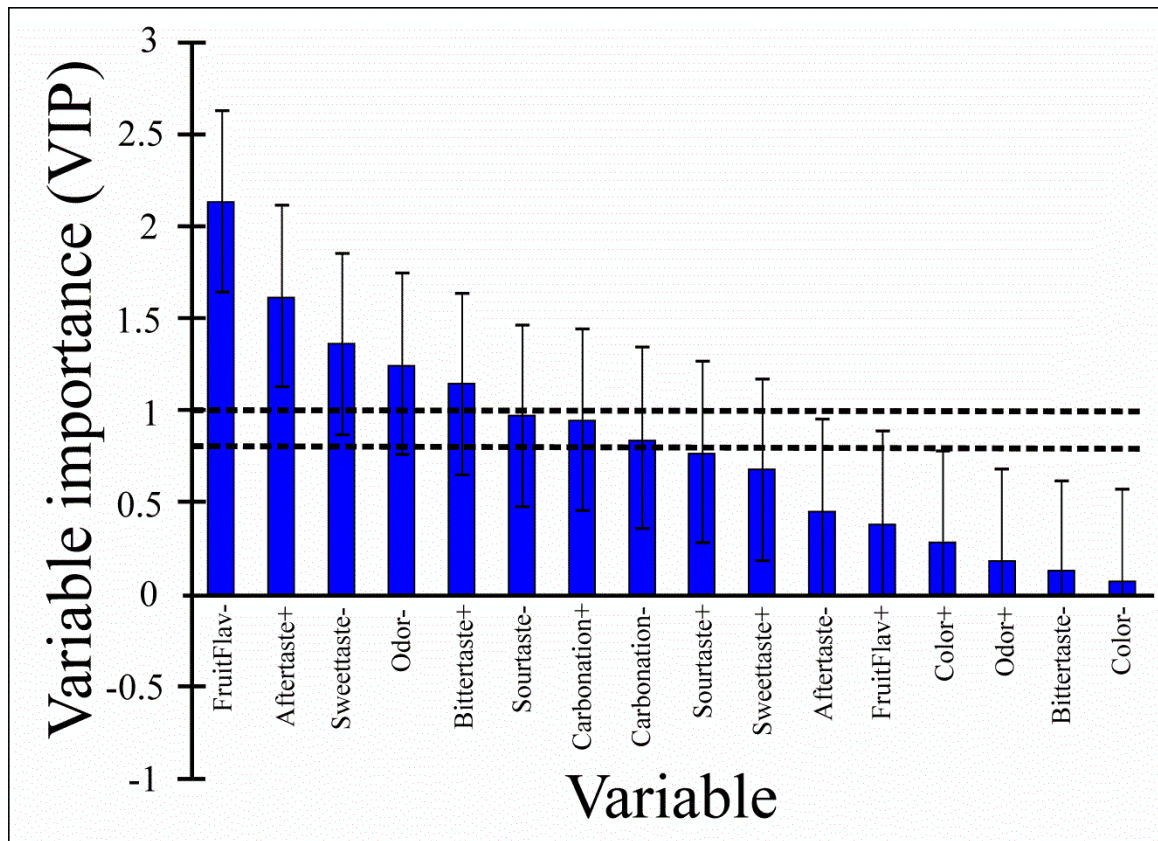
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1 Figure 5



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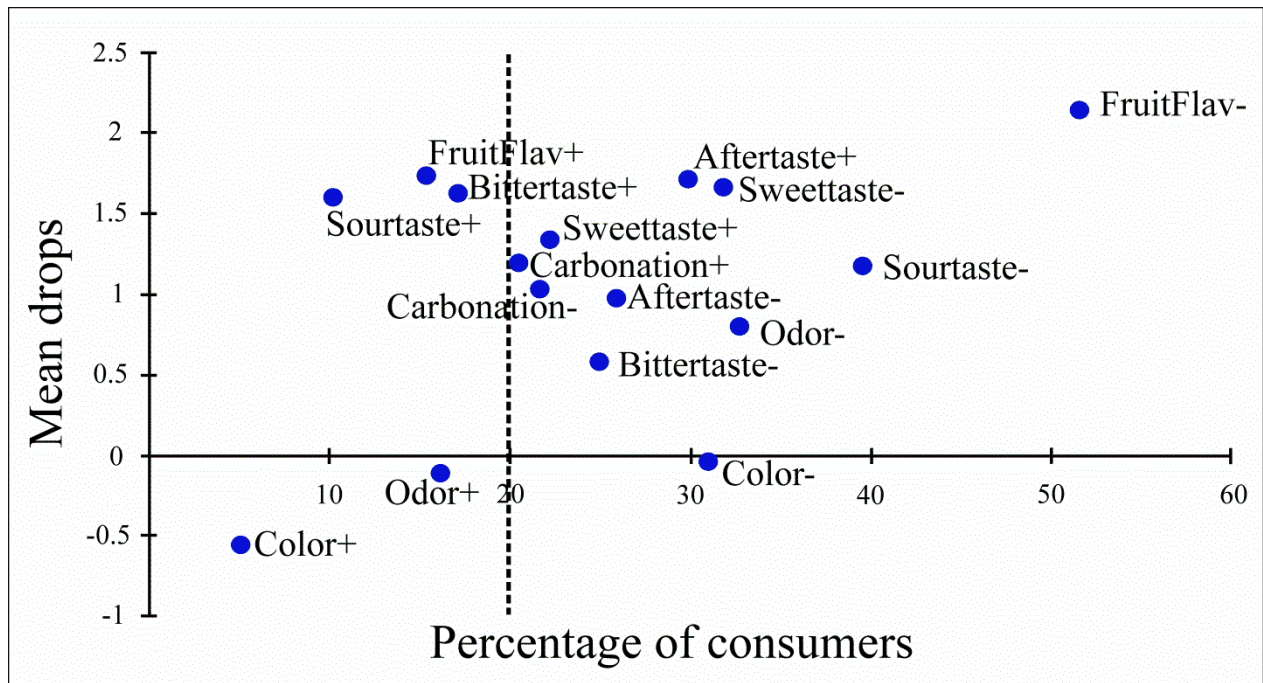
1 Figure 6



2

3

1 Figure 7



2