MULTIVARIATE DATA ANALYSIS IN SENSORY AND CONSUMER SCIENCE

by

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This book served as my Ph.D. thesis, at the department of Datatheory, at the University of Leiden. The main threat to the thesis ever coming to an end was I. Every now and then I would lose myself in a "very interesting" side-track of Multivariate Data Analysis. It was Willem Heiser who, by patiently and repeatedly telling me that I should focus on "sensory applications", put me back on the track again. Over the years he must have told me this several times, and it helped.

Ann Noble (University of Davis, California, USA) had become a kind of e-mail consultant to me. I thank her for her prompt answering of my questions, providing references, and commenting on some of my writing.

My current job is at the Food Science Department of ID-DLO, the Institute for Animal Science and Health (Lelystad, the Netherlands), leading their sensory laboratory. ID-DLO is one of the major research institutes on animal production. In their Food Science Department resides the research on the eating quality and safety of meat, eggs and dairy products mainly, in relation to the processing required to produce a palatable food. At this sensory laboratory I plan to explore some of the newer directions in sensory and consumer science outlined in this book.

Finally there are a number of people that, in some way or another, helped with the finishing of this book. To be sure to include them all, I do not give names, but I thank them all. However, one name must be mentioned. Because the preparation of the thesis was not part of my job, a lot of the writing took place at home, Gerjo is thanked for her patience, enthusiasm and organisational talents I needed to finish this project.

GARMT B. DIJKSTERHUIS
AMMERSTOL

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CHAPTER 1

Introduction

Summary

In this introduction the basic terminology of the subject matter of this book is introduced. The underlying research question of the study is presented and the four main themes that the chapters cover are described and related to this question. The kind of data that are analysed throughout the book is explained. Furthermore, the aim and the structure of the book are explained.

1.1 Research Question

This book is concerned with problems from sensory and consumer research. What exactly these kinds of research are is defined later. The tools used to study the problems are the apparatus of Multivariate Data Analysis. The underlying question that is addressed by the research in this book is:

What has Multivariate Data Analysis to offer for studying problems in sensory research?

Asking a question like this is more or less "upside down". Usually when one is confronted with a scientific problem, an experiment is designed to study it or to test a hypothesis. The reason that this is turned around in this book is that the problems in sensory science that the author was confronted with, were often such that the data were already collected. It was the feeling of both the sensory researchers and the author that "There's more than meets the eye in this data set."

1.2 Sensory Science

Sensory science is the general heading under which the study of many different problems and the application of methods can be found. No complete picture of sensory science will attempted to be given here. A concise history and overview of the field can be found in Stone and Sidel (1985, 1993), McBride (1990) and Punter (1991).

1.2.1 Some Definitions

The part of Sensory Science that this book is concerned with can be defined as follows:

> Sensory evaluation is a scientific discipline used to evoke, measure, analyse and interpret reactions to those characteristics of foods and materials as they are perceived by the senses of sight, smell, taste, touch and hearing.

This definition was used by the (U.S.) Institute of Food Technologists in 1975 and quoted by Stone and Sidel (1985). The definition is very general, but it contains most ingredients of the discipline as it will be presented in this book. The focus in this book will be on the *analysis* of the *reactions* to certain *characteristics* of *food* products (italics refer to the ingredients of the definition). The *reactions* to *characteristics* will be in the form of scores given to attributes perceived in the *food*-stimuli, the analyses will be multivariate and the *senses* will mainly be the senses of *smell* and *taste*.

The field has many names, which may stress different aspects of Sensory Science, but globally the same problems underlie all sub-disciplines. Thomson (1988) poses the question:

> What are the attributes that consumers perceive in a particular new food product and in what ways will these combine to determine future purchase decisions?

as one of the most obvious questions to be answered by the scientific discipline coined "Food Acceptability". He also describes "Food Acceptability" as a somewhat uncomfortable marriage between food science and behavioural psychology. In an attempt to consolidate this marriage, a third party is introduced in this book: data analysis.

McBride (1990) gives an overview of the position of sensory evaluation in between the other disciplines:

1. research and development with a food-technical focus
2. consumer and marketing research with a behavioural and psychological focus

Note that the marriage Thomson (1988) referred to is reflected here too. A lot of bridges can be, and are being, built between the different disciplines involved (see e.g. Thomson *et al.* 1988). In this book a bridge is being developed based on statistics and data analysis.

1.2.2 Sensory and Consumer Science and Related Disciplines

A brief layout along simple lines will be given here to explain further the subject matter of this book. From now on the term *Sensory and Consumer Science* will be adopted, because it reflects reasonably well the contents of the field. It is set apart from the study of the chemical senses, which is commonly referred to as Sensory Psychology and Sensory Physiology (e.g. Köster 1971, de Wijk 1989). Such research is not of concern in this book. The (chemical) senses can also be studied in connection to psychological properties of the experimental subject. In this case behavioural responses may (be attempted to) be modelled mathematically and the properties of the models studied. This kind of research is historically linked to psychophysics and psychometrics. Recent psychophysical studies with applications in sensory science and psychophysics were performed by Frijters (1980) and Ennis (1991). This field is again not the subject of this book.

Figure 1[1] presents an overview of the different parts *Sensory and Consumer Science* contains.

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[1]This figure is based on a suggestion by Pieter Punter.

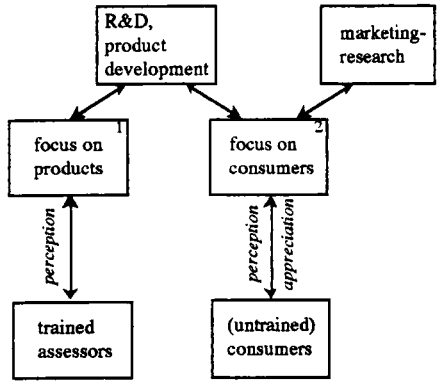

Figure 1 Overview of Sensory and Consumer Science, illustrating the differences in focus (1: on products; 2: on consumers).

As is illustrated in Figure 1, Sensory and Consumer Science and marketing/consumer research can be subdivided into two main fields:

1. the study of products
2. the study of consumers

In the study of products, mainly trained assessors are used to judge the products on rather technical or analytical attributes. This is what is meant by *perception*, in the figure, in contrast to *appreciation*. The hedonic quality *appreciation* of the products is of no concern in this type of sensory research.

Both appreciative and perceptive aspects are used in the consumer focused studies. The perceptive part uses consumer characterisations of the products, rather than technical/analytical attributes. The appreciative part may include measurement of the ideal intensity of the attributes and/or the preferences of the consumers.

Product-oriented research has a clear relation to R&D and product development. Consumer-oriented sensory research in addition has a relation to marketing research.

In this book, the focus is on the products rather than on the consumer. The perception will mainly involve taste and smell properties of the products, though visual, auditory (e.g. Vickers 1983, 1991) and kinaesthetic perceptions are by no means excluded from Sensory and Consumer Science.

The distinction in Figure 1 is not so strict as the figure may suggest. Sensory profiling studies are usually of an analytical nature, hence often found in perception-studies. They try to answer the question: "What are the important

attributes of the products?" They can be applied in appreciation studies too. Then the question: "What products are preferred/accepted/appreciated by the consumers?" is answered. It is a matter of choosing the attributes. In appreciation studies, the attributes are fixed and will be mostly hedonic and focusing on aspects of the quality of the products. Profiling studies will be introduced in more detail in later sections (§1.4).

In Sensory-Instrumental research, the relations between physical/chemical (*instrumental*) properties and the sensory properties of products are studied. The focus of these studies is mainly analytical, i.e., they are perception-studies. However, they may be conducted in an appreciation context, provided that special attention is given to the relations between the instrumental and the sensory-appreciative (see e.g. Noble 1975). Sensory-Instrumental research is covered in more detail in section 1.7 and is the subject of Part III.

Time-Intensity research (§1.8 and Part IV) is focused on perception only. The time-course of a particular perceived property of a product is studied.

1.3 Sensory Research and Sensory Profiling Data

The questions dealt with in this book are from the field of sensory and consumer science. In general terms, this is the field of research in which *people* use their senses to *describe* certain *properties* of *objects*. Admittedly this definition is too general and needs narrowing.

Three entities constitute the research and the resulting data in this book:

- Objects
- People
- Descriptions (of properties)

Objects can be interpreted very broadly. People can describe physical objects, other people, services, etc. Other terms used are *products* or, borrowed from psychology, *stimuli*.

The *descriptions* can take different forms. They can be a judgement of the quality of an object, its hedonic value or another specific property. In this book, the descriptions will take the form of judgements of a particular sensory property of the object, e.g. its sweet taste, its colour, its bitterness or the roughness of its surface. These properties will be called *attributes*, and they constitute the *variables* of the research in the sequel. A variable may consist of numerical scores, or of a number of (ordered) categories.

In sensory research the data are almost exclusively elicited from *people*. One of the directions in sensory and consumer science is research of products with the use of sensory panels, sensory profiling studies. A sensory panel is a group of people who give judgements about products. There are different kinds of sensory panels, some of which will be introduced in a following section.

The products in the case of sensory research are food products, drinks, cosmetics or luxuries like snacks, candy or tobacco. The products are evaluated using essentially all senses (sight, hearing, smell, touch and taste) though depending on the specific research question the focus may be on just one or two of them. In purely analytical taste and/or smell studies, the appearance of different products will be controlled for by e.g. using special lighting conditions. Another modality is texture perception in the mouth. This sense is important when judging products where texture plays a role e.g. in meat. Sight and even hearing also play a part in sensory research. The appearance of products may be important, depending on the kind of research. The sound of potato chips during chewing is an example of use of the auditive sense in judging edible goods (see also Vickers 1991).

1.3.1 Sensory-, Consumer- and Marketing Research

Sometimes the line between sensory, consumer and marketing research is very thin indeed. Often a sensory panel receives a certain amount of training in the judging task that is expected of them. The term *consumer panel* is sometimes reserved for a group of judges that are not trained with respect to their task. They are sometimes described as (or in fact) "picked up from the street", but it also happens that such a panel receives a limited amount of training. No clear standard terminology seems to exist. Matters may get more complicated when the term marketing-research is included in the picture too. Is sensory research a special case of consumer research, which is a special case of marketing research? It proves hard to answer this question and perhaps it is even harder to consolidate sensory researchers with consumer and marketing researchers. Van Trijp (1992, see also Figure 2) makes a distinction between the different types of product that are studied by the different disciplines. Sensory research studies the *core product*, i.e. a product with certain physical/chemical ("instrumental") characteristics of which the sensory characteristics are sought. This is the study of the *perception* of products as presented in §1.2.2. The *generic product* possesses certain derived "benefits" as usage utility, ease of use, perceived durability and a "status". This generic product is different from the

core product, though the same physical product may underlie both. Consumer or marketing research is concerned with studying the generic products.

Figure 2 illustrates the relations between the fields of sensory, consumer and marketing research.

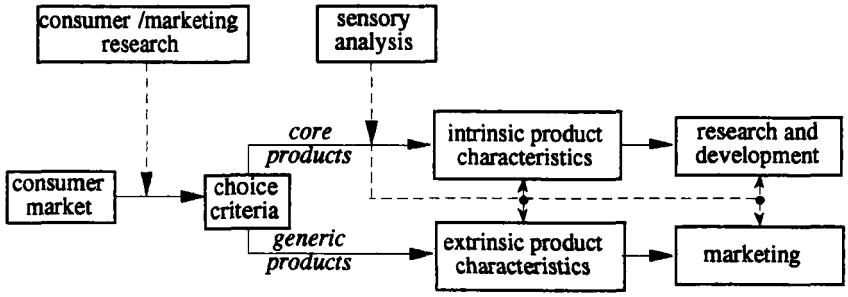

Figure 2 Relations between sensory, consumer and marketing research, showing the differences between *core products* and the *generic products* (slightly adapted from van Trijp 1992).

Figure 2 shows the "classic" point of impact of sensory analysis, studying the intrinsic product characteristics (the *core* product) for research and development. The two double arrows between the intrinsic and extrinsic product characteristics, and between R&D and marketing, indicate an interesting potential application of sensory analysis and marketing, viz. the study of to what extent sensory perception is influenced by properties of the "generic" product such as price, packaging, brand labelling, and the derived characteristics of the generic product.

Sensory research and consumer/marketing research have different, though both psychological, origins. Sensory research is based in sensory physiology and psychology and has, through psychophysics, always had a link with statistics and psychometrics (see e.g. Punter 1991). Marketing/consumer research has its origins in social psychology, and it has a strong link to direct applications in marketing. Sensory research is perhaps less applied than marketing/consumer research, in that it is closer to research and development of products, and further away from the market (see also §1.2.1, Thomson 1988, McBride 1990).

1.3.2 Sensory Panels and Ditto Data

There are a number of different ways to collect sensory profiling data, using different kinds of sensory panels. One important aspect in which these methods of data collection differ is in the amount of training of the panels receive prior to the actual experiment. Figure 3 arranges the different panel-types along a continuum with respect to the amount of training they receive.

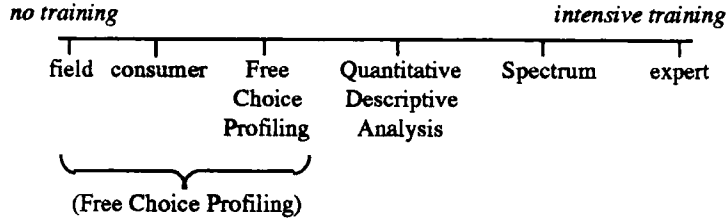

Figure 3 "Sensory panel method continuum", ranging from untrained panels at the left to panels that receive much training at the right.

The sensory analytical panels are located at the right extreme of this continuum. These panels judge a limited set of products on a number of strictly defined properties, with respect to which they have been intensively trained. They are sometimes referred to as *expert* panels. At the other end of the continuum in Figure 3 the consumer panels reside. Here one moves closer to marketing research. The most extreme example is probably found in "mobile testing" where the research takes place in a prepared bus which drives up to a shopping centre and invites people in to judge products. These panels may be called *field* panels, to distinguish them from *consumer* panels in which inexperienced consumers are invited to take place in a sensory experiment inside a laboratory, or at least in a somewhat more controlled environment than a bus. In between the field-panels and the expert-panels a lot of different sensory-panel methods exist of which some are indicated in Figure 3. The differences between the *QDA* panel and the *Spectrum* panel method are not fundamental, and they are not explained here (see Stone and Sidel 1985, 1993 for QDA, Meilgaard *et al.* 1990 for Spectrum). These two methods have in common that a standard vocabulary of descriptive attributes is formed. These attributes are used in the sensory experiment after the panel receives training with respect to the

attributes. The differences between the methods lie in the amount of and procedures of training of the sensory panel.

Another way of distinguishing between different panels is in terms of the kind of questions the judges are asked. A sensory panel is also referred to as an *analytical* sensory panel when the questions in the experiment apply to analytical, as opposed to hedonic, properties of the products. This division is also present in Figure 1, where the term "perception studies" is used for "analytical," and "appreciation studies" for "hedonic studies." Examples of analytical attributes are sweet taste, nutty taste, sticky odour, rubbery texture, etc. The further we move to the right on the continuum in Figure 3, the less likely it is that hedonic questions will be asked. Hedonic studies are not explicitly covered in this book. However, when analytical attributes are replaced by hedonic attributes, or just by one hedonic attribute, most MVA methods discussed in this book can be used for hedonic sensory profiling studies as well.

Free Choice Profiling panels differ not only in the amount of training, but also in another property (see §1.4.2). This is why it is hard to include FCP panels in Figure 3. The panels that are usually called FCP panels are at the approximate position indicated in Figure 3. They often contain consumers, or somewhat more experienced panelists, who receive only a limited amount of training with respect to the attributes. The important property of FCP panel studies is that the assessors can choose their own attributes. When field or consumer panels are allowed to choose their own attributes they become FCP-panels too, hence the brace in Figure 3. The panels at the right hand side of FCP on the continuum are not FCP panels by definition. These, so-called Conventional Profiling panels, are trained with respect to a fixed set of attributes.

Because the distinction between different types of sensory and consumer panels is not always clear, and because the data that result from all profiling-type panels are not very different, both terms *sensory* and *consumer* research appear in this book. Another reason for this is that the Multivariate Analyses applied can be used for both Sensory and Consumer data. As a result, when the term *sensory research* is used it can be read to mean *sensory and consumer research*.

1.4 Sensory Profiling

A large number of sensory studies are of the sensory *profiling* type. There are two different kinds of profiling studies: *Conventional profiling* studies and *Free Choice Profiling* studies (Williams and Langron 1984, Williams and Arnold 1985). The data from either profiling method are usually derived from

the position of marks along a line scale or scores on a rating scale or from a category scale. The assessor marks his/her perceived intensity of an attribute on a line scale or indicates the appropriate category of a category-scale. Figure 4 gives an example of four line-scales for four attributes.

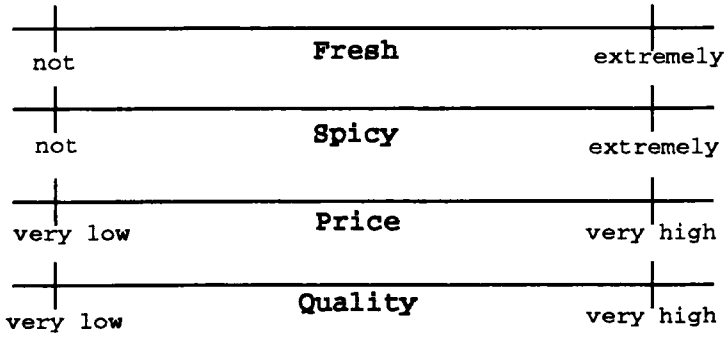

Figure 4 Example of four line-scales, for the attributes fresh, spicy, price and quality.

Figure 5 shows two examples of another type of scale, the category scale. These scales have a limited number of categories of which the assessor can choose one. A comparison of the results of using line-scales and category-scales can be found in Chapter 6 (van der Burg and Dijksterhuis 1993). A disadvantage of that study is that the line-scale data were converted into a low number of categories *a posteriori* (see also Chapter 5, van der Burg and Dijksterhuis 1989). In this way the effect of a different response behaviour of the assessor, resulting from the presentation of a different kind of response scale, is excluded from the study. It would be interesting to study this particular aspect of the differences in use of response-scales.

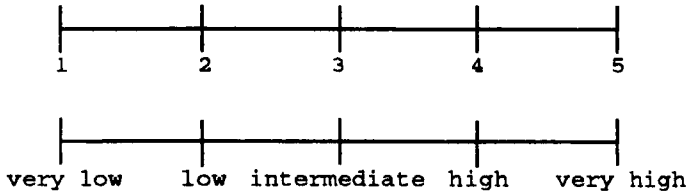

Figure 5 Two different category scales, a 5-point numerical and a 5 category adjective scale.

The type of response scale used is intimately connected to the problem of the measurement level and the admissible scale transformations of the data. This point is returned to in §1.6 and in Part II.

There are other types of response-scales too. King (1986) reports the use of an audio method in which the assessors give their scores by adjusting a tone to a certain pitch. Non-graphical response scales, as King's pitch-scale, deserve to be studied too. A disadvantage is that special devices are needed, and graphical scales are much easier to employ.

1.4.1 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 e.g. 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 may take months. 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 minimised due to the training. When one assumes no individual differences or ascribes them to noise or random error, individual judgements can be averaged and e.g. Principal Component Analysis can be applied to the average scores.

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 6).

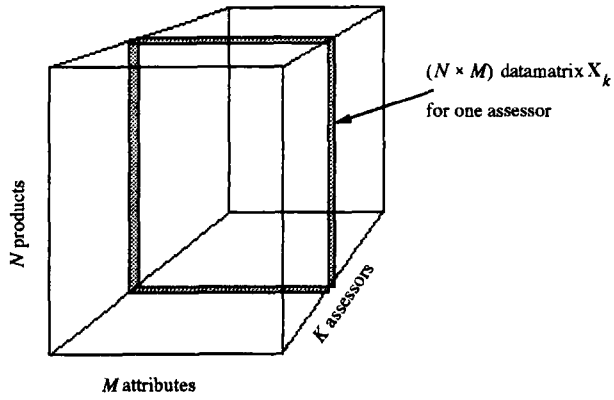

Figure 6 3-mode data structure representing Conventional Profiling data: N products are judged by K assessors using M attributes.

1.4.2 Free Choice Profiling

In Free Choice Profiling (FCP, Williams and Langron 1984, Arnold and Williams 1985), the assessors are free to come up with their own attributes, which they use for judging the products. So there is no *a priori* agreement on attributes between the assessors. As a result, it is impossible to average the individual data directly, because it makes no sense to add different attributes. The data from Free Choice Profiling experiments *must* be analysed by individual difference models which come up with some kind of average after transformation of the data. Unlike Conventional Profiling data, Free Choice Profiling data cannot be arranged in a kind of 3-mode data structure because each assessor $k=1,\ldots,K$ may have a different number of attributes (M_k). More importantly, the jth attributes of the assessors are not necessarily the same. Figure 7 illustrates the structure of an FCP data set.

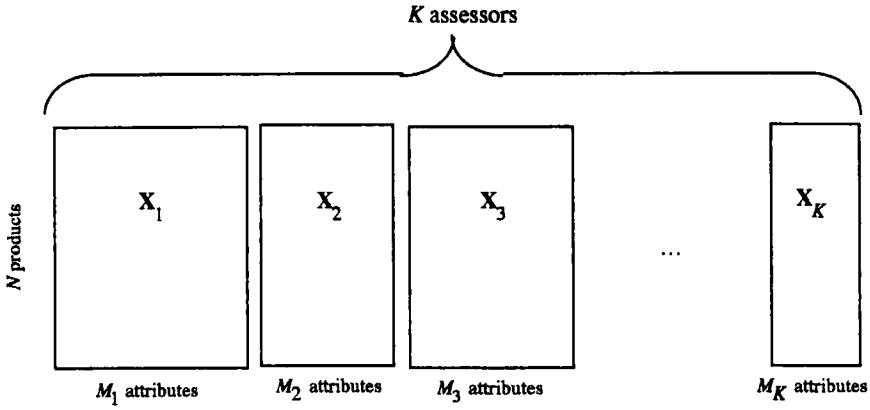

Figure 7 Data structure representing Free Choice Profiling data: N products are judged by K assessors each using M_k attributes.

Figure 7 shows that the individual data matrices $\mathbf{X}_k$ cannot be arranged such that the attributes match because each assessor's individual data matrix contains different attributes.

1.5 Individual Differences

Differences between the data of the assessors in a sensory panel are a concern in most sensory studies. Because in sensory research the chemical senses (smell and taste) play an important role, there are rather large individual differences between the judges. These differences may be larger than with the visual, auditory and other senses. The lack of consensus is for a large amount due to two effects, one physiological, and one psychological:

- large individual differences in the internal milieu of the chemical senses, i.e. the nose and mouth;
- there is no clear standard vocabulary concerning the sensations of taste and smell.

The first effect results in different perceived intensities of stimuli and different time courses of the perceptions. The differences in time course are found clearly in TI-studies (see also §1.8 and Part IV).

The second effect results in problems with the interpretation of the behavioural responses elicited from the assessors. The four basic tastes, sweet, sour, salty and bitter are clear, but flavours involve the sense of smell and there are no basic smells known. Everyone may use another term to describe the same sensation. This is the main reason that sensory panels are trained when exact and consistent sensory *analytical* data are needed.

Under the assumption of only a physiological effect, proper standardisation of scores should correct for much of the individual differences. In that case, individual scores could be averaged and analysed subsequently by e.g. PCA. When the psychological effect plays a role too, and it most often does, standardisation is not enough, and special methods that correct for the so-called interpretation-effect are needed.

When averages are computed over individuals, both the physiological and the psychological effect can be interpreted to give rise to random error only. But, when more elaborate data analysis is employed, as will be illustrated in this book, some of this error appears not to be random and may contain interesting information.

1.5.1 Subjects, Objects and Variables: Three-Modes and Three-Ways

A typical sensory profiling experiment consists of presenting a group of people, the *panel*, with a number of products and asking them to judge the products on a set of attributes. In more formal terms: *subjects* are presented with *objects* which they judge using a set of *variables*. The data resulting from such an experiment can be characterised as consisting of three ways, corresponding to the three *modes*: objects, subjects and variables (see also §1.4.1 and Figure 6). The data can be classified as three-way, three-mode data (Carroll and Arabie 1983). When K assessors judge N products on M attributes, the corresponding data can be presented as a three dimensional table (see Figure 6). An element x from such a three-way data matrix X can be identified by three subscripts:

$$x_{ijk} \epsilon \mathrm{X},\ i=1,\ldots,N;\ j=1,\ldots,M;\ k=1,\ldots,K \qquad (1)$$

Such data are typically multivariate, at least it will be assumed they are (see Heiser 1992). For the multivariate analysis of this kind of data special three way techniques exist (see e.g. Law *et al.* 1984, Coppi and Bolasco, 1989).

1.5.2 Averaging and Individual Differences

A common way of analysing sensory data is by using averages. The first step in these analyses is the averaging of the individual data matrices. An individual data matrix is one slice X_k of order (N×M) from the three-dimensional structure in Figure 6. The average data matrix looks just like this slice of Figure 6, with the difference that it contains averaged scores, $i=1,\ldots,N$; $j=1,\ldots,M$, instead of individual data x_{ijk}:

$$x_{ij\cdot}=K^{-1}\sum_{k=1}^{K}x_{ijk} \tag{2}$$

The average data matrix $\bar{\mathbf{X}}$ can be analysed by means of Factor Analysis or Principal Component Analysis. The averaging of the raw data naturally results in loss of individual differences.

As an alternative to averaging it is possible to perform a PCA on all variables of the concatenated sets which amounts to an analysis of an $(N\times MK)$ data matrix. Such an analysis results in MK component loadings which can be inspected. In a plot the loadings from the same assessor can be marked for easy identification of which variable goes with what assessor. The disadvantage of this strategy is that the individual assessors may not be represented fairly. Weighting variables per assessor may help but eventually other methods will be more appropriate. To solve problems like these an individual difference model can be useful.

Three-way models offer a solution because they respect the third mode, here the different assessors, in the data. However, these models assume equality of variables over subjects. This assumption may be justified for data which contains clear and unambiguous variables but probably not for most sensory data.

1.5.3 Sets in K-sets Analyses

The assessors in a sensory panel are the measuring devices with which the data are collected. The human being acting like a measurement device can measure e.g. the shape, the colour, the apparent length, the taste, the smoky odour, and lots of other characteristics of objects. Each individual device (assessor) produces and uses these variables in its own idiosyncratic way. It is as if all devices were differently, and obscurely, calibrated, and it is unknown what it is they measure. This confusion is the reason that the attributes used by