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PANCA: Panel concordance analysis

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ABSTRACT

This paper proposes panel concordance analysis (PANCA) as a tool for panel leaders to identify disconsensus between the panelists on the sensory attributes used. PANCA summarizes the sensory data ([products × panelists × replicates] × attributes) by a low-rank approximation which is penalized for disconsensus (disagreement) between the panelists. When all the panelists agree on the sensory attributes used, the disconsensus penalty will have a negligible effect. However, if the assumption of good consensus is not supported by the data, considerable residual errors will arise. Consequently, PANCA can be used to identify difficult sensory attributes or even poor/deviating panelists which requires further training or could call for an alternative data processing strategy. It is also demonstrated that PANCA can be used to apply a multivariate ANOVA decomposition like in ASCA (ANOVA simultaneous component analysis). Theory and applications are explained by means of a real-life example from industrial sensory practice.

1. Introduction

QDA®-panels (quantitative descriptive analysis) are frequently used in the food industry to obtain descriptive sensory profiles (e.g. flavour, texture, appearance) to support product development, manufacturing and communications. The descriptive sensory profiles are commonly obtained by computing (weighted) average profiles across panelists and replicates, assuming good mutual agreement between the panelists on the attributes used. Good agreement (consensus or concordance) can be achieved by extensive selection and training procedures and is one of the major reasons why QDA®-panels are often considered as expensive.

The last decade, a number of different methods for studying panel consensus have emerged in the literature. Brockhoff presented a parametric model which takes account of individual scaling and reproducibility differences (see Brockhoff & Skovgaard, 1994; Brockhoff, 1998). Kermit and Lengard (2006) proposed various performance metrics in descriptive sensory evaluations (a.o. assessor sensitivity, reproducibility, agreement and cross-over effects) and described some ANOVA models to estimate their effects. Other authors (see Naes & Risvik, 1996) suggested the use of unfolding methods (Tucker-1 type models) to study the different positions of the panelists in the descriptive space. Other authors from the same group proposed special diagnostic displays like the Eggshell (see Naes, 1998; Hirst & Naes, 1994), Manhattan and Hiding plots (see Dahl, Tomic, Wold, & Naes, 2008) to study panelist performances.

In this paper, a simple extension of principal component analysis (PCA) is proposed as a tool to identify panel disconsensus in QDA® with respect to the panelists and the sensory attributes used. The paper is structured as follows. First the theory of PCA and PANCA is explained and it is demonstrated how restrictions can be embedded in the PANCA objective function to penalize for panel disconsensus. Thereafter it is explained how PANCA can be extended with additional restrictions, for example to simultaneously control the disagreement between panelists and disagreement between products. The relationships between (extended) PANCA with methods like ASCA (see Smilde et al., 2006; Luciano & Naes, 2008) and soft-ASCA (see Westerhuis, Derks, Hoefsloot, & Smilde, 2007) are briefly explained and discussed. Finally, a practical example of PANCA is presented based on QDA®-data from industrial sensory practice and it is demonstrated how outlying panelists and suspect attributes can be identified.

2. Theory

2.1. PCA

Principal component analysis (PCA) is a well-known working horse in the sensory sciences to compute low-rank summaries of highly collinear QDA® data. The algorithmic details of this method have extensively been described elsewhere in Jollife (1986), Wold (1987), Jackson (1991) whereas good examples of QDA® applications with different data (unfolding) structures can be found in Brockhoff, Hirst, and Naes (1996, chap. 10), Qannari et al. (2000), Dahl et al. (2008). Consequently, the PCA objective function will

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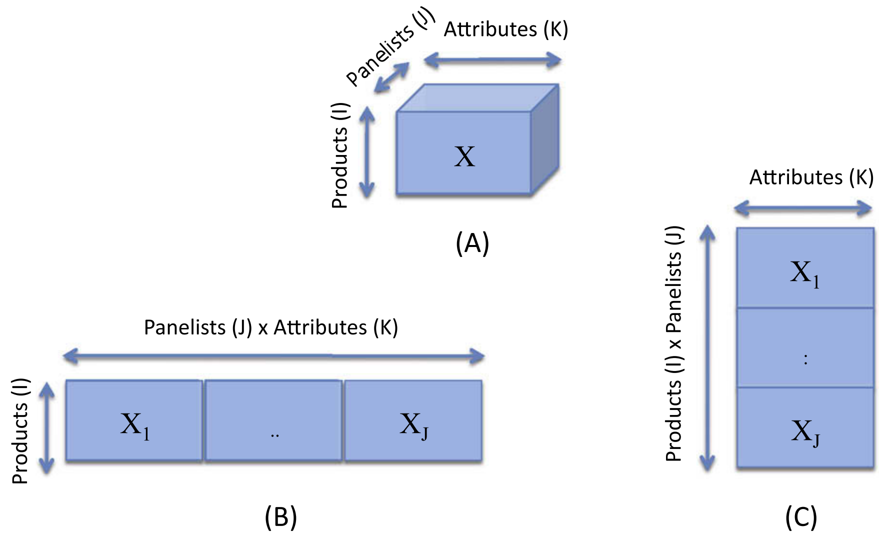

Fig. 1. Unfolding of three-way QDA® data into bilinear substructures.

only be defined here very briefly as it constitutes the theoretical framework for PANCA.

In short, PCA tries to explain maximum variance in $\mathbf{X}$ (typically structured as I products versus K attributes or I products $\times J$ panelists versus K attributes) by minimizing the residuals between estimated and real data

$$\min\left(\|\mathbf{X}-tp'\|^2\right) \tag{1}$$

for the first r principal components ($r < K$). The vectors t represent the scores and p' the normalized loadings (i.e. $p'p = 1$). In QDA®-applications, the scores commonly represent the products and/or assessors (depending how the data are structured) whereas the loadings are commonly used to represent the sensory attributes. The successive r components can simply be computed by deflation ($\mathbf{X} = \mathbf{X} - tp'$) like in NIPALS, preserving the orthogonal base ($\mathbf{P}'\mathbf{P} = \mathbf{I}$). Naturally, the scores and loadings can also more efficiently be computed by a direct singular value decomposition but the NIPALS approach has been favored here as it was also used for PANCA, as shown in the following section.

2.2. PANCA

PANCA can be considered as PCA on unfolded QDA® data restricted by a panel disconsensus penalty. When there actually is high consensus between the panelists, the disconsensus penalty will have a negligible effect on the total sum of squares. However, if the assumption of good consensus is not supported by the data, residuals will arise for the sensory attributes of interest. Consequently PANCA provides convenient means to identify sensory specific disconsensus. This information can be used by panel leaders to decide on next training strategies.

There are different ways to unfold the QDA® data into bilinear substructures which also has consequences for the organization of the disconsensus penalty and the way PANCA needs to be applied. Fig. 1 shows how the three-way dataset $\mathbf{X}_{IJK}$ can be reshaped into $\mathbf{X}_{I\times JK}$ in which the J panelists have the I products in common or into $\mathbf{X}_{IJ\times K}$ in which the J panelists have the K sensory attributes in common. These bilinear data structures were introduced by Brockhoff et al. (1996, chap. 10) as common scores and common loading unfolding for Tucker-1 type models. As argued in Brockhoff et al. (1996, chap. 10), the choice for the unfolding method depends on the assumptions one is willing to make about the data. For example, it is often observed in practice that common scores structures are used for similar purposes as for generalized procustes analysis (GPA) (see Gower, 1975; Dijksterhuis, 1996) like in flavour language studies and expert comparisons (see Derks, Westerhuis, Smilde, & King, 2003) for which it is assumed that the different evaluators have a similar latent sensory perception but differ in the way they express what they perceive due to insufficient training or different (flavour) language. On the other hand, for the common loading structure it is often assumed that QDA® panelists are highly trained and should have a similar understanding about the sensory attributes used and that the differences should mostly be assigned to individual and product differences and not to a lack of sensory specificity. In this paper, the common loading unfolding was applied for the arguments described above, i.e. dealing with a QDA® panel. However, as suggested by one of the reviewers it is also outlined how PANCA can be applied with common products unfolding and how the results could be interpreted.

2.3. PANCA and common attributes unfolding

Common attributes unfolding (see Fig. 1C) reshapes the QDA® dataset $\mathbf{X}_{IJK}$ into the bilinear structure $\mathbf{X}_{(I\times J)\times K}$, where I, J and K represent the number of products, panelists and sensory attributes, respectively. For convenience it is assumed here that $\mathbf{X}_{IJK}$ was already averaged across replicates.

The PANCA objective function for common products unfolded data is defined in Eq. (2). The first term on the left handside can be recognized as the PCA objective function. The second term on the right handside represents the disconsensus penalty which is organized as the sum of squared differences of assessors j to the panel mean, excluding[1] assessor j. For low values of λ, Eq. (2) resembles PCA, i.e. explaining maximum variance, whereas for high values for λ the scores are directed to minimize the within group variance for panelists as well. If there is good panel consensus, the disconsensus penalty wil hardly affect the first term (PCA-fit). On the other hand the explained variance will reduce significantly for each attribute with poor panel consensus.

$$\min\left(\|\mathbf{X}-tp'\|^2+\lambda\sum_j\|t_j-\bar{t}_{/j}\|^2\right) \tag{2}$$

Eq. (2) can be simplified by the introduction of a difference matrix Δ which simplifies Eq. (2) into

[1] The backslash symbol is used as exclusion operator.