Multivariate Analysis of Data in Sensory Science
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PROCRUSTES ANALYSIS IN SENSORY RESEARCH

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1. INTRODUCTION

Since its adoption in the seventies (e.g. Banfield and Harries 1975, Harries and MacFie 1976), Procrustes analysis has become a popular tool for sensory scientists (Williams and Langron 1984, Arnold and Williams 1985), and still the method is used frequently and is studied and extended by several authors (Oreskovich et al. 1991, Dijksterhuis and Gower 1991/2, Wakeling et al. 1992). Procrustes analysis was originally developed as a technique to match the solutions of two Factor Analyses (Hurley & Cattell 1962). The method was generalised to match more than two data sets by Kristof and Wingersky (1971) and Gower (1975). Recently the method has received increasing attention, partly through the availability of software programs for generalised Procrustes analysis (GPA), partly through some critisisms on the method.

In this chapter the kinds of sensory data to which GPA can be applied are introduced, along with the rationale for using the method. Next some background and theory of GPA is provided with special attention for the Procrustes analysis of variance. Finally, two applications of GPA to sensory profiling data, one conventional and one free-choice, are shown.

1.1 Sensory profiling

A very large number of applications of generalised Procrustes analysis is found in the analysis of sensory profiling data. There are two different kinds of profiling data, that can both be analysed by means of generalised Procrustes analysis. Conventional profiling data can also be analysed by averaging and applying factor analysis or PCA to it. Free choice profiling FCP, (Williams & Langron 1984, Williams and Arnold 1985) results in data that can not be averaged over assessors, generalised Procrustes analysis or other, so-called, *K*-sets methods are suited for the analysis of free choice profiling data.

The scores from either profiling technique are derived from the position of marks along a line-scale. The assessor marks his/her perceived intensity of some attribute along a line scale (Figure 1). Often the scores range from 0 to 100, but the range is unimportant, in the following a range from 0 to 100 is assumed.

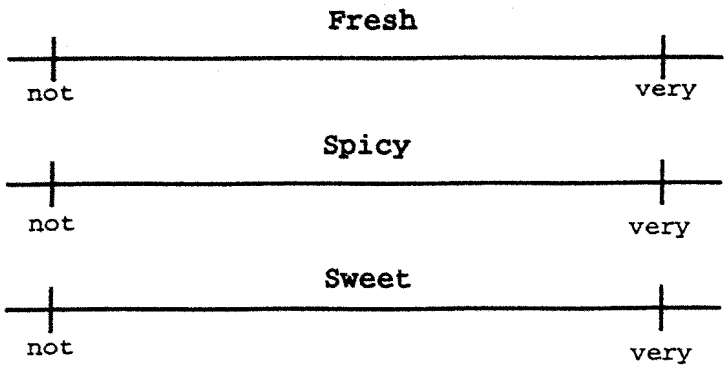

Figure 1. Example of a line-scale often used in sensory profiling experiments.

1.1.1 Conventional profiling

In conventional profiling a fixed vocabulary of descriptive terms is used by the sensory panel to judge the products. A sensory panel is often trained in the use of these terms. In the case of QDA (Quantitative Descriptive Analysis, see Stone & Sidel 1985) the panel starts with the generation of a lot of terms that are thought useful to describe the products under consideration. The whole procedure of attribute generation and training can take considerable time. Because of this training it is assumed that all assessors are able to use the attributes in the same way, so individual differences in use of the attributes are minimized. Because of this the individual judgements are sometimes averaged and factor analysis or PCA is applied to the average scores. However, methods as generalised Procrustes analysis can of course also be applied to conventional profiling data. Such analyses show that the assumption of all assessors using the attributes in the same way is not always justified (see e.g. Dijksterhuis & Punter 1990).

The data from conventional profiling experiments can be seen as a 3-mode data structure built from N products, M attributes and K assessors (see Figure 2).

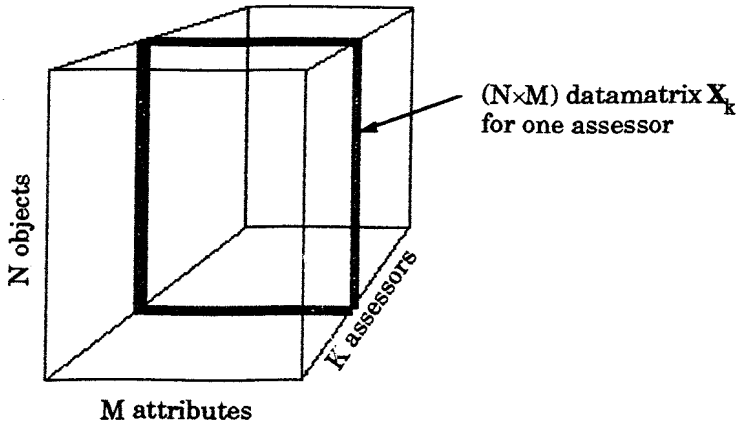

Figure 2. 3-Mode data structure representing conventional profiling data: N products are judged by K judges using M attributes.

The ($N \times M \times K$) data block in Figure 2 consists of K layers, each with the ($N \times M$) datamatrix of one assessor. Other slices of this block may be analysed but generalised Procrustes analysis focusses on the agreement of the K matrices from the individual assessors.

1.1.2 Free choice profiling

In free choice profiling the assessors are free to come up with their own attributes, which they use for judging the products. So between the assessors there is no agreement about attributes. As a result it is impossible to average the individual data, because it makes no sense to combine different attributes. The data from free choice profiling experiments must be analysed by individual difference methods, or rather 'K-sets' methods, of wich generalised Procrustes analysis is one. Unlike conventional profiling data, free choice profiling data cannot be rearranged in some kind of 3-mode data structure. Because each assessor k=1,...,K may have a different number of attributes (M_k), furthermore the jth attributes of the assessors are not the same. Figure 3 shows the structure of a FCP data set.

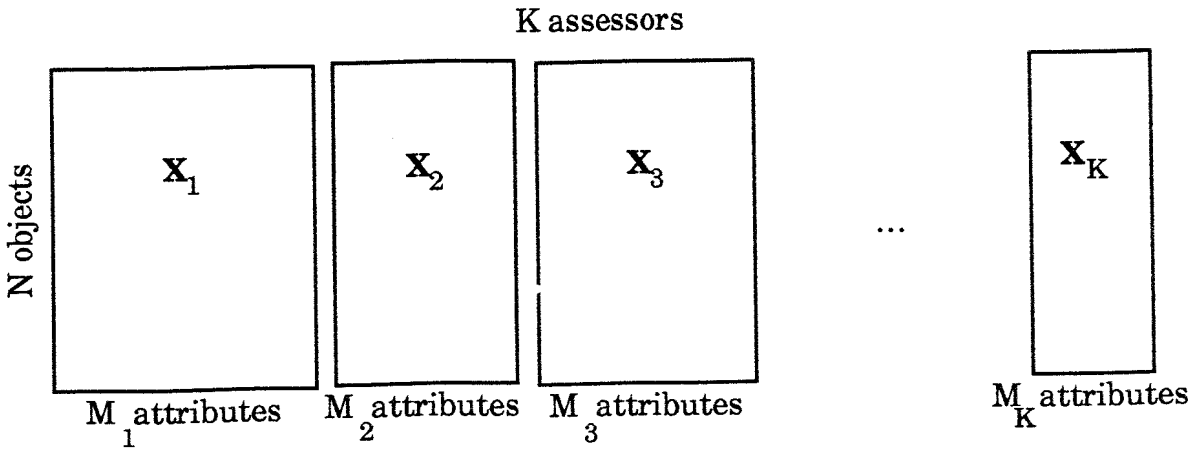

Figure 3. Data structure representing free choice profiling data: N products are judged by K judges using M_k attributes.

Figure 3 shows that the individual datamatrices $\mathbf{X}_k$ cannot be arranged such that the attributes match because each assessor's individual datamatrix has different attributes.

1.2 Sensory-instrumental Relations

One of the fields in which Procrustes analysis can be applied is the study of sensory-instrumental relations. Though Procrustes analysis appears not to be often used in this field it can be a useful method to analyse sensory-instrumental relations (see e.g. Dijksterhuis 1994). The idea behind the study of sensory-instrumental relations is that sensory perceptions have chemical/physical counterparts in the substance under investigation. A simple example is e.g. the amount of caffeine in a certain drink, which of course determines the bitterness perceived by someone drinking it. In real life the sensory-instrumental research is much more complicated, and involves multivariate, not univariate, data, and consequently needs multivariate data-analysis.

The original, not generalised, Procrustes analysis can be applied to sensory-instrumental data, because two-data sets are involved. One data set contains the sensory judgements on a number of, say N, products. The second data set contains a number of instrumental measures on the same N products. These can be results of chemical analyses, physical properties or of other measurements.

1.3 Designed experiments and incomplete data

In some cases it is conceivable that at a profiling experiment, be it conventional or free choice, the data may be gathered according to some experimental design. When the design has been an incomplete one, the datamatrices of the assessors may not all have scores on the same set of N products. In this case it is impossible to analyse these data by means of ordinary generalised Procrustes analysis. Special generalised Procrustes analysis methods that can handle missing data must be used. They are outside the scope of this chapter but can be found in Commandeur (1991) and Ten Berge, Kiers & Commandeur (1993).

2. THEORY AND BACKGROUND OF PROCRUSTES ANALYSIS

In this section generalised Procrustes analysis is introduced in two different ways, first in a geometrical way and next in a somewhat more formal mathematical way.

2.1 A geometrical look

Each assessor's datamatrix, $\mathbf{X}_k$, consists of N rows with scores on M_k attributes. This datamatrix contains elements $\mathbf{X}_{ijk}$, where i is the index over the N products, j=1,...,M_k, the number of attributes of the kth assessor and k=1,...,K the number of assessors. In this section no distinction between conventional profiling and Free choice profiling will be made.

The scores in an assessor's datamatrix describe N objects using M attributes. Geometrically the N points can be seen as to lie in an M-dimensional space. With M=2 attributes we can draw a plane with the N points in it, but in general M will be (much) larger. Figure 4 shows a configuration of N points from the data of an assessor judging on only 2 attributes. Mathematically high dimensional spaces are no problem, though we may have trouble imagining them, but this we don't need to. When the analysis is done we don't look at the high dimensional space but at a projection onto an imaginable lower dimensional space, often two dimensions, so it can be plotted on paper. This projection is often accomplished by means of performing a principal component analysis and plotting the first two dimensions.

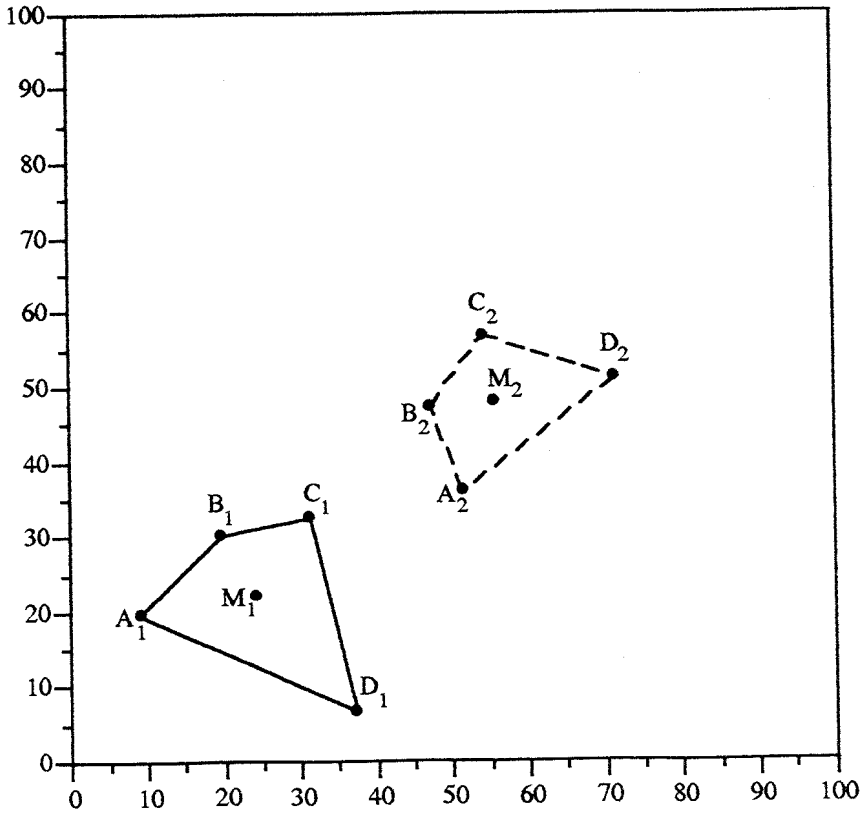

Figure 4. Two configurations with points representing scores on four products from assessor 1 (A_1, B_1, C_1, D_1) and from assessor 2 (A_2, B_2, C_2, D_2) with their centroids M_1 and M_2.

We have M-dimensional configurations of N points for all K assessors. Suppose that we deal with two assessors, to keep this example simple. We can draw the two different configurations of the N=4 points (Figure 4). The objective of generalised Procrustes analysis is to try to get the same objects as close to each other as is possible by shifting entire configurations, rotating them and reflecting them if necessary. The important underlying assumption is that the distances between the N objects for one assessor may not be changed during these transformations. When the configurations are also allowed to stretch or shrink the *relative* distances between the objects remain the same.

The distances between the objects reflect the relations between the objects. Objects close together are similar, objects far apart are different. The reason to keep the *distances* invariant is that in the process of matching, the *relations* between the N objects of one assessor should not change. Similar objects must remain similar, different objects must remain different.

2.2 Transformations

The transformations mentioned above, i.e. shifting, rotating, reflecting and stretching or shrinking, that make up a generalised Procrustes analysis, turn out to correct for a number of assessor effects (see Arnold & Williams 1985).

2.2.1 The Level-Effect: Translation

The so-called level-effect manifests itself by the different average scoring position on a line scale of different assessors. One assessor may give all N products scores that lie between, say, 5 and 25 and another assessor may use scores from 60 to 100 (assuming a 1 to 100 line-scale score). These two extreme assessors could very well perceive the objects identically, and would perhaps agree with one another completely, had not they possessed such different scaling behaviour. This level-effect can easily be corrected for by expressing the scores as deviations from the average score of an assessor on an attribute. Geometrically this results in translating the entire configuration of an assessor such that the centre of the N object-points coincides with the origin of the space (see Figure 5). The centres M_1 and M_2 in Figure 4 are shifted onto each other and this point is labled C in Figure 5. Mathematically this translation operation is known as column-centring, in 'Analysis of Variance' terms the *assessor main-effect* is removed.

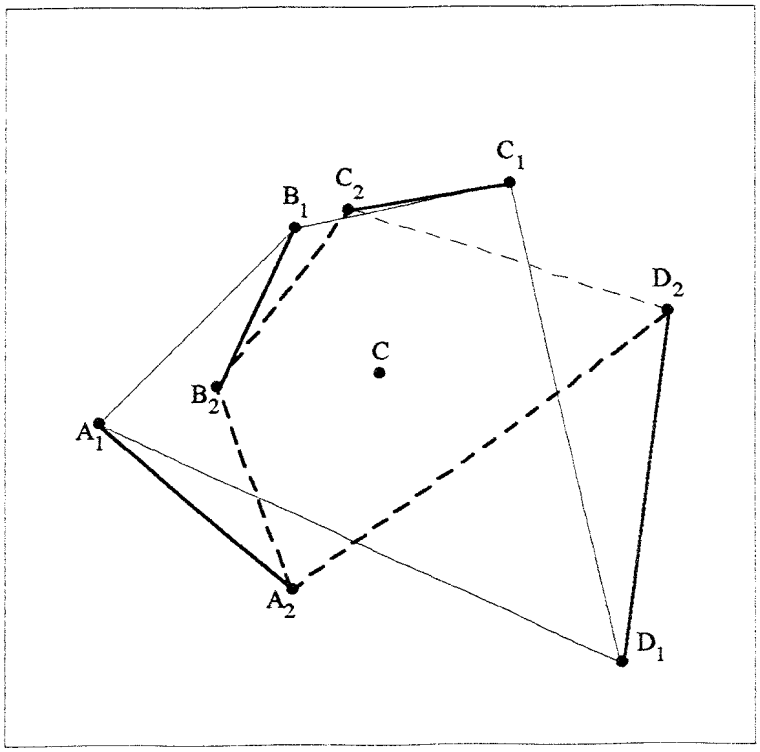

Figure 5. Centred configuration of two assessors.

2.2.2 The interpretation-effect: Rotation/Reflection

The transformations which allow for the fact that the attributes do not have to be the same (the interpretation-effect) for all assessors are rotation and reflection. The entire configuration of an assessor can be rotated to bring the N object-points in agreement with the N points of the other configurations. If necessary the configuration can be reflected in a particular dimension too. As can be seen from Figure 5, the object-points are not very close yet, the lines between the pairs

of points (A_1, A_2), (B_1, B_2) etc. indicate the distance that is to be minimised. Mathematically the rotation and (reflection) are represented in a rotation matrix $\mathbf{H}_k$, for the configuration of assessor k.

Figure 6 shows the two example configurations after rotation. Note that the N points actually are closer (A_1 to A_2, B_1 to B_2, C_1 to C_2, D_1 to D_2) than in Figure 5.

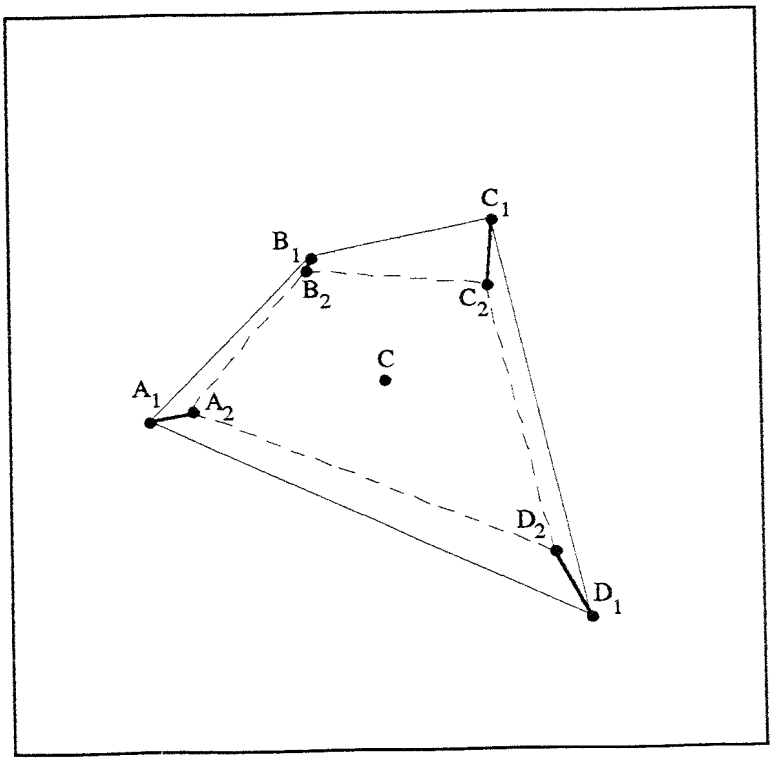

Figure 6. Configurations after centring and rotation.

2.2.3 The range-effect: Isotropic Scaling

Another individual scaling effect is the so-called range-effect. This is shown by the different ranges of scoring that the assessors use. One assessor may give scores ranging between 10 and 95 and another assessor uses scores from 60 to 80. This difference in range is another unwanted effect caused by individual differences in scoring behaviour. The underlying perception is believed not to depend on these differences in scaling range, so the effect is controlled for. The correction that is used is called isotropic scaling, which means that a configuration is shrunk or stretched in its entirity, i.e. alike in all directions of the space.

A different scaling range shows as a different extensiveness of the configurations. Figure 6 showed the two example configurations after centring and after rotation. It can be seen that the second configuration is contained whithin the first. The second assessor must have used a smaller range of the line-scale. The thick lines can now be shortend by stretching the inner configuration a little bit. The result of this operation is shown in Figure 7.

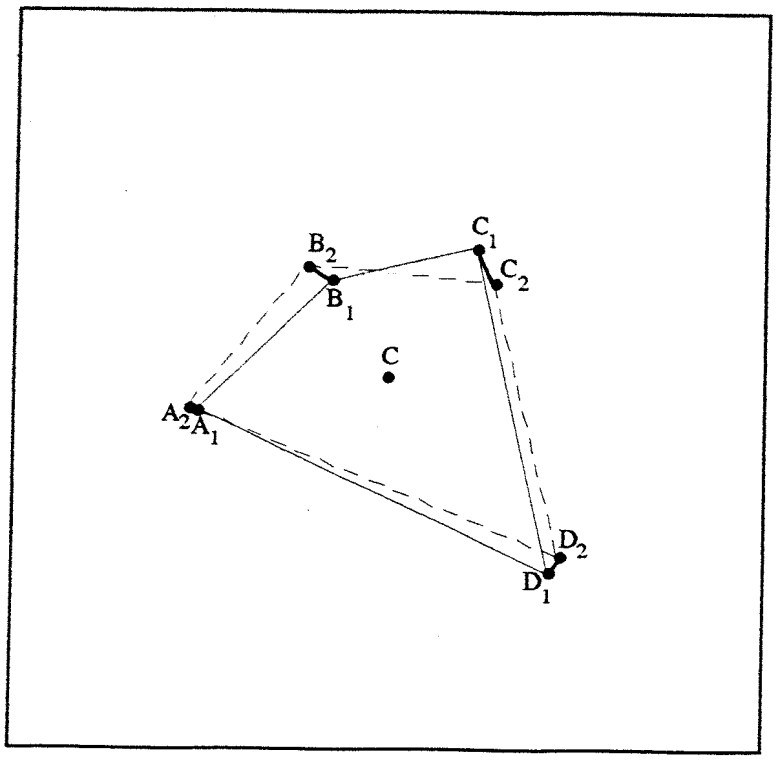

Figure 7. The two example configurations after centring, rotating and isotropic scaling.

The scaling factors are represented by a number ρ_k. A configuration k is shrunk when $0<\rho_k<1$ and stretched when $1<\rho_k$.

2.3 Generalised Procrustes analysis more formally

Mathematically the matching process is expressed by minimizing the distances between the same objects for different assessors, under the conditions that the distances between the objects of one assessor may not change. Gower (1975) gives a mathematical derivation of generalised Procrustes analysis.

The above mentioned distances can be expressed as the differences between the individual matrices:

$$\sum_{k<l}^{K} \left\| \mathcal{T}(\mathbf{X}_k) - \mathcal{T}(\mathbf{X}_l) \right\| \tag{1}$$

$\mathcal{T}(\mathbf{X}_k)$ stands for a certain transformation $\mathcal{T}$ of the matrices $\mathbf{X}_k$, and

$$\|\mathbf{M}\| = \mathrm{tr}(\mathbf{M}\mathbf{M}') = \sum_{i,j} m_{ij}^2$$

for the sum of the squared elements of **M**. The transformation $\mathcal{T}$ has to maintain relative distances between the product-points. Such transformations were introduced in §2.1, now they are presented more formally. Firstly minimising (1) can be shown to be equivalent to minimising:

$$\sum_{k=1}^{K} \left\| \mathcal{T}(\mathbf{X}_k) - \mathbf{Y} \right\| \tag{2}$$

when

$$\mathrm{Y} = K^{-1} \sum_{k=1}^{K} \mathcal{T}(\mathrm{X}_k)$$

the mean of the individudal transformed datamatrices $\mathcal{T}(\mathbf{X}_k)$. The transformations applied in Procrustes analysis are translations, rotations and isotropic scaling and they can be expressed as follows:

$$\mathcal{T}(\mathbf{X}_k) = \rho_k \mathbf{X}_k \mathbf{H}_k + \mathbf{T}_k \tag{3}$$

where ρ_k is the isotropic scaling factor, $\mathbf{H}_k$ the rotationmatrix and $\mathbf{T}_k$ the translation. The translation can be taken care of by column centring the matrices $\mathbf{X}_k$, as was shown by Gower (1975). To keep the formulae in this section from growing long, the translation is not mentioned anymore. It is assumed that the columns in $\mathbf{X}_k$ are expressed in deviations from their means. Removing the means in this way is effectively removing the assessor main effect.

The criterion minimised by generalised Procrustes analysis is the sum of all the squared distances between the individual transformed matrices which by (2) can be written as:

$$\sum_{k<l}^{K} \left\| \rho_k \mathrm{X}_k \mathrm{H}_k - \rho_l \mathrm{X}_l \mathrm{H}_l \right\| = K \sum_{k=1}^{K} \left\| \mathrm{Y} - \rho_k \mathrm{X}_k \mathrm{H}_k \right\| \tag{4}$$

Some constraints are necessary, to assure non-trivial solutions. One constraint is in the $\mathbf{H}_k$ being rotation matrices, which are orthonormal matrices, hence:

$$\mathbf{H}_k' \mathbf{H}_k = \mathbf{H}_k \mathbf{H}_k' = \mathbf{I} \tag{5}$$

A constraint on the isotropic scaling factors ρ_k is needed to prevent them from becoming zero to minimise (4) in a trivial way. The constraint scales the total variance to K, the number of sets:

$$\sum_{k=1}^{K} \left\| \rho_k \mathbf{X}_k \mathbf{H}_k \right\| = K \tag{6}$$

It has been assumed hitherto that all the matrices $\mathbf{X}_k$ are of the same order ($N \times M$), which is the case with conventional profiling data. When Free choice profiling data are analysed this assumption does not hold. In this case the $\mathbf{X}_k$ are made of the same order by padding columns of zero's until all $\mathbf{X}_k$ are of the same order ($N \times \max\{M_k\}$). See Dijksterhuis and Gower (1991/2) for some discussion about this custom. Another possibility is using Projecting Procrustes analysis (Peay 1988) which differs from the classical (Gower 1975) Procrustes analysis. The criterion maximised by Projecting Procrustes analysis is

$$K\left\|\mathbf{Y}^{[p]}\right\| = \left\|\left(\sum_{k=1}^{K} \rho_k \mathbf{X}_k \mathbf{H}_k\right)^{[p]}\right\| \tag{7}$$

where the superscript $[p]$ stands for the first p dimensions of the configuration $\mathbf{Y}$. Note that the variance contained in the resulting, p-dimensional group average space is maximised, while in the classical Procrustes analysis the residual variance beteween the corresponding objects in the entire M-dimensional individual configurations is minimised. The important difference with GPA is that the rotationmatrices are no longer proper *rotation*matrices but they include a projection onto p dimensions as well. This means that it is not necessary to pad all $\mathbf{X}_k$ to the same order. This also means that it is not needed to perform a PCA on the group average space afterwards, because this space already exists in p dimensions.

Another difference proposed by Peay (1988) is the constraint on the isotropic scaling factors ρ_k as follows:

$$\sum_{k=1}^{K} \left\|\rho_k \mathbf{X}_k \mathbf{H}_k\right\| = \left(\max\{M_k\}\right)^{-1} \sum_{k=1}^{K} M_k \tag{8}$$

which is equal to (6) in case all sets are of the same order ($N \times M$). The scaling of the variance, formula (6) or (8), does not influence the GPA solution. Dijksterhuis and Punter (1990) suggest to scale the total variance to 100. This means that all subsequent variances can be read as percentages explained, or residual, variance.

More about GPA and some variants can be found in Ten Berge (1977) and Ten Berge and Knol (1984, see also Dijksterhuis and Gower 1991/2).

2.4 Variables and dimensions

When analysing the raw data from the assessors in a sensory panel the columns of the datamatrices are the variables or attributes the assessors used in judging. When analysing sensory-instrumental data, often only two datamatrices are involved of which one may contain the results of some previous analysis like PCA or even another GPA. Such a datamatrix with the PCA or GPA result does not have variables as columns but dimensions. This is a different situation from the analysis of raw, sensory, datamatrices from different assessors. Different ways of scaling and standardizing are needed when analysing sensory-instrumental data compared to the data from a sensory panel.

The result of prior analyses (e.g. factor analysis, or MDS) will often be normalised configurations, which do not need pre-scaling for the Procrustes analysis. Different instrumental measures (e.g. pH, Instron-measures etc.) will have very different ranges and

levels of scores. In these cases standardisation of each variable may be useful. The sensory scores of a panel are much more homogeneous than different instrumental measures, so they may not need to be standardised individually.

For an application of generalised Procrustes analysis to sensory-instrumental data see Dijksterhuis (1994). Dijksterhuis & Gower (1991/2) also discuss some matters related to the pre-scaling of the datamatrices.

3. RESULTS OF A PROCRUSTES ANALYSIS

This section presents matters related to the results of a GPA. The analysis of variance is an important tool in interpreting the results, as is the PCA which enables inspection of a low-dimensional projection of the group average.

3.1 Analysis of variance

After the analysis, the distances between the corresponding points can be interpreted in the translated, scaled and rotated configurations. These distances are precisely those which are minimized by the generalised Procrustes analysis process. It is not possible to get the objects closer under the assumptions of generalised Procrustes analysis. There are different ways of looking at these distances.

3.1.1 Total fit/loss

Squaring the distances, resulting in 'variances', and adding them, gives a overall measure of loss which can be compared with the squared distances before the generalised Procrustes analysis. It is convenient to express these variances relative to the total variance before the generalised Procrustes analysis (see also Dijksterhuis & Punter, 1990). The thick lines remaining in Figure 7 cannot be made shorter, and these lines represent the *loss*, i.e. that what cannot be modelled by the GPA process. The complement of the percentage loss to 100% gives the *fit* of the obtained solution. Remember that the group average is subjected to a PCA to find a projection onto a low-dimensional space. The aforementioned *fit* can be broken down per dimension, to infer an optimal dimensionality to best represent the results in. Dijksterhuis & Punter (1990) use a scree-graph to infer an optimal dimensionality.

When the variances -squared distances between the objects- are added over the N objects, per assessor, a measure results which shows the agreement of a particular assessor with the group average. When these variances are added over the K assessors, a measure for each product can be obtained, which shows how much agreement there is among the assessors about a particular product. Both outlying assessors and products can be thus identified.

These variance measures for assessors and for objects can be split over dimenions too, this enables identification of assessors or objects which need an extra dimension, or cases in which one assessor or one object accounts for an extra dimension by itself.

3.1.2 Geometry of the variance measures

The different variances in a Procrustes analysis have a clear geometrical meaning. In Figure 8 the different variance measures ('group average', 'Residual' and 'Total') for the different products are illustrated. In this figure the position of product A is shown for three assessors

(A_1, A_2, A_3), their 'group average' point is labelled A. The variances are, as variances usually are, measured relative to the origin, labelled C (Centre).

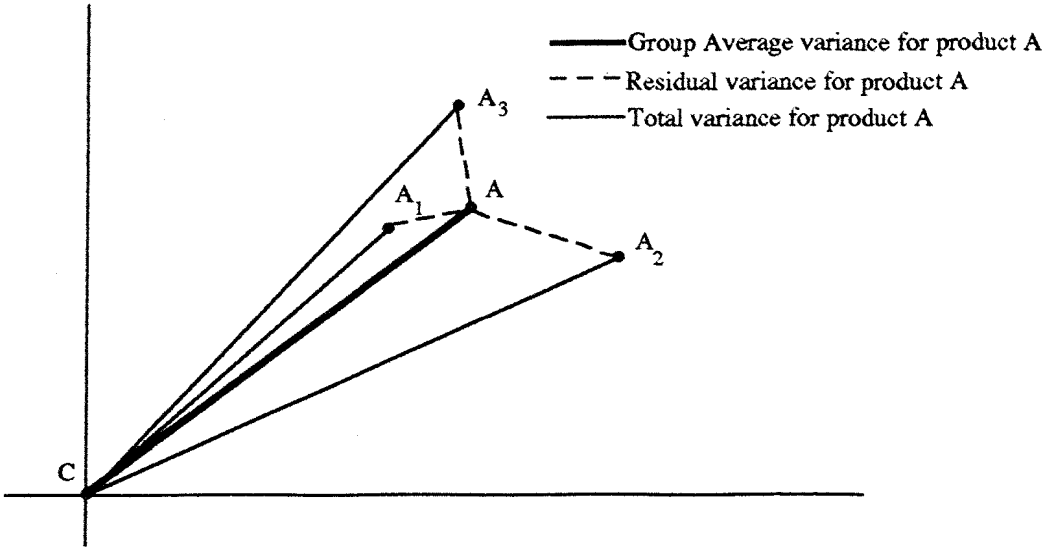

Figure 8. Geometrical interpretation of the group average, residual and total variances for the objects in a Procrustes analysis.

In Figure 8 the lines between the points represent the variances. The squared lenghts of these lines is the variance.

When the residuals or total variances are regarded per subject instead of per product, variance measures for assessors result (see Figure 9). In this figure only three assessors (1, 2 and 3) and two products (A and B) are used to keep the plot from cluttering.

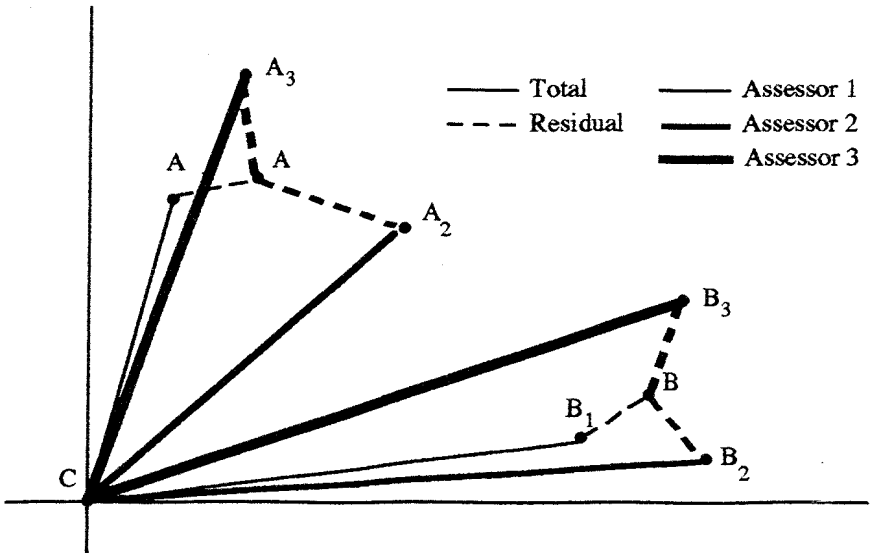

Figure 9. Geometrical interpretation of the group average, residual and total variance for two assessors in a Procrustes analysis.

In Figure 9 the dashed lines represent the residual variances, the plain lines the total variances. The three assessors are represented by different thicknesses of the lines. For assessor 1 the residual is computed by adding all its residual parts from all products, the same holds for the total parts. Note that the residuals and the totals are not part of the same 'average assessor-point', as was the case with the product-points. This is the reason that a group average variance is not available for assessors but only for products.

3.2 Principal component analysis

It is time to expand a little on the matter of the dimensionality of the solution. The classical generalised Procrustes analysis according to Gower (1975) applies all the transformations (translation, rotation/reflection, scaling) in the highest possible dimensionality, i.e. 100% of the data is involved throughout the entire analysis. When the optimal solution is obtained, it is in this high, say M, dimensional space. In order to obtain a convenient representation in a low number of dimenions, say two, a PCA is applied to the M dimensional GPA group average. This final PCA gives a number of dimensions of which the first two can be plotted for inspection. The percentages explained variances of these dimensions can be used to infer a dimensionality of the solution. Perhaps a third or fourth dimension is decided to be needed in order to interpret the results. A scree graph of the explained variance of this PCA can help in deciding on the dimensionality of the representation.

The final PCA on the group average space results in a low-dimensional representation of this space. The PCA gives this space a certain orientation. Because one wants to compare the group average space to all individual spaces, the latter are given the same orientation as the low-dimensional group average space.

3.2.1 Representing the original variables

The original variables, the attributes of a sensory panel or instrumental variables in sensory-instrumental data, can be represented in the GPA group average. Basically there are two ways of doing this. One is to use the coordinates of the rotationmatrices, these are called the loadings of the variables. These matrices, $\mathbf{H}_k$ rotate the individual datamatrices $\mathbf{X}_k$ to $\mathbf{X}_k\mathbf{H}_k$ The matrices $\mathbf{H}_k$ are of order $(M \times M)$ and their rows represent the M columns of $\mathbf{X}_k$ on the new -rotated- M dimensions $\mathbf{X}_k\mathbf{H}_k$. These dimensions are represented in the $\mathbf{H}_k$ as their M columns. Plotting the column-points from $\mathbf{H}_k$ thus result in points that represent the original variables in the rotated spaces $\mathbf{X}_k\mathbf{H}_k$.

Another way of representing the original variables is to calculate their correlation with the dimensions of the group average space. Plotting the correlations results in a representation of the original variables often much alike the one using the loadings.

Theoretically the loadings may be interpreted as biplot axes (see e.g. Gower and Dijksterhuis 1994), which can be a reason to prefer the loadings. Others may prefer the correlations because sometimes they may give more explicit results. Which one prefers seems to amount to a matter of taste.

3.3 Statistical matters

There is no formal test of significance available for the results of a generalised Procrustes analysis. In Langron and Collins (1985) such a test is derived, but the assumptions may be unrealistic (cf. Dijksterhuis and Gower 1991/2). GPA is most often used as an exploratory

tool, especially in sensory analysis. Recently some papers are publised which address the matter of significance in a generalised Procrustes analysis context. King and Arents (1991) devise a test based on the analysis of random data-matrices. Their approach is the same as the one used by Langeheine (1982). In this approach random datamatrices, the size of the original data, are analysed, and this is repeated a number, say 100, of times with different random data. The position of the original result in the distribution of the results from the random data analyses, is an indication of the statistical significance of the GPA result. The permutation test approach (see e.g. Wakeling et al. 1992) uses the same distribution as the original data, in fact it uses the very same data, to obtain a measure of the statistical significance. In a permutation test the null hypothesis of no structure in the data, or no relation between the data sets, is simulated by means of permuting the rows of the datamatrices. For the permuted data set a relevant statistic, here e.g. the Procrustes-loss, is calculated. This process is repeated a large number of times, say 100. The empirical result, i.e. the Procrustes loss of the unpermuted, original, data set, is compared to the distribution of the loss-values obtained after permutation of the data sets. Analogously to the random data approach, the position of this empirical loss-value in the distribution of loss-values gives the statistical significance. In Dijksterhuis and Heiser (1995) a brief evaluation of the random data- and the permutation methods is given.

Analytical approaches (Sibson 1978, Langron and Collins 1985) to find a theoretical distribution for the Procrustes loss values, suffer from the fact that the data must follow a multivariate normal distribution, which may not occur in practice. As a result the results of these studies may not work satisfactory in practice.

3.4 Methods for missing data

Generalised Procrustes analysis as an exploratory research tool in sensory analysis presupposes a complete data set for each assessor. Until recently there were no Procrustes models which would hanlde missing values properly. Commandeur (1991) developed a generalised Procrustes analysis in which it is allowed to have arbritrary rows of individual data sets missing. The model is able to fit data sets which are of unequal row-order. This situation could arise in a sensory context when not all assessors tasted or smelled all objects because e.g. some assessors failed to appear at a certain experimental session. Ten Berge et al. (1993) expanded the method of Commandeur to include missing cells. This means that each of the individual data sets can have missing values for some products on some attributes.

3.5 Comparison with other MVA techniques

3.5.1 Procrustes variants

The original generalised Procrustes analysis is developed by Gower (1975). Earlier Procrustes analysis methods were developed to match two data sets. Table 1 presents a concise overview of the most cited contributions to the development of Procrustes analysis.

Table 1
Some papers in the history of Procrustes analysis.

Author	Year
Green	1952
Hurley & Cattell	1962
Cliff	1966
Schönemann	1968
Schönemann & Carroll	1970
Kristof & Wingersky	1971
Gower	1975
Ten Berge	1977
Ten Berge & Knol	1984
Peay	1988
Gower	1995

Another approach to generalised Procrustes analysis is described by Peay (1988). The 'classic' generalised Procrustes analysis of Gower (1975, see also Ten Berge 1977) performs all transformations in the highest possible dimensional space. The results are subjected to PCA afterwards to create a low-dimensional representation. The method according to (Peay 1988) has a different approach to make a low dimensional representation. The rotation/reflection step of the process includes a *projection* onto a low dimensional space. Hence this method will be called *projection Procrustes analysis* in contrast with *orthogonal Procrustes analysis* (see Gower 1995). A PCA is not needed afterwards. A result of the projecting approach of projecting Procrustes analysis is that the dimensions of the result of this method are not *nested.* This means that a P-dimensional solution is not the same as the first P dimensions of a $P+p$ ($p>0$) solution as is the case with classical GPA.

What method is to be preferred is perhaps more a matter of philosophy than of supremacy of one of the methods. Dijksterhuis & Gower (1991/2) compare the 'classical' Gower (1975) method with the Peay (1988) method.

3.5.2 Other MVA techniques

Before talking about the relationship of GPA with other MVA methods there are two distinctions to make:

- between 2-way methods and individual difference methods
- between 3-way and K-sets techniques.

Section II ('Analysing aggregated sensory data') treats a number of different 2-way MVA methods. These methods work on matrices that are aggregated. The aggregation is often done by means of averaging over assessors, so there are no individuals present in the data. It is argued by some (see e.g. Dijksterhuis and Punter 1991, Dijksterhuis 1995a, 1995b) that it is seldom justified to average over assessors in sensory data analysis because the attributes actually are different for each assessor, despite training of the panel.

The methods that respect the individuals in the data are called 'individual difference methods' and they are treated in Section III ('Analysing individual sensory profiles'). Two kinds of individual difference methods must be distinguished: 3-way methods and K-sets methods. There is a fundamental difference between these two methods and between the corresponding two kinds of data: 3-way data and K-sets data. Figure 2 shows the structure of

a 3-way data matrix, in sensory applications this means that all attributes are the same for all assessors. In Figure 3 it is illustrated that the attributes are different for the assessors. 3-Way MVA methods assume that all sets -the assessors- have the same variables, hence it is useless to use these methods for *K*-sets data. *K*-sets methods do not make this assumption, so they are fit for the analysis of *K*-sets data as well as for the analysis of 3-way data. Analysing 3-way data by a *K*-sets method provides a manner to find out if the variables are really commensurate in all sets.

The 3-way factor analytic methods in Chapter 10 ('Analysing individual profiles by three-way factor analysis') are, as their name suggests, 3-way methods. GPA and GCA, Chapter 7 ('Procrustes analysis in sensory research') and Chapter 8 ('Generalised canonical analysis of individual sensory profiles and instrumental data') respectively, are *K*-sets methods. Chapter 6 ('Analysing differences and similarities among products and among assessors by Multidimensional Scaling') treats Multidimensional Scaling methods, which come in a 2-way and an individual-difference variety. The individual-difference MDS methods work differently from GPA and GCA, but they effectively analyse *K*-sets data. This is because individual difference MDS methods study the relationships (distances) between the *objects* of each individual data set, so that the variables dissapear in the process. When the variables dissapear it does not matter anymore whether the data were *K*-sets, or 3-way.

4. CONVENTIONAL PROFILING

In this section a data set is analysed using the program Procrustes-PC v2.2 (OP&P, 1992, Dijksterhuis et al. 1991).

4.1 Data

The cheese data set analysed in this paragraph is made available by Matforsk and is part of a study by Hirst et al. (1994). This data set is also analysed in Dijksterhuis (1995a) in the context of a study of 'panel consonance', i.e. the agreement of the individuals in a sensory panel on each attribute separately.

The data consist of the scores of 10 judges scoring 12 kinds of hard cheese using 19 attributes. The QDA procedure (Stone and Sidel 1985) is used so the data are 'conventional profiling' data. GPA is applied to this data set to study individual differences between judges and to construct a 'group average' configuration of the 12 cheeses. It is the same data set that is studied in the chapter on 3-way factor analysis (chapter 4.4, 'Analysing individual profiles by three-way factor analysis'). The analysis in this chapter is to illustrate the method of generalised Procrustes analysis, it is not meant as a study of the cheese data.

Each of the 12 cheeses is presented twice to each subject. Each replication is analysed as a separate 'product' in the GPA, so 24 'products' are used in the analysis.

4.2 Dimensionality of the GPA group average

Most often the results of GPA are displayed in a two dimensional plot. At this point it is useful to consider the differences between the projection Procrustes analysis according to Peay

(1988) and the original Procrustes analysis according to Gower (1975). The differences between the two methods will be illustrated using the cheese data.

4.2.1 Projection Procrustes analysis

This variant of GPA combines the Procrustes transformations with a projection onto a low dimensional space. This means that when the researcher chooses to calulate a two-dimensional GPA solution, the data are projected onto a 2-dimensional space and that higher dimensions are not used for the calculation of the optimal solution. This does not mean that the solution is sub-optimal, it is the best solution in two-dimensions, but at the cost of loosing sight of any interesting information that could have been captured in the third, forth or higher dimensions. To be sure, in addition a three-, four-, five-, etc. dimensional analysis should be carried out.

4.2.2 Classical Procrustes analysis

The original GPA applies all Procrustes transformations in the full dimensional configuration, and the result of the analysis is a group average in the maximum number of dimensions possible. Any potentially interesting information is available. The resulting high-dimensional configuration is subjected to a principal component analysis in order to be able to give a low dimensional representation of it. The researcher can *a posteriori* decide to use only two or three dimensions of the total result.

4.2.3 Cheese group average

To find-out the optimum dimensionality to represent the group average in, all dimensions are considered. Note that a projection Procrustes analysis with the maximum number of

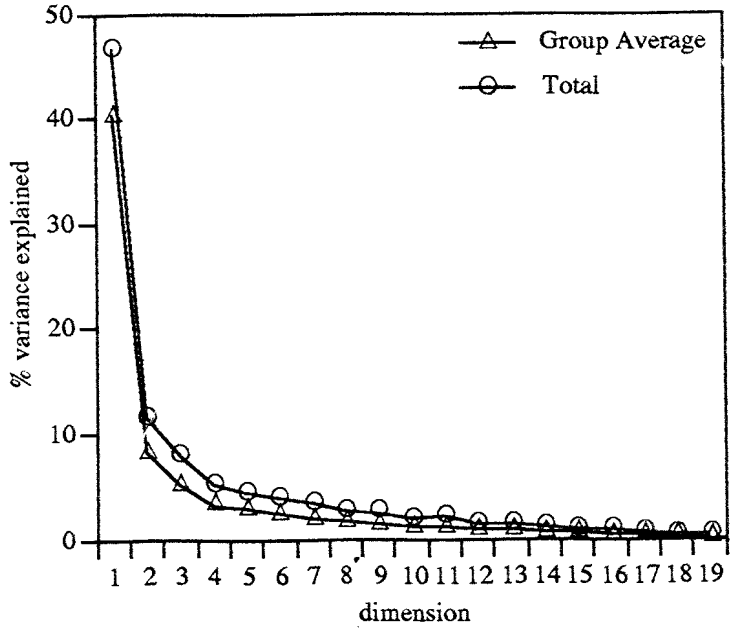

Figure 10. Percentages group average- and total variance explained in the dimensions of the group average space.

dimensions is identical to the classic Procrustes analysis because there are no dimenions left to project onto. In this case the projections are onto the full dimensional space, which is of course the same thing as not projecting at all.Figure 10 presents a scree-graph in which the percentages explained variance of all dimensions are shown.

Figure 10 shows that approximately 40% of the group average variance and 46% of the total variance is explained in the first dimension. Remember that the total variance is the variance explained by the configurations of all the assessors. When these configurations are averaged, becoming the 'group average' configuration, the group average variance remains. The averaging of individual configurations results in the loss of variance. It is exactly this loss, the residual variance, which is minimized by the classical orthogonal procrustes analysis. The projection procrustes analysis maximises the group average variance, in a particular number of dimensions. In this full-dimensional analysis, the two are identical.

Table 2

Cumulative explained variance for the dimensions of the group average and of the individual configurations ('Total') of the GPA result of the (10 × 12 × 19) Cheese data set.

Dimensions	group average	Total
1	40.37	46.62
2	48.59	58.09
3	53.78	66.08
4	57.08	71.19
5	59.92	75.61
6	62.33	79.62
7	64.32	82.98
8	65.97	85.73
9	67.48	88.28
10	68.68	90.25
11	69.81	92.38
12	70.73	93.87
13	71.55	95.33
14	72.20	96.51
15	72.76	97.51
16	73.22	98.40
17	73.59	99.12
18	73.86	99.62
19	74.04	100.00

In Table 2 it can be seen that a two dimensional solution explains 48.59% variance of the group average configuration. The total variance in two dimensions is 58.09%, i.e. the variance explained by the inidividual configurations of all the assessors. Both from Table 2 and Figure 10 two- or three-dimensions seem enough to represent the results in. When we decide that two (or three) dimensions will suffice we can use the first two (three) dimensions of the results of the full-dimensional analysis above. Alternativeley we can perform a new analysis using the projecting Procrustes technique in two (or three) dimensions, which will result in a slightly increased fit in the first two (three) dimensions. The disadvantage is that there are no higher dimensions available, all higher dimensions are explicitely regarded as noise by this decision. Table 3 shows the percentage variance explained by these additional Projecting Procrustes Analyses[1].

Table 3

Cumulative explained group average variance for the separate 2 and 3 dimensional Projection Procrustes Analyses of the Cheese data (corresponding classic GPA percentage from Table 2 between brackets).

Dimension	2D analysis	3D analysis
1	49.764	40.628
2	49.540 (48.59)	49.238
3	-	54.940 (53.78)

Table 3 shows a slight increase in explained variance for the dimensions of the group average compared with the results in Table 2. For the presentation of the cheese data analysis we will choose the result of the two dimensional projection Procrustes analysis.

4.3 Group average configuration

One of the most interesting results from a Procrustes analysis is the 'group average-', or 'Consensus-'configuration. This configuration contains the products, here the 24 cheeses. Figure 11 shows this configuration.

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1 Note that the PROCRUSTES-PC v2.2 program, that was used for the analyses in this chapter, allows for both 'classical' orthogonal procrustes analysis and projection procrustes analysis. Most other Procrustes software is based on the 'classical' orthogonal procrustes analysis

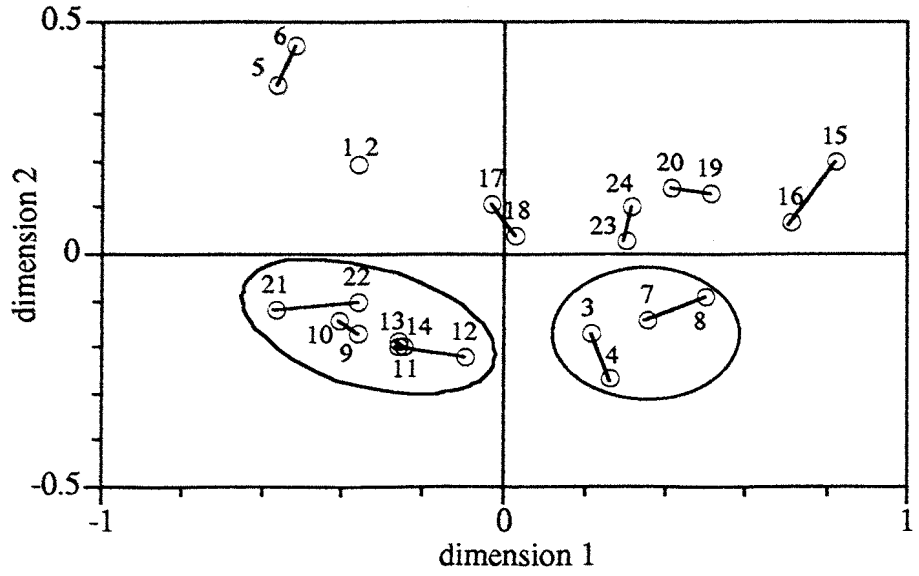

Figure 11. Group average configuration of the Procrustes analysis of the cheese data. Replicate cheeses are connected by a line.

The configuration in Figure 11 shows the 24 cheeses. The replicates are connected by a line. Including replicates in a profiling study is very important, especially when the data are analysed by Procrustes analysis or another multivariate analysis. In Figure 11 the lines connecting the replicates are relatively short, which is an indication that the judges assessed the replicates almost identically, hence an indication of the validity of the obtained result. In this case interpretations of this configuration can be made safely.

Taking a closer look at Figure 11 reveals some groups of cheeses. Two releatively clear groups are indicated in the figure. At the lower left part are the cheeses (9, 10, 11, 12, 13, 14, 21, 22), at the lower right part of the plot are (3, 4, 7, 8). At the upper right part there is a group, though looser than the previous two groups, that seems to consist of the cheeses (15, 16, 19, 20, 23, 24). At the upper left part of the figure clearly the pair (5,6) is different from the other cheeses. Cheese number 1 and 2 lie in that part of the plot too. The numbers 17 and 18 lie almost at the centre of the plot, this usually means that there is no clear agreement between the judges on these cheeses. The numbers 17 and 18 will probably show a relatively high residual variance. The Procrustes 'analysis of variance' can be used to further interpret the results.

4.4 Analysis of variance

In this section the Procrustes analysis of variance tables are shown and interpreted. To illustrate the tables they are plotted as bar-charts (cf. Dijksterhuis and Punter, 1990).

4.4.1 Analysis of variance for objects (cheeses)

Figure 12 shows the group average (explained) variance and the residual (not explained) variance for the 24 cheeses. The 'Total' variance can directly be read from the plot as the total hight of the bars because:

total variance = residual variance + group average variance

The order of the cheeses along the horizontal axis in Figure 12 is in increasing size of their residual variance.

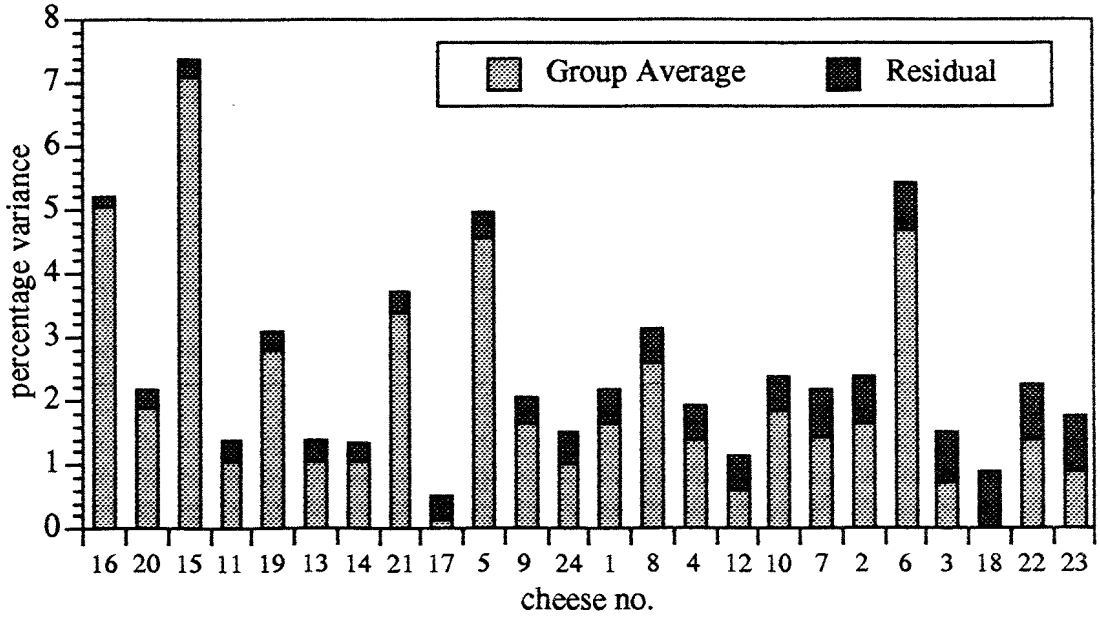

Figure 12. Percentage variance explained (group average) and unexplained (Residual) for the cheeses. The order of the cheeses is in increasing size of Residual variance.

The cheeses at the left hand side of Figure 12 have the smallest residuals. This means that there was not much difference between the scores of the assessors on these cheeses. The panel agreed well on these cheeses.

The cheeses with a larger part of residual variance (right hand side of the picture) did not fit well in the group average, there were differences between the scores of the assessors. In Figure 12 the cheeses 3, 18, 22 and 23 have relatively large residual variances. There must have been less agreement on these cheeses.

4.4.2 Analysis of variance for assessors

In this section the residual variances for assessors are studied. Table 4 shows the residual variance per assessor.

Table 4.
Percentage unexplained ('residual') variance for the assessors.

judge no	Residual
9	0.772
7	0.818
5	0.970
2	1.015
10	1.075
4	1.344
6	1.418
1	1.489
3	1.624
8	1.882

From Table 4 it can be seen that assessors 1, 3 and 8 have the highest residual variances. These assessors' individual configurations of the 24 cheeses differ most from the group average configuration. Assessors 7 and 9 are among the lowest-residual assessors.

When selecting an analytical sensory panel, an homogeneous group of judges is desired. Suppose that a selection of judges is to be made from Table 4, judges with high residual variances will be deleted from the panel, or subjected to extra training.

4.4.3 Individual configurations

To illustrate differences between individual configurations Figure 13 and Figure 14 show the group average position of the 24 cheeses, connected with the position of the same cheeses in the individual result of respectively assessor 7 -a low-residual assessor- and assessor 8 -a high-residual assessor.

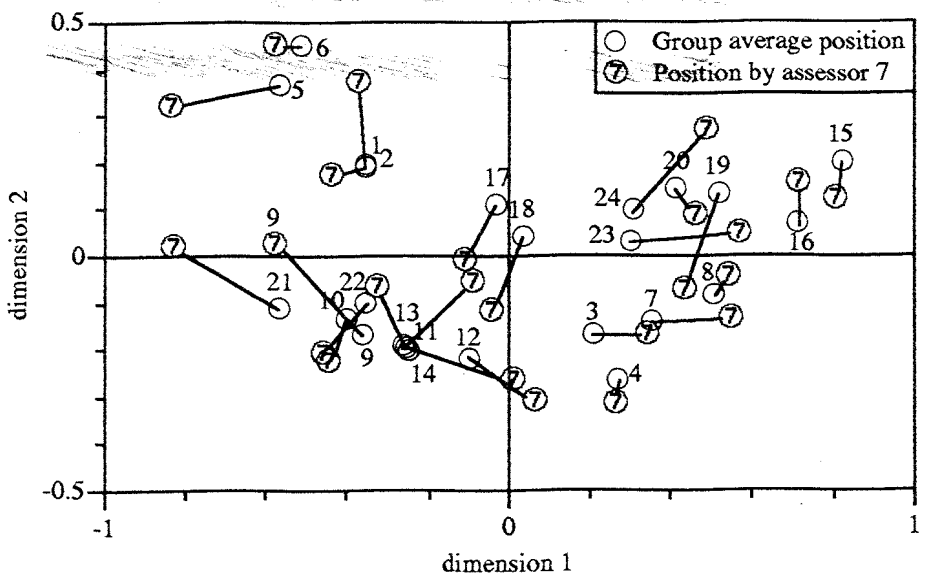

Figure 13. Group average position of the 24 cheeses, connected to the position of the same cheeses according to the configuration of assessor 7.

Though the differences are not large, over-all the lines in Figure 14 are longer than the lines in Figure 13. The sum of the squared lengths of the lines is the residual variance for the assessors 7 and 8, and is shown in Table 4.

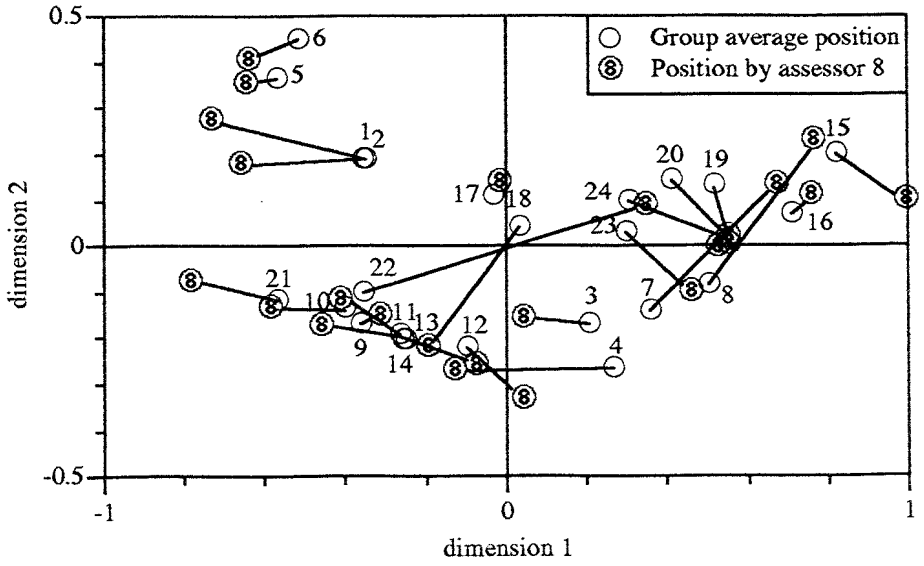

Figure 14. Group average position of the 24 cheeses, connected to the position of the same cheeses according to the configuration of assessor 8.

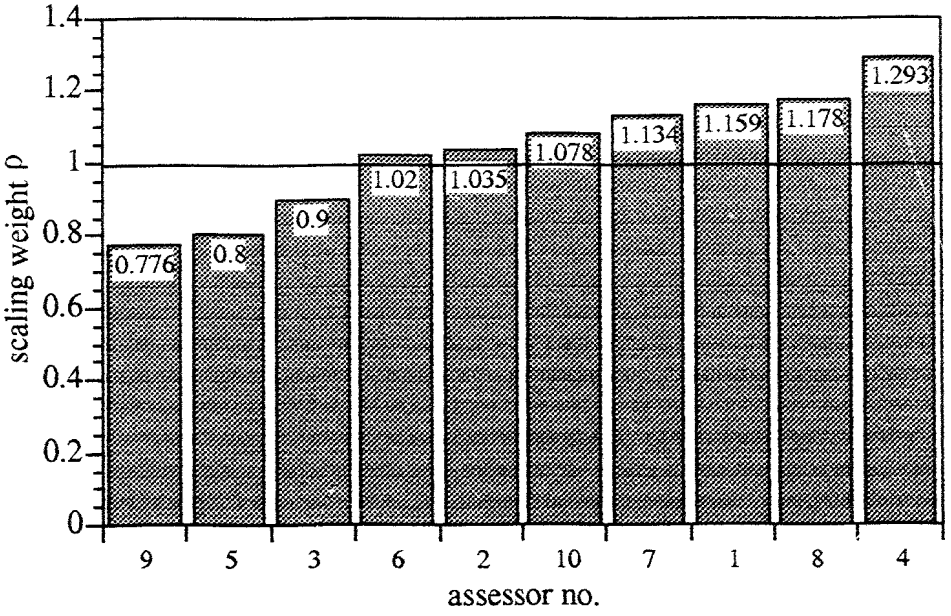

Figure 15. Isotropic scaling factors (sorted) for the 10 individual assessors' configurations.

4.5 Scaling factors

The isotropic scaling factors (see §2.2.3) reflect the amount of stretching or shrinking the individual configurations of the 10 assessors underwent in the Procrustes analysis. Figure 15 presents the 10 scaling weights.

The horizontal line in Figure 15 is at $\rho = 1$. Bars extending above this line show stretched configurations ($\rho > 1$), bars below this line represent shrunk configurations ($0<\rho<1$). Assessor 9, 5 and 3 have their configurations shrunk, they used a larger range of scores than the other assessors. It's the other way around for assessors 1, 4 ,7 and 8, their configurations are stretched. They used a limited range of scores. The assessors 6, 2 and 10 had their configurations hardly changed by the scaling.

4.6 Representing the original variables

Until now the objects, i.e. the 24 cheeses, and the assessors are studied. The 19 attributes the assessors used remain to be studied now. The attributes can be subdivided into odour-, flavour and texture attribtutes and are presented in Table 5.

Table 5.

Attributes used in the cheese study (Hirst et al. 1994).

	odour		flavour		texture
1	odour intensity	7	flavour intensity	15	hardness
2	creamy/milky	8	creamy/milky	16	rubbery
3	ammonia/sulphur	9	sour	17	doughy
4	nutty	10	ammonia	18	grainy
5	sour	11	nutty/fruity/sweet	19	sticky
6	other	12	bitter		
		13	salty		
		14	other (cheddar)		

Note that the arrangement in the table does not indicate any relation between attributes in the same row.

The loadings or correlations from the Procrustes analysis output give representations of the original attributes. Both the coordinates of the loadings and of the correlations can be used to draw the original attributes in the group average configuration. In this example the correlations will be used.

Each assessor used these 19 attributes, this means that each individual configuration contains 19 attributes. The total configuration with all judges together will consequently contain $10 \cdot 19 = 190$ attributes. These are far too many attributes to draw in a picture. With conventional profiling data, like this cheese data set, it is possible to average the attributes over the assessors, to make group average attributes. This is analogous to the averaging of the individual product-positions to make group average product points. Figure 16 presents the resulting group average attribute points based on the correlations of the original attributes with the group average dimensions. Of course averaging is only justified with a reasonable fit. When the fit is very low, the group average configuration is to be doubted.

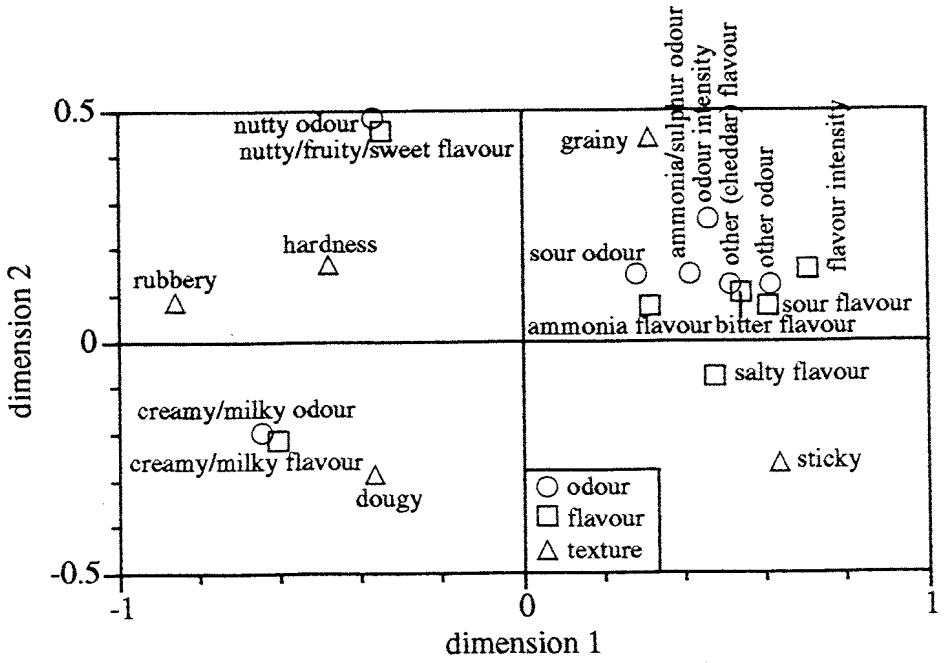

Figure 16. Averaged ('group average') attributes in the group average space of the cheese data.

In Figure 16 the relations between the attributes can be inferred. It shows that some odour and flavour attributes match: nutty odour with nutty flavour, creamy/milky odour with creamy/milky flavour, sour odour with sour flavour, ammonia odour with ammonia flavour, and odour intensity with flavour intensity. The texture attributes seem to divide the cheeses into sticky, doughy, grainy and rubbery/hardness. When dimensions have to be reified the first dimension may be approximately interpreted as a bitter/sour odour/taste and rubbery versus sticky dimension, and the second dimension as a nutty/sweet odour/taste and doughy versus grainy dimension.

Figure 16 can be compared to Figure 11 to infer properties of the cheeses. The lower left group of cheeses (9, 10, 11, 12, 13, 14, 21, 22) appear to be characterised by creamy/milky flavour and taste, their texture is mainly doughy. The cheeses 9, 10, 21, 22 seem to tend to a rubbery texture. The group at the lower right part of the plot (3, 4, 7, 8) has a sticky texture and a somewhat more salty and sour flavour. The cheeses 19, 20, 15 and 16 have a high flavour and taste intensity, a bitter/sour/ammonia flavour/taste. Because these cheeses lay opposite to the texture attributes rubbery and hardness, they do *not* have these properties, they are mainly soft cheeses. The cheeses number 5 and 6 (1 and 2 to a lesser extent) are the nutty/fruity/sweet cheeses. These cheeses are among the harder, more rubbery and grainy cheeses.

The above interpretation of the GPA group average space and the positions of the correlations of the original attributes is a kind of *biplot*-interpretation. For more about biplots in a GPA context see Gower and Dijksterhuis (1992), for biplots in general see (Gabriel 1971, Gower 1992).

5. FREE CHOICE PROFILING

In this section a free choice profiling data set is analysed by means of GPA. For this analysis the Procrustes-PC v2.2 program (OP&P 1992) was used. This same data is analysed by GCA in Chapter 8 too.

5.1 Data

The data consist of the judgements of 20 different mineral waters by eleven assessors[2]. Each assessor used her/his own attributes to judge the waters, so the data are FCP data. FCP data can only be analysed by an individual difference method of the *K*-sets type, or an individual-difference MDS method (e.g. Indscal; Carrol and Chang 1970). In this section GPA is used to analyse this data set. What is presented here is a standard GPA analysis of an FCP data set. The GPA method used is the classic GPA (Gower 1975) so the smaller data sets are padded with zero's to make all sets of the same order.

Some of the 20 mineral waters were presented, blindly, two or three times. These replications are very useful, they will be represented as connected points in the Group Averge plot (compare Figure 11).

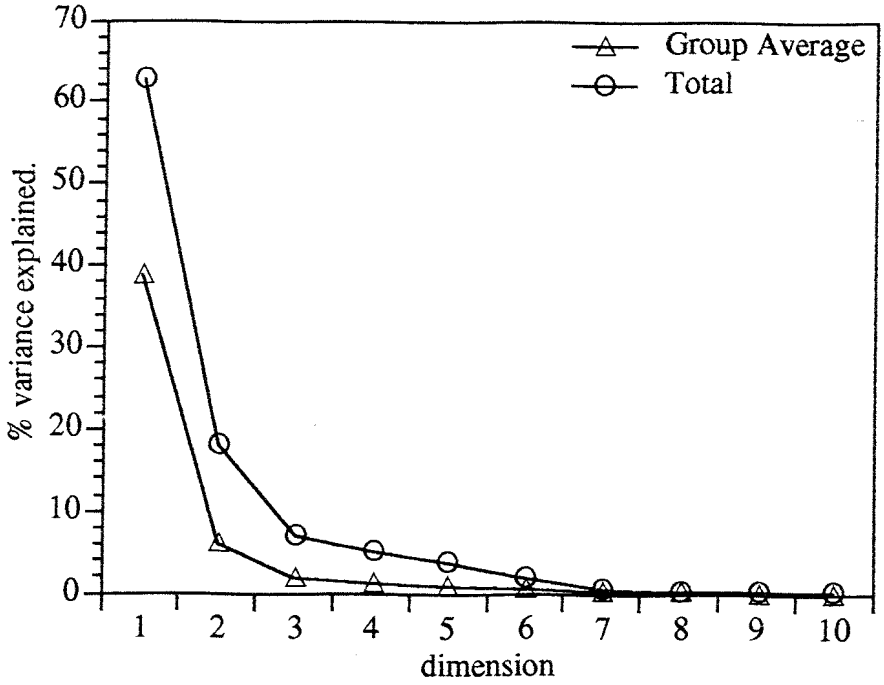

Figure 17. Percentages group average and total variance explained by the dimensions of the GPA group average space.

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2 The data were made available by Dr. Pascal Schlich, INRA, Dijon, France.

5.2 Analysis of variance

First the dimensionality to represent the results in must be chosen. To this end the explained variance, distributed over the dimensions are needed. Figure 17 presents this scree for the dimensions of the water data.

The scree for the total variance shows that the first dimension explains 63% of the variance, the second dimension adds about 18%, the third adds another 7%. The line for the group average variance has the same shape, but the variances are lower. They should be, the differences are the residual variances per dimension. It seems that a 2-dimensional solution would do as a reasonable approximation of the data. In Table 6 the cumulative percentages explained variance are given, a two-dimensional solution explains 81% in all individual configurations together and 45% in the group average.

Table 6

Cumulative explained variance for the dimensions of the group average and of the individual configurations (Total) of the GPA result of the water data.

dimension	group average	Total
1	38.837	62.908
2	44.729	80.963
3	46.607	88.084
4	47.918	93.231
5	48.722	97.078
6	49.091	99.05
7	49.155	99.46
8	49.202	99.765
9	49.231	99.945
10	49.240	100

Note that in Table 6 the total explained variance in 10 dimensions is 100%, as it should be because in the maximum dimensionality all data are included and of course nothing is lost.

5.3 Configurations

5.3.1 Group average configuration

Figure 18 shows the GPA group average configuration of the 49 mineral waters. Replications are connected by lines. It can be seen from Figure 18 that e.g. water no. 15, 16 and 17, are judged more different than the waters 21 and 22, because the lines connecting the former are much longer than the lines connecting the latter.

Figure 18 enables identification of four approximate groups. At the left are two waters: 15, 16, 17 and 21, 22. Somewhat more to the right are two other waters: 1, 2 and 43, 44. The big cluster of the remaining waters may be subdivided into the waters 25, 26; 47, 48, 49; 10,11, which appear at the rightmost bottom part. This group also includes 45, which is connected by a rather long line to 46, these two waters were not very consistently assessed, they are rather far apart. In the set remaining waters it is hard to distinghuish separate groups. Note that the lines connecting replicates cross through this cluster, so there apear no clearly separated groups of waters.

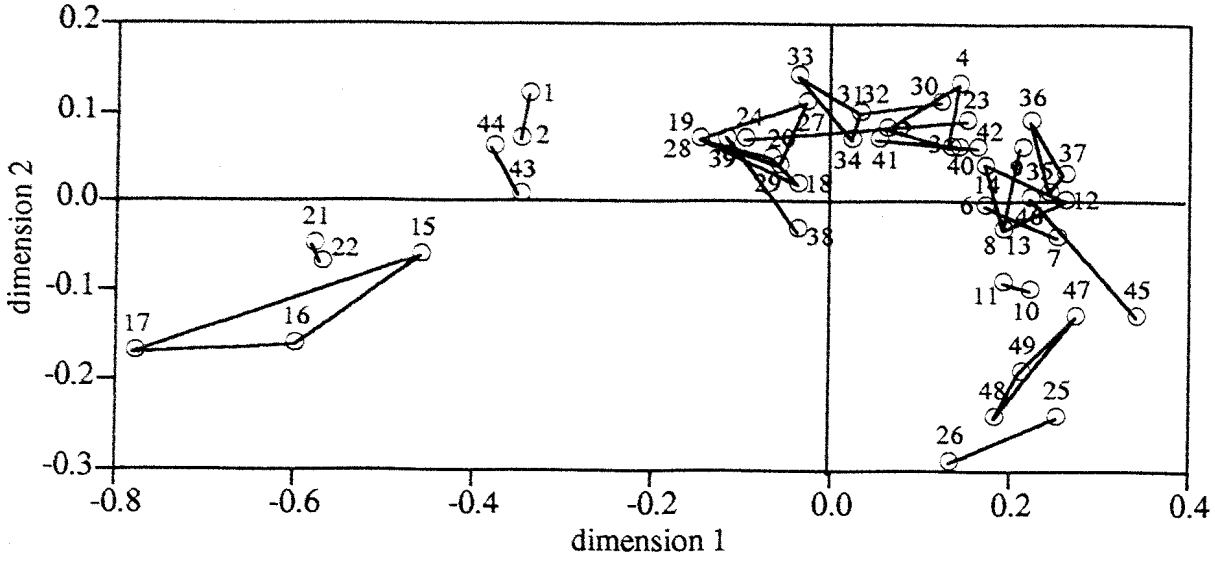

Figure 18. GPA group average configuration of the 49 mineral waters. Replicate waters are connected by lines.

Figure 19 shows the residual and total variances of the ten judges in the mineral water data set. Note that all the residual variances are about equal, and the total variances differ.

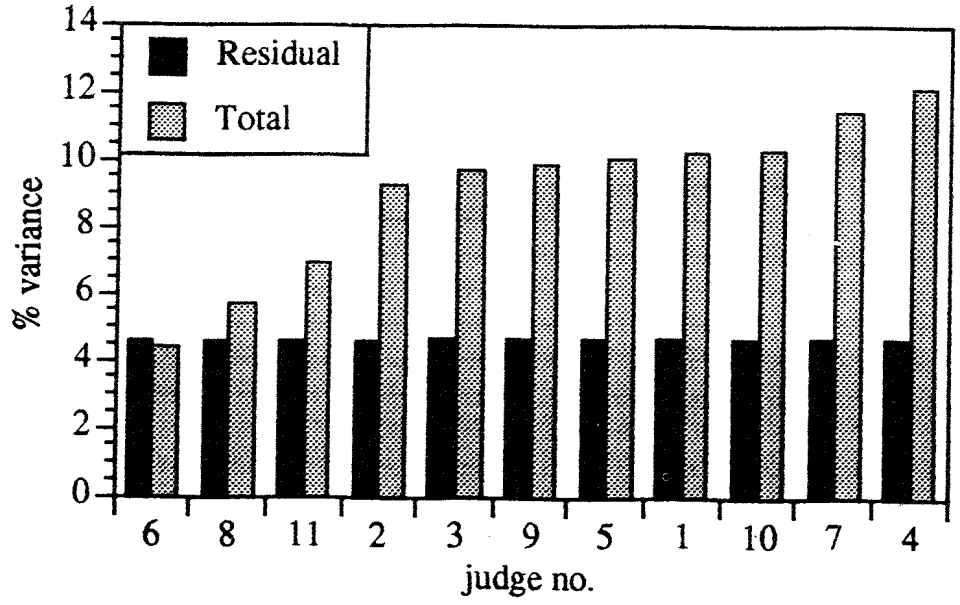

Figure 19. Total and residual variances of the assessors in the water study.

The judges 6 and 4 differ the most in the amount of total variance. It may be interesting here to study the total variances per judge, for dimensions separately. Table 7 presents these variances.

Table 7
Total variance in the first four dimensions, per judge.

judge no.	1	2	3	4
1	8.920	0.509	0.134	0.486
2	5.895	1.831	0.598	0.224
3	5.293	1.819	1.444	0.572
4	9.361	0.725	0.285	0.498
5	4.891	3.540	0.451	0.320
6	1.134	1.933	0.288	0.527
7	7.352	1.401	1.011	0.572
8	2.439	2.210	0.969	0.051
9	7.605	0.514	0.816	0.553
10	6.993	1.811	0.633	0.545
11	3.027	1.761	0.490	0.799

Table 7 shows that some judges (1, 4, 9) have a large proportion of variance in the first dimension, and relative low proportions in the second. In contrast judge 5, 6, 8 have relatively much more variance in the second dimensions, compared to what they have in the first.

5.4 Scaling factors

Table 8 gives the isotropic scaling factors for the individual sets. Two sets (7 and 10) needed to be stretched by a factor 2.6 and 2 respectively. Apparantly the judges 7 and 10 used a rather small range of scores. Judge 11 used a large range of scores, the corresponding configuration is shrunk by a factor 0.6.

Table 8
Scaling weights of the judges in the GPA of the water data.

judge	weight
11	0.627
6	0.769
8	0.785
1	0.855
2	0.920
3	0.959
4	1.007
9	1.065
5	1.389
10	2.001
7	2.571

5.5 Representing the original variables

Table 9 shows the attributes and their use by the assessors. Note that 8 of the 11 judges used the term bitterness, the terms neutral and metal were used by six assessors. There are a lot of

unique attributes, i.e. which were only used by one assessor. Notably assessor 4 and 5 generated most unique attributes.

Table 9

Attributes used in the FCP of the mineral waters and the no. of the judge that used it.

Attribute	judge no.	Attribute	judge no.
bitter	1, 2, 3, 5, 6, 8, 9, 11	balanced	4
neutral	1, 2, 4, 6, 8, 9	persistent	4, 6
taste	1	mineral	5
metal	1, 3, 7, 9, 10, 11	stagnant	5
fluid	1	river	5
salty	2, 4, 7, 8	cool	5
earth	2, 4, 7, 11	sugar	6
hard	2	old	6
acid	3, 4, 11	mushroom	7
paper	3, 10	milky	7
flat	4, 5	energic	9
dry	4	hazelnut	10
pungent	4	soft	11
rubber	4		

Note that the arrangement in the table does not indicate any relation between attributes in the same row.

For the interpretation of the clusters of waters that appeared in Figure 18 it is needed to represent the original attributes in the group average configuration. In Figure 20 the correlations of the original attributes with the dimensions of the group average space are presented.

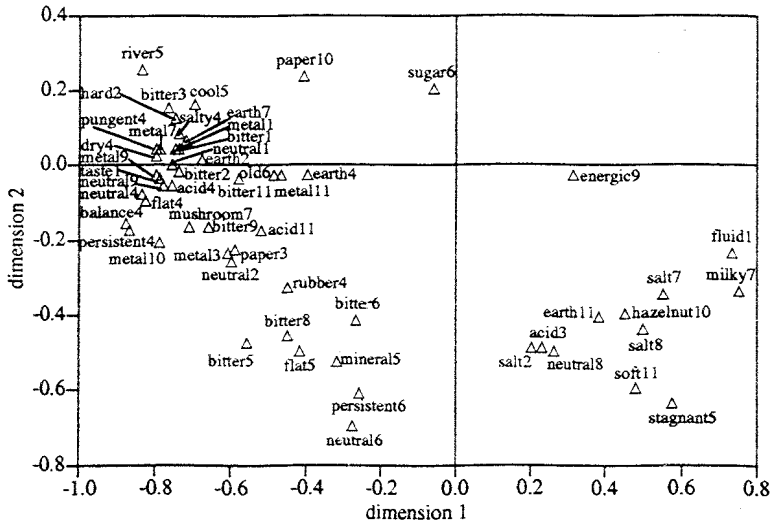

Figure 20. Configurations of the individual attributes based on the correlations of the attributes with the dimensions of the group average. The number following the term indicates the assessor number.

In Figure 20 there appear two main groups of attributes. In the lower right quadrant: fluid, milky, hazelnut, salt (2, 7, 8), soft, stagnant, neutral (8), acid (3), earth (11) (assessor numbers between parentheses) and in the upper left quadrant most other attributes.

Inspecting the configuration in Figure 20 enables one to draw some interesting conclusions with respect to the use of the attributes. The term 'metal' was used by six assessors (1, 3, 7, 9, 10, 11), and there seems to be reasonable agreement between them. This agreement is larger than the agreement found between the use of the term 'neutral', also used by six assessors (1, 2, 4, 6, 8, 9). The agreement on 'bitter' appears less than that on 'neutral', assessors 5, 6 and 8 have scored bitter somewhat differently than assessors 1, 2, 3, 9, 11.

Figure 20 and Figure 18 show the same plane, so they can be superimposed. This results in a kind of biplot, containing both the mineral water object points and the positions of the attributes. This plot is not presented here -it would be too cluttered-, but through comparison of the figures Figure 20 and Figure 18 a biplot-like interpretation can also be given. The set of waters {15, 16, 17, 21, 22} lies in a region in the plane that is characterised by a lot of attributes, including most 'metal' and 'bitter' attributes. The set {25, 26, 47, 48, 49, 10, 11, 45} lies in a region characterised by the attributes salt (for 3 assessors), soft, stagnant, acid, earth, hazelnut, milky, fluid. The remaining waters are mainly characterised as not having a certain property. Most lay opposite the remaining attributes.

It is conceivable that mineral waters have rather low amounts of clear tastes. So, after the attributes are generated, a lot of the waters will turn out not to possess this attribute, or just have it in a very low intensity. In addition, when the tastes are not clear, the differences between the assessors may become rather outspoken. A clear bitter taste may not cause much confusion in a sensory panel, but when the taste is only just above the detection threshold, as it may be in mineral waters, individual differences may arise. This could result in the use of other terms.

6. ALGORITM AND SOFTWARE FOR PROCRUSTES ANALYSIS

6.1 Generalised Procrustes analysis algorithm

The original generalised Procrustes analysis algorithm is presented in Gower (1975). Ten Berge (1977) presents a slightly modified algorithm. These algorithms concern the heart of the Procrustes analysis: the rotation and isotropic scaling. In a somewhat broader view, and in most applied situations a Procrustes analysis consists of three different parts:

- Pre-steps (translation, 'pre-scaling')
- Analysis (rotation/reflection, isotropic scaling)
- Post-steps (PCA, analysis of variance)

6.1.1 Pre

The pre-steps consist of the translation operation which amounts to centering the individual datamatrices $\mathbf{X}_k$. It is also possible to give differential weights to sets or to variables. This is all pre-scaling, it is not part of the actual Procrustes analysis. Depending on the wishes of the analist the data may be pre-scaled to have a certain total variance.

6.1.2 Procrustes analysis

The heart of the analysis consists of the two Procrustes transformations, rotation/reflection and isotropic scaling. The rotation/reflection is computed for all individual matrices $\mathbf{X}_k$ to fit the group average matrix. This computation results in a rotationmatrix $\mathbf{H}_k$. The reflection is a part of this rotationmatrix and will not be mentioned any further for this reason. After each individual rotationmatrix is computed, the new rotated individual matrix is $\mathbf{X}_k\mathbf{H}_k$ and the group average matrix is recomputed (see Ten Berge 1977). This is repeated for all sets k=1,...,K. After one run over the K sets the isotropic scaling is performed.

The isotropic scaling factors ρ_k are computed for each $\mathbf{X}_k$. At this point one iteration of the generalised Procrustes process is completed and a new average matrix, now with inclusion of the scaling factors, is computed. One iteration is seldom enough. The decrease of the sum of squared distances between the individual sets $\rho_k\mathbf{X}_k\mathbf{H}_k$ over two subsequent iterations is taken as the criterion to judge whether a satisfactory result is obtained. This criterion is usually set to a very small value, e.g. 0.001. After a number of iterations the criterion approaches this value and will finally become smaller than 0.001. Then the process is said to have converged and the iterative process is terminated.

6.1.3 Post

As said before, the result is in the highest possible dimensionality and PCA is applied to the resulting average configuration. Suppose we take two dimensions from this PCA to inspect the group average space. In order to be able to compare this two-dimensional representation with the individual sets, the individual matrices $\rho_k\mathbf{X}_k\mathbf{H}_k$ are given the same orientation as the PCA result of the group average. We must assure that we compare the individual sets and the group average in the same plane.

Further post-steps include the computation of several ways of partitioning of the residual, explained and total variance, and the computation of the correlations of the original attributes with the dimensions. Finally the tabling and plotting of the results is the obvious final step of the Procrustes program.

6.2 Software for Procrustes analysis

There are several computer programs available that can perform a GPA. A macro in the GENSTAT language was written by Arnold (1986). Schlich (1989) wrote a GPA macro in the SAS IML language. These programs work fine, but have the disadvantage that they run as macro's whithin a large statistical program. The user needs to be able to 'speak' either SAS or GENSTAT. In 1988 a special Procrustes program for the personal computer was developed, which is called Procrustes-PC (OP&P 1988, Dijksterhuis and van Buuren 1988). At the moment version 2.2 is the latest one (OP&P 1992, Dijksterhuis et al. 1992). Recently a new GPA program -Procrustes for Windows- has been developed (OP&P 1995).

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