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Abstract. The industrial development of innovative and succesful food items and the measuring of food quality in general is difficult without actually letting human beings evaluate the products using their senses at some point in the process. The use of humans as measurement instruments calls for special attention in the modelling and data analysis phase. In this paper the focus is on sensometrics – the „metric" side of the sensory science field. The sensometrics field is introduced and related to the fields of statistics, chemometrics and psychometrics. Some of the most commonly used sensory testing methods are introduced and some of the corresponding sensometrics methods reviewed and discussed.

Keywords: Sensometrics, Statistics, Chemometrics, Psychometrics, Sensory.

1 Introduction

The current contribution is an extended version of [1]. The use of humans as measurement instruments is playing an increasing role in product development and user driven innovation in many industries. This ranges from the use of experts and trained human test panels to market studies where the consumer population is tested for preference and behaviour patterns. This calls for improved understanding on one side of the human measurement instrument itself and on the other side the modelling and empirical treatment of data. The scientific grounds for obtaining improvements within a given industry span from experimental psychology to mathematical modelling, statistics, chemometrics and machine learning together with specific product knowledge be it food, TVs, Hearing aids, mobile phones or whatever.

In particular in the food industry sensory and consumer data is frequently produced and applied as the basis for decision making. And in the field of food research, sensory and consumer data is produced and used similar to the industrial use, and academic environments specifically for sensory and consumer sciences exists worldwide. The development and application of statistics and data analysis within this area is called sensometrics.

2 Sensometrics

2.1 Sensometrics and Sensory Science

As the name indicates sensometrics really grew out of and is still closely linked to sensory science, where the use of trained sensory panels plays a central role. Sensory science is the cross disciplinary scientific field dealing with human perception of stimuli and the way they act upon sensory input. Sensory food research focuses on better understanding of how the senses react during food intake, but also how our senses can be used in quality control and innovative product development. Historically it can be viewed as a merger of simple industrial product testing with psychophysics as originated by G. T. Fechner and S.S. Stevens in the 19th century. Probably the first exposition of the modern sensory science is given by [2]. Rose Marie Pangborn(1932-1990) was considered one of the pioneers of sensory analysis of food and the main global scientific conference in sensory science is named after her. The 1st Pangborn Symposium was held in Helsinki, Finland in 1992 and these conferences are approaching in the order of 1000 participants - the 9th will take place in Toronto, Canada in 2011. Jointly with this, international Sensometrics conferences have been held also since 1992, where the first took place in Leiden, Holland (as a small workshop) and the 10th took place in Rotterdam, Holland in 2010. The sensometrics conferences have a participation level of around 150. Both conferences are working together with the Elsevier Journal Food Quality and Preference which is also the official membership journal for the Sensometrics Society (www.sensometric.org).

2.2 Sensometrics: Statistics, Psychometrics or Chemometrics?

The “sensometrician” is faced with a vast collection of data types from a widespread number of experimental settings ranging from a simple one sample binomial outcome to complex dynamical and/or multivariate data sets, see e.g. [3] for a recent review of quantitative sensory methodology. So what is really (good) sensometrics? The answer will depend on the background of the sensometrician, which for the majority, if not a food scientist, is coming from one of the following fields: generic statistics, psychophysics/experimental psychology or chemometrics.

The generic statistician arch type would commonly carry out the data analysis as a purely “empirical” exercise in the sense that methods are not based on any models for the fundamental psychological characteristics underlying the sensory phenomena that the measurements express. The advantage of a strong link to the generic scientific fields of mathematical and applied statistics is the ability to employ the most modern statistical techniques when relevant for sensory data and to be on top of sampling uncertainty and formal statistical inferential reasoning. And this is certainly needed for the sensory field as for any other field producing experimental data. The weakness is that the lack of proper psychophysical models may lead to inadequate interpretations of the analysis results. In e.g. [4] the first sentence of the abstract is expressing this concern rather severely: “Sensory and hedonic variability are fundamental psychological characteristics that must be explicitly modeled if one is to develop meaningful statistical models of sensory phenomena.” A fundamental challenge of this ambitious approach is that the required psychophysical (probabilistic) models of behavior is on one hand only vaguely verifiable, since they are based on models of a (partly) unobserved system, the human brain and perceptual system, and on the other may lead to rather complicated statistical models. [4] is published in a special sensory data issue of The Journal of Chemometrics, see [5]. Chemometricians are the third and final arch type of a sensometrician. In chemometrics the focus is more on multivariate data analysis and for some the explorative principle is at the very heart of the field, see e.g. [6] and [7]. The advantage of the chemometrics approach is that usually all multivariate features of the data are studied without forcing certain potentially inadequate model structures on the data. The weakness is exactly also this lack of modelling rendering potentially certain well understood psychophysical phenomena for the explorative modelling to find out by itself. Also, linked with the explorative approach, the formal statistical inferential reasoning is sometimes considered less important by the chemometrician.

Now, none of these arch types are (at their best) unintelligent and they would all three of them understand (some of) the limitations of their pure versions of analysis approach. And they all have ways of dealing with (some of) these concerns for practical data analysis, such that often, at the end of the day, the end results may not differ that much. There is though, in the point of view of this author, a lack of comprehensive comparisons between these different approaches where they all are used at their best.

3 Sensory Profile Data

Probably the most used sensory technique is the so-called sensory profiling – a quantitative descriptive analysis, where a number of products are evaluated on a continuous line scale with respect to a number of properties. In sensory profiling the panellists develop a test vocabulary (defining attributes) for the product category and rate the intensity of these attributes for a set of different samples within the category. Thus, a sensory profile of each product is provided for each of the panellists, and most often this is replicated, see [8]. Hence, data is inherently multivariate as many characteristics of the products are measured.

The statistics arch type would focus on the ANOVA structure of the setting and perform univariate and multivariate analysis of variance (ANOVA) and would make sure that the proper version of a mixed model ANOVA is used, see e.g. [9] and [10]. For studying the multivariate product structure the Canonical Variates Analysis (CVA) within the Multivariate ANOVA (MANOVA) framework would be the natural choice, see eg. [11], since it would be an analysis that incorporates the within product (co)variability.

The chemometrics arch type would begin with principal components analysis (PCA) on averaged and/or unfolded data. For more elaborate analysis maybe 3-way methods, see [12], [13] or other more ANOVA like extensions would be used, see e.g. [14]. Analysis accounting for within product (co)variability could be provided by extensions as presented in [15] or in [16].

In [4] the approach for this type of data is that of probabilistic multidimensional scaling (PROSCAL). In short, a formal statistical model for product differences is expressed as variability on the (low-dimensional) underlying latent sensory scale. It is usually presented as superior to the use of e.g. standard PCA, focussing on the point that it naturally includes models for different within product variability, which in the standard PCA could be confounded with the “signal” – the inter product distances.

One recurrent issue in sensometrics is the monitoring and/or accounting for individual differences in sensory panel data also called dealing with panel performance. A model based approach within the univariate ANOVA framework was introduced in [17] leading to multiplicative models for interaction effect expressing the individual varying scale usage. In [18] the open source stand alone software PanelCheck (www.panelcheck.com) was introduced as a general tool for panelist performance analysis. PanelCheck was developed in a Danish/Norwegian consortium of industrial and research partners to optimize the industrial use of the tool while still maintaining the proper statistical methodology. PanelCheck also gives tools for the heavily used univariate attribute-by-attribute analysis of variance (ANOVA). Standard univariate mixed model analysis of variance is then used to investigate the product differences for each attribute, see [10]. In [19], [20] and [21] random effect versions of such analyses were put forward leading to either a multiplicative (nonlinear) mixed model or a linear random coefficient model. This approach offers a synthesis of the individuality focus with the random effect approach that really applies when product differences are in focus.

Specifically, scaling differences will often constitute a non-trivial part of the assessor-by-product interaction in such sensory profile data, [22], [23] and [24]. In [21] a new mixed model ANOVA analysis approach is suggested that properly takes this into account by a simple inclusion of the product averages as covariates in the modeling and allow the covariate regression coefficients to depend on the assessor. This gives a more powerful analysis and provides more correct confidence limits that are deduced as an adjusted version of the linear random scaling model confidence limits. In 52 sensory profile data sets with all together 564 attributes, 344 (61.1%) showed significant (P-value<0.10) scaling difference. Among almost all these 344 attributes, the product difference P-values were for the new approach smaller than for the traditional analysis. In 15 cases an attribute was significant on level 5% by the new approach and not so by the classical approach and in 5 more cases on level 10%. These 20 changed conclusions were among 37 attributes showing significant scaling differences in spite of being claimed NS by the traditional analysis - and all together only 87 attributes out of the 564 were claimed NS by the traditional approach. Among these 344 attributes, 33.432 post-hoc comparisons were calculated. In 13.503 cases the classical analysis claimed significance (5%) but the new analysis claimed so in 15.137 cases. Still, generally the new, and non-symmetrical, confidence limits are more often wider than narrower compared to the classical ones: in 19.926 cases the new lower limit was wider and in 26.591 cases the new upper limit was wider. In the final paper the meta study will be extended to include an investigation in SensoBase (www.sensobase.fr), using in the order of 500 profile data sets with around 9000 attributes.

4 Basic Sensory Difference and Similarity Test Data

The so-called difference and/or similarity tests are a commonly used sensory technique resulting in binary and/or categorical frequency data - the so-called triangle test is a classical example. In the triangle test an individual is presented with 3 samples, two of which are the same, and then asked to select the odd sample. The result is binary: correct or incorrect. Such sensory tests were already in the 1950s treated by the statistical community, see e.g. [25] and [26]. These types of tests and results have also been treated extensively from a more psychophysical approach, often here denoted a Thurstonian approach. The focus in the Thurstonian approach is on quantifying/estimating the underlying sensory difference d between the two products that are compared in the difference test. This is done by setting up mathematical/psycho-physical models for the cognitive decision processes that are used by assessors in each sensory test protocol, see e.g. [27]. For the triangle test, the usual model for how the cognitive decision process is taking place is that the most deviating product would be the answer – sometimes called that the assessors are using a so-called tau-strategy. Using basic probability calculus on 3 realizations from two different normal distributions, differing by exactly the true underlying sensory difference d, one can deduce the probability of getting the answer correct for such a strategy. This function is called the psychometric function and relates the observed number of correct answers to the underlying sensory difference d. Different test protocols will then lead to different psychometric functions.

In [28] probably the first systematic exposition of the psychological scaling theory and methods by Thurstone was given. This included a sound psychological basis as well as a statistical one with the use and theory of maximum likelihood methods. Within the field known as signal detection theory, see e.g. [29] or [30], methods of this kind were further developed, originally with special emphasis on detecting weak visual or auditory signals. Further developments of such methods and their use within food testing and sensory science have developed over the last couple of decades with the numerous contributions of D. Ennis as a corner stone see e.g. [31]. In [32] it was emphasized and exploited that the thurstonian based statistical analysis of data from the basic sensory discrimination test protocols can be identified as generalized linear models using the inverse psychometric functions as link functions. With this in place, it is possible to extend and combine designed experimentation with discrimination/similarity testing and combine standard statistical modeling/analysis with thurstonian modeling. All this was implemented in the R-package *sensR*, cf [33]. So *sensR* now offers a complete tool for the planning and analysis of sensory discrimination and similarity experiments. The *sensR* package includes easily accessible tools for handling the six basic sensory test protocols: duo-trio, triangle, 2-AFC, 3-AFC, A-not A and Same-Different test. For all of these sensR provides:

- power and sample size calculations
- simulation
- hypothesis tests
- standard and improved (likelihood based) confidence intervals
- thurstonian analysis
- plotting features

In addition to this sensR currently offers:

- Analysis of A-not-A tests with or without sureness response
- ROC curve computations and plotting
- Signal Detection Theory (SDT) Computation of d-prime
- Beta-Binomial (standard and corrected) analysis for replicated data
- Replicated Thurstonian Model for discrimination analysis
- A link between standard statistical (regression/anova/ancova) modeling and thurstonian modeling.
- Simulation of replicated difference tests

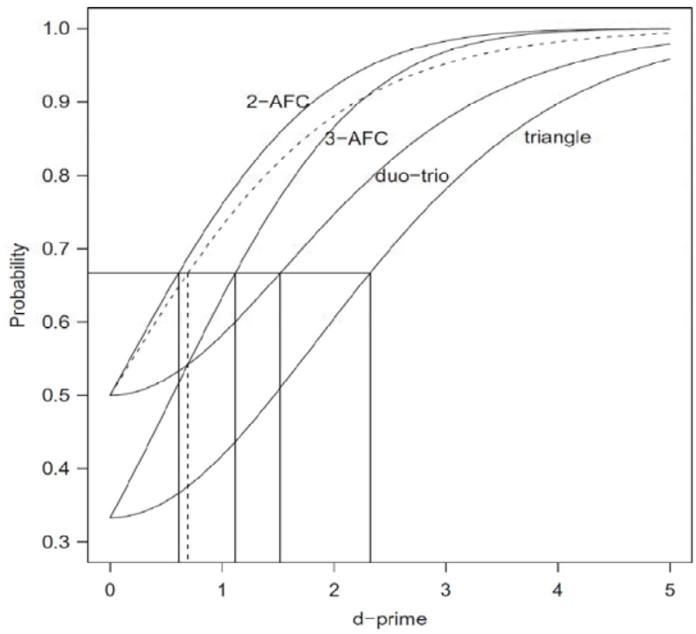

Fig. 1. The four psychometric functions used for the four basic testing protocols. The logistic link function is shown as the dashed curve. A response of 2/3 correct answer leads to four different estimates of sensory difference in the four different protocols (neither of which equals the logistic based estimate)

The basic idea from [32] is shown in Figure 1 illustrating the four basic psychometric functions together with the logistic link function. It is emphasized how a response of 2/3 correct answers has quite different interpretation depending on how the sensory testing protocol was actually carried out. Or expressed in more popular terms: The answer you get depends on the question you pose! The thurstonian modeling approach offers an approach to explicitly include the modeling of the question dependency into the data analysis framework. Linking this more to general statistical theory and methods than traditionally done in the literature offers an extended and improved toolbox of methods. This becomes evident, when turning to mixed effect versions of these models, which, as for the profile data above, becomes highly relevant to capture and model individual differences in such data. Due to the complexity of this challenge, these issues are still discussed in the sensory and sensometrics literature, and much more work is called for here. A friendly introduction to the analysis of the basic discrimination and similarity testing data is given in Chapter 8 in [10].

5 Other Types of Data

5.1 Ranking and ordinal data

Another commonly used sensory and consumer survey methodology is to use rankings or scoring on an ordinal scale. In [34] a general approach for non-parametric analysis based on orthogonal polynomial decompositions is presented. The methods are applicable in a variety of situations but were not well suited to handle ties in the data. In [35] a method is developed based on polynomials that are orthogonal with respect to the given tie structure that allows for ties in this kind of analysis. Among other things it is shown that the generalized decomposition of the Anderson χ-statistic for randomized block designs allowing for ties has a first component that equals the well known tie corrected version of the Friedman statistic. The second component is a novel tie corrected test for dispersion effects. This is an important aspect of consumer preference data as this may reflect segmentations in the population. In [36] and [37] this extended methodology is presented in a more applied oriented way. In [38] the methods are extended and exemplified for the incomplete block design setting. In [39] the methods are presented in a user friendly way to the sensory practitioner including a website with relevant R code (http://www2.imm.dtu.dk/stat/nonparametrics/).

The disadvantage of this classical nonparametric approach to such data is the lack of models and hence the lack of the ability to easily quantify the effects and their (proper) uncertainty including random effects of individuals. A model based approach is taken in [40] and [21]. The close link between certain Thurstonian models and well established statistical models are extended to these data and the consequence of including proper random effect models are illustrated. In the new R-package *ordinal*, cf. [41], likelihood based models for ordinal (ordered categorical) data based on cumulative probabilities are implemented in the framework of cumulative link (mixed) models. This includes the important proportional odds model but also allows for general regression structures for location as well as scale of the latent distribution, i.e. additive as well as multiplicative structures, structured thresholds (cut-points), nominal effects, flexible link functions and random effects.

5.2 Linking multivariate data

Another recurring issue is the relation of multivariate data sets, e.g. trying to predict sensory response by instrumental/ spectroscopic and/or chemical measurements. Similarly there is a wish to be able to predict how the market(consumers) will react to sensory changes in food products – then called Preference Mapping, [42]. This links the area closely to the chemometrics field and also naturally to the (machine) learning area. When analyzing consumer data a possible market segmentation is a key issue. So for relational models the so-called latent class regression models have been used frequently in market research. In [43] and [44] a `latent class random coefficient' regression model is formulated, handled and applied. It is a combination of the typical latent class regression model and the typical random coefficient model. Furthermore it is combined with principal component regression.

For such regression and/or correlation analyses often average sensory data is used. The issue of correcting for the ``measurement error'' of these averages is treated in [45], [46] and [47]. In [47] it is among other things described how simple F-test statistics can be used for the diagnostics and correction of measurement error in simple correlations in even rather complex settings.

One of the big challenges in the food industrial R&D process is the comparability/predictability of different levels of testing procedures/protocols applied throughout the development process – many of which may involve human perception. This goes from in house fast screening methods through more elaborate sensory evaluations to larger scale consumer surveys. A coherent theme is hence to develop methodology that can disentangle product differences from human differences, and jointly to be able to do so for data with multi-protocol origin. The multi-protocol data setup is a current research topic.

Another important open source tool for the analysis of sensory and consumer data is the the R-based SensoMiner, [48].

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