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A comparison of methods for analyzing multivariate sensory data in designed experiments – A case study of salt reduction in liver paste

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ABSTRACT

This paper presents a comparison of different methods for analyzing designed experiments. The methods used are based on PCA, PLS and ANOVA, used either separately or in combination. Special emphasis will be on how to obtain information about medium and less important factors in the presence of very dominating ones. It will be shown that this could be done by splitting the dataset in two. Our propositions will be illustrated on a data set obtained for studying the effect of salt reduction in liver paste.
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1. Introduction

Designed experiments play an important role when developing new products in industry. Typically one is interested in how different formulations and different process conditions influence the properties of end products. Such properties may be technological, health related or related to taste and odour. In most cases one is interested in several aspects of the output at the same time, i.e. one is interested in multivariate output data. In addition to improved insight one is typically also interested in optimizing the responses for the purpose of satisfying for instance consumer needs and wishes. The focus of the present paper is on a methodology for obtaining improved insight.

A number of different methods exist for analyzing multivariate output from designed experiments. The classical approach is multivariate analysis of variance (MANOVA, see e.g. Mardia, Kent, and Bibby (1979)) which provides tests of significance for the different input factors on the entire vector of responses. That is useful as a starting point, but provides little insight into correlation structures among the output variables and similarities and differences between the objects or samples in the study. A possible solution is to use PC-ANOVA (principal components-analysis of variance, see e.g. Ellekjær, Ilseng, and Næs (1996), Luciano and Næs (2009) and Næs, Brockhoff, and Tomic (2010)), which is based on first using principal component analysis (PCA) on multivariate response values followed by regular analysis of variance (ANOVA) on the first few components vs. the design. The main drawback of such an approach is that if the different design factors represent very different correlation structures among responses, the information in the first few components may be too complex. A possible remedy to that is to use the ASCA (analysis of variance – simultaneous components analysis, see e.g. Jansen et al. (2005)) method which reverses the two operations of ANOVA and PCA. The method first estimates the effects of the factors for each response variable using regular ANOVA parameter estimation and then uses a PCA on the individual effects matrices separately. The method provides plots that are easy to interpret, but more limited information on the significance of effects. A third possibility is to use partial least squares (PLS) regression of the response variables onto the design factors represented as dummy variables. This gives one score plot and two loadings plots, one for the responses and one for the design factors. Cross-validation can be used for assessing overall performance of the model, but more specific information about the significance of design factors on component scores is more difficult to obtain using this approach.

The purpose of this paper is to compare and discuss advantages and disadvantages of the approaches mentioned previously in a situation of product development in the food sector. In addition

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to discussing and comparing those established approaches, we will also propose a couple of new variants which may be useful. Focus will also be on how to obtain improved insight about effects of moderately important factors in the presence of very dominating ones. The case study presented is based on a designed experiment conducted for the purpose of investigating the effect of reducing salt content in liver paste without losing important sensory properties (based on sensory profiling). The design used is a full factorial design based on 16 combinations of 4 factors. Special focus will be on the salt content control factor and its possible interactions with other factors. Some replicates are also present and some attention will be given to how these can be used for assessing the validity of the sensory panel and the conclusions drawn.

2. Methodology

2.1. General framework

The response data matrix is here written as $\mathbf{Y}$. Columns represent the sensory variables and rows represent the experimental runs or products. The design matrix is denoted by $\mathbf{X}$. The $\mathbf{Y}$ matrix may as usual be seen as a function of the design matrix $\mathbf{X}$, $\mathbf{Y} = \mathbf{f}(\mathbf{X})$ plus a matrix of noise $\mathbf{E}$. Since the design considered is a two-level design, we will here only consider the linear model situation, i.e.

$$\mathbf{Y} = \mathbf{XB} + \mathbf{E} \tag{1}$$

In some cases we will also add interaction terms to the model, which corresponds to extending the $\mathbf{X}$ matrix with some additional columns. Although our focus is on factorial designs, some of the methods discussed here may be easily extended to other designs.

2.2. PC-ANOVA

The main analytical tools of PC-ANOVA are PCA and ANOVA (Ellekjær et al., 1996). The PCA is first run on all response variables $\mathbf{Y}$ or only on a subset of them if one is interested in a special focus. In this way one obtains scores $\mathbf{T}$ and loadings $\mathbf{P}$, which may be plotted and interpreted directly using standard scatter plots. Scores from the PCA model $\mathbf{Y} = \mathbf{TP}' + \mathbf{F}$, where $\mathbf{F}$ represents the residuals after a number of factors, are then used as dependent variables in an ANOVA model with $\mathbf{X}$ as independent variables ($\mathbf{T} = \mathbf{XA} + \mathbf{E}$). Note that one then has full freedom to define the ANOVA model according to which design that is underlying the study (included interactions), and the error structure that is the right one to use (split-plot, repeated measures etc.; see Luciano and Næs (2009)). Note also that all tools available in the regular ANOVA toolkit will be available here (LS-means, random effects, post hoc testing etc.). In particular in situations with many objects, the additional ANOVA step may be very useful to aid interpretation of the effects. If the two models are put together, one can write the result as a regular regression model (as model (1)) with $\mathbf{B} = \mathbf{AP}'$.

In Luciano and Næs (2009) it was also proposed to provide scores plots based on estimates of the parameters corresponding to the levels of the most interesting factors in order to highlight the factor effects in the same multivariate space as the raw data. Note that this is identical to first averaging all raw observation vectors for each of the actual design factor levels and then projecting these average vectors onto the space spanned by the principal components of the analysis of all the data. In the same paper it was also proposed to incorporate line segments associated with the principal component (PC) axes with a length indicating for instance the least significant differences (LSD's) or standard deviation of the random error. That can be very useful for assessing visually the importance of the effects seen in the plot. A sophisticated modification of the standard PC-ANOVA was proposed in Langsrud (2002). It is denoted 50/50 MANOVA and it is based on an interesting splitting of the information in both data blocks for the purpose of significance testing.

For handling replicates there are several possibilities. One is to incorporate all data in the PCA and also in the ANOVA, thus utilizing the extra data for improved precision (Myers and Montgomery, 1995). This will, however, lead to unbalanced models, possibly with repeated measurement error structure, and one needs to be more cautious in the analysis. If only few replicates are available, the improvement will be marginal. A better choice is to simply project the replicates onto the PCA space for the purpose of visually assessing the variation. The focus is then not on improved precision, but merely on information about the uncertainty in the measurements and experimentation.

The use of ANOVA on the scores also implicitly represents a type of validation of the PCA model. If some of the effects are clearly significant and the effects look reasonable, that supports the validity of the PCA model. Cross-validation (CV) is also sometimes used for validation of PCA models, but in small designed experiments with possibly unique samples the applicability of CV is questionable. In this case study, however, it seems that there is enough similarity between the objects to give reasonable CV results for the PCA. Another possibility for validation is the bootstrap or other randomization techniques such as permutation tests (Endrizzi, Gasperi, and M., 2014), but this will not be considered here.

An extra tool that should be mentioned is the use of passive variables in the analysis, in that design factors (dummy) and interactions are incorporated in the PCA, but in such a way that they are given very low weights. This means that they do not influence the analysis, but still play a meaningful role in the interpretation of the correlation loadings plot (Martens and Martens, 2001).

Standard ANOVA testing is based on certain assumptions on the residuals in order to give valid test results. These assumptions are never exactly fulfilled in sensory analysis, but often they are close enough to provide *p*-values that are good indications of the level of significance (see Næs et al. (2010)). Luciano and Næs (2009) show that normality assumptions may be better satisfied for the principal components than for the original variables.

The main advantages of this approach are its simplicity, that it provides several useful interpretation tools and also statistical tests. In addition, the results are easy to obtain in most statistical software packages.

2.3. ASCA related methods

The main advantage of ASCA (Jansen et al., 2005, 2008) as opposed to PC-ANOVA is that it can explicitly handle different correlation structures for different groups of design factors. If for instance the variation of $\mathbf{Y}$ associated with design factor(s) in $\mathbf{X}_1$ is completely different from the variation associated with design factor(s) in $\mathbf{X}_2$ (where the $\mathbf{X}_1$ and $\mathbf{X}_2$ together span the same space as $\mathbf{X}$), the regular PCA plot is a compromise of the two effects and then possibly difficult to interpret. The idea is then to switch the order of the operations, i.e. to use ANOVA to first estimate the effects in the model and then to use PCA for each of the effect matrices separately. In more detail, if the model is

$$\mathbf{Y} = \mathbf{X_1B_1} + \mathbf{X_2B_2} + \mathbf{E} \tag{2}$$

the first step is to estimate the coefficients $\mathbf{B}_1$ and $\mathbf{B}_2$ and then to use PCA for each of the effect matrices, $\mathbf{X}_1\hat{\mathbf{B}}_1$ and $\mathbf{X}_2\hat{\mathbf{B}}_2$ separately. This means that each $\mathbf{X}_i\hat{\mathbf{B}}_i$ is decomposed as $\mathbf{T}_i\mathbf{P}_i$ and the results plotted as usual. This method is also very flexible with respect to the model used, the error structure, etc. A similar procedure is proposed in Harrington et al. (2005) (see also Zwanenburg, Hoefsloot, Wester-

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