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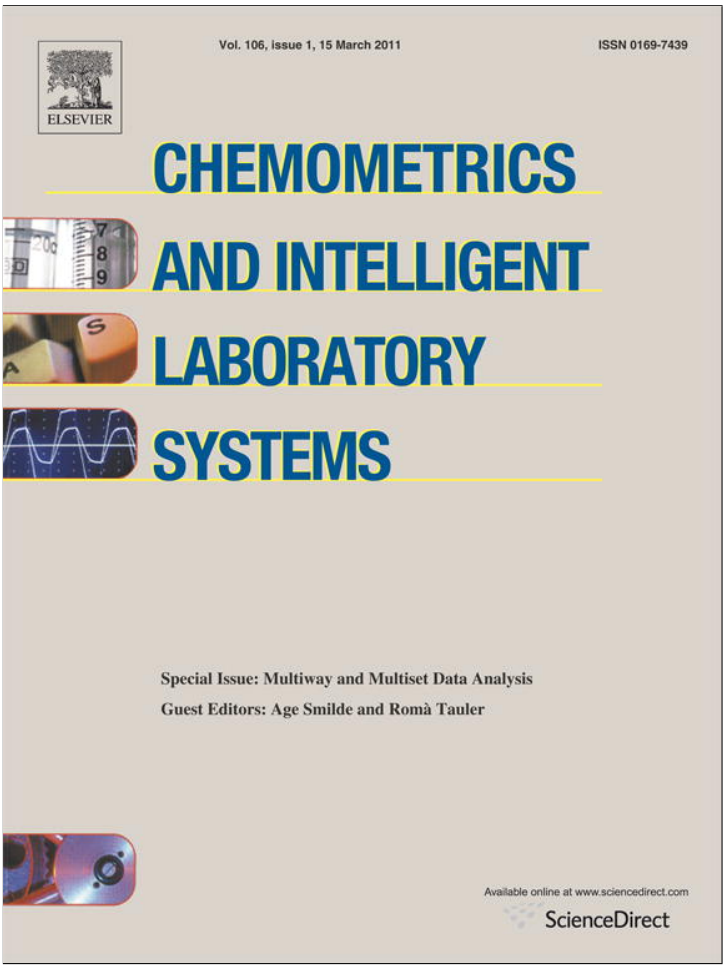

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The CHull procedure for selecting among multilevel component solutions ☆

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ABSTRACT

Recently, Timmerman [1] proposed a class of multilevel component models for the analysis of two-level multivariate data. These models consist of a separate component model for each level in the data. Specifically, the between-differences are captured by a between-component model and the within-differences by a within-component model. Within the class of multilevel component models a number of variants can be distinguished. These variants differ with respect to the within-component model, in that different sets of restrictions are imposed on the within-component loadings and on the variances and correlations of the within-component scores. The following question then may be raised: given a specific two-level data set, which of the multilevel component model variants should be selected, and with how many between- and within-components? We address this question by proposing a model selection procedure that builds on the CHull heuristic of Ceulemans and Kiers [2,3]. The results of an extensive simulation study show that the proposed CHull heuristic succeeds very well in assessing the number of between- and within-components. Tracing the underlying multilevel component model variant is more difficult: Whereas differences in within-loading matrices and differences in variances are very easy to detect, the precise correlational structure of the within-components is much harder to capture.

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1. Introduction

In many research domains, multilevel multivariate data are encountered. For instance, in sensometric research, panelists are asked to rate food samples on a number of descriptor variables (e.g., [4]). Such studies yield food samples by panelist data, with the food samples (level 1) being nested within the panelists (level 2). As another example, in contextualized emotion psychology, one gathers information about the emotions that people experience in different situations or on randomly selected time points during the day (e.g., [5]). This way, multilevel data are obtained in that the measurement occasions (level 1) are nested within the persons (level 2). In this paper, we limit ourselves to multilevel data with two levels. In what follows, the level 2 units will be denoted by 'subjects' and the level 1 units by 'measurement occasions'.

Given two-level multivariate data, one often wants to gain insight into the latent processes underlying the data. Analyzing such data, it is important to take the multilevel structure of the data into account, as the data may be driven by different processes at the different levels. For instance, in sensometric research, one is interested in capturing individual differences between panelists, where the panelists may on the one hand have different offsets for the descriptor variables — differences at level 2 — , and on the other hand may perceive the separate food samples differently — differences at level 1. Moreover, the interrelations of the variables may be completely different at levels 1 and 2. For instance, in contextualized emotion research, some authors claim that, whereas positive and negative emotions are independent across subjects (level 2), these emotions are negatively related across the measurement occasions of a single subject (level 1; [5]).

To reveal the mechanisms that drive the data at the different levels, Timmerman [1] proposed a class of multilevel component models. These models consist of a separate component model for each level in the data, which summarizes the most important differences between the observations at that level by reducing the variables to a few components. Specifically, the differences between the subjects are captured by a between-component model and the differences within the data of each subject by a within-component model.

Within the class of multilevel component models a number of variants can be distinguished. These variants differ with respect to the within-component model, in that different sets of restrictions are imposed on the within-component loadings, and on the correlations and the variances of the within-component scores. The restrictions on the within-component loadings are useful to find out whether or not the same set of within-components underlies the data of the different subjects. The restrictions on the variances and the correlations of the within-component scores are imposed to detect similarities among

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[1] The cheese data can be downloaded from http://www.models.kvl.dk/research/data/.

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individuals in stability across measurement occasions and in correlations between within-components, respectively. Multilevel component analysis has proved to be useful in a wide range of applications, such as cross-cultural psychology [6], functional genomics [7], social psychology [8], developmental psychology [9], and process control [10].

Applying multilevel component analysis in practice, it is usually unclear beforehand which model variant with which number of between- and within-components should be fitted to the data. In most cases, this uncertainty is dealt with by fitting the different model variants with varying numbers of between- and within-components. Subsequently, one looks for a solution that is well interpretable and yields a good description of the data at hand, without being overly complex. As it is very time consuming to assess the interpretability of all the different solutions, it is desirable to have a formal model selection criterion to find the solution with an optimal balance between goodness-of-fit and complexity. Subsequently, it can be verified whether the retained solution is well interpretable.

Up to now, the model selection criterion that is almost always used in multilevel component analysis is a generalization of the well-known scree test [11]. Specifically, one visually inspects a plot with the number of between- or within-components of the solutions on the X-axis and a measure of their goodness-of-fit on the Y-axis. At the within-level, it is common to first select the number of within-components and then, given the selected number of within-components, the specific model variant. The choices between different numbers of within-components and different model variants are thus made successively, whereas, obviously, these choices are interrelated. Indeed, the complexity of models increases both with the number of components and with a decrease in constraints on the model. Thus, an important disadvantage of this model selection method is that the restrictiveness of the different multilevel component analysis variants is not properly taken into account.

In this paper, we will present a formal model selection procedure in which the differences in restrictiveness between the different models are reflected in the complexity measures of the obtained solutions. Specifically, building on the work of Ceulemans and Kiers [2,3] for the related family of three-mode component analysis models, we propose a numerical convex hull based model selection (CHull) procedure, which selects the solution with the best balance between goodness-of-fit and a complexity measure. This complexity measure equals the number of free parameters, corrected for the number of observations. In this procedure, more restrictive model variants will yield solutions with a lower number of free parameters than less restrictive variants. The performance of the proposed model selection procedure is systematically evaluated in a simulation study.

The remainder of this paper is organized as follows: In Section 2, the class of multilevel component analysis models is recapitulated. In Section 3, we discuss the CHull procedure. Subsequently, we show how this procedure can be used to select among the different multilevel component analysis variants and to establish the appropriate number of between- and within-components. In Section 4, the performance of the CHull procedure is evaluated by means of an extensive simulation study. Section 5 illustrates the use of the CHull procedure by applying it to a sensory profiling data set. Finally, Section 6 contains some concluding remarks.

2. Multilevel component analysis and multilevel simultaneous component analysis

As stated in the Introduction, the class of multilevel component models can be used to analyze a two-level data matrix **X**. Because of the hierarchical structure of the data — observations being nested within individuals, **X** consists of I data matrices $\mathbf{X}_i$ ($K_i \times J$), which contain the observed scores x_{ijk_i} of individual i ($i = 1...I$) on variable j ($j = 1...J$) at measurement occasion k_i ($k_i = 1... K_i$).

All multilevel component models yield separate component models for the between- and within-parts of the data. The between-model capture the differences among the I individuals and the within-model the differences among the measurement occasions of each individual. The different variants of multilevel component analysis differ only with respect to the restrictions that are imposed on the within-model.

In the remainder of this section, we first introduce the least restrictive variant, multilevel component analysis (MCA), followed by four more restricted variants (MSCA). Note that in the original publications, the models are called MLCA and MLSCA, respectively; however, in this paper we adopt the nomenclature used in [7]. Finally, we briefly discuss how the models are fitted.

2.1. The MCA model

The MCA model decomposes each of the I data matrices $\mathbf{X}_i$ as follows:

$$\mathbf{X}_i = \mathbf{1}_{K_i}\mathbf{m}' + \mathbf{1}_{K_i}\mathbf{f}_i^b B^{b'} + \mathbf{F}_i^w \mathbf{B}_i^{w'} + \mathbf{E}_i, \quad (1)$$

where $\mathbf{1}_{K_i}$ is a $K_i \times 1$ vector of which each element is set to 1, $\mathbf{m}$ ($J \times 1$) contains the offsets of the J variables across all measurement occasions of all individuals, $\mathbf{f}_i^b$ ($1 \times Q_b$) is the i-th row of the $I \times Q_b$ between-component scores matrix $\mathbf{F}^b$, $\mathbf{B}^b$ ($J \times Q_b$) denotes the between-loading matrix, $\mathbf{F}_i^w$ ($K_i \times Q_{wi}$) denotes the within-component scores matrix of individual i, $\mathbf{B}_i^w$ ($J \times Q_{wi}$) denotes the within-loading matrix of individual i, and $\mathbf{E}_i$ ($K_i \times J$) denotes the matrix of residuals. Finally, Q_b is the number of between-components and Q_{wi} the number of within-components of subject i. For identification purposes it is required that the mean between-component scores across all measurement occasions and subjects are zero, thus

$$\sum_{i=1}^{I} K_i \mathbf{f}_i^b = \mathbf{0}', \quad (2)$$

and the mean within-component scores across the measurement occasions per subject are zero, i.e.,

$$\sum_{k_i=1}^{K_i} \mathbf{f}_{k_i}^w = \mathbf{0}', \quad (3)$$

with $\mathbf{f}_{k_i}^w$ the k_i^{th} row of $\mathbf{F}_i^w$. The latter constraints are sufficient to ensure that the offset term, the between-part and the within-part of the model are uniquely separated. Moreover, these restrictions imply that the MCA model reconstructs the data in an ANOVA-like way by summing terms that model the overall means ($\mathbf{1}_{K_i}\mathbf{m}'$), the deviations of the subjects from these overall means $\left(\mathbf{1}_{K_i}\mathbf{f}_i^b\mathbf{B}^{b'}\right)$ and the deviations of the measurement occasions from the subject means $\left(\mathbf{F}_i^w\mathbf{B}_i^{w'}\right)$.

Note that the between-loading matrix $\mathbf{B}^b$ as well as the within-loading matrices $\mathbf{B}_i^w$ has transformational freedom. Specifically, $\mathbf{B}^b$ and $\mathbf{B}_i^w$ may be orthogonally or obliquely transformed without changing the fit of the model, provided that such transformations are compensated for in the component score matrices $\mathbf{F}^b$ and $\mathbf{F}_i^w$, respectively.

2.2. Four MSCA models

Applying MCA as formalized in Eq. (1) can be rather problematic in practice, as it yields a different set of within-components for each individual i. Comparing these different sets of components is burdensome, unless the number of individuals under study is very small. As a way out, Timmerman [1] proposed multilevel simultaneous component analysis (MSCA) in which the within-loading

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Table 1
The restrictions that are imposed by the four MSCA variants on the correlations and the variances of the within-component scores of the individuals.

MSCA variant	Correlations	Variances
MSCA-P	Free	Free
MSCA-PF2	Equal across individuals	Free
MSCA-IND	Equal to 0	Free
MSCA-ECP	Equals across individuals	Equal across individuals

matrices $\mathbf{B}_i^w$ of the individuals are restricted to be the same. Specifically, the decomposition rule of an MSCA model reads

$$\mathbf{X}_i = \mathbf{1}_{K_i}\mathbf{m}' + \mathbf{1}_{K_i}\mathbf{f}_i^b\mathbf{B}^{b'} + \mathbf{F}_i^w\mathbf{B}^{w\prime} + \mathbf{E}_i, \quad (4)$$

where $\mathbf{B}^w$ ($J \times Q_w$) denotes the within-loading matrix that is shared by all individuals. For identification purposes, the variance across all the measurement occasions of the I individuals of each within-component is set to 1. In case the data are standardized across subjects and measurement occasions (i.e., across the columns of $\mathbf{X}$), a nice consequence of this restriction is that the between-loadings and the within-loadings can be interpreted as correlations between the variables and the components, provided that the associated between- and within-component scores are orthogonal to each other.

To gain further insight into the individual differences in the mechanisms that underlie the data, Timmerman [1] made a further distinction between four MSCA variants, which differ with respect to the constraints that are imposed on the variances and correlations of the within-component scores in the matrices $\mathbf{F}_i^w$. As can be read from Table 1, the least restrictive variant, which is called MSCA-P, imposes no constraints on the within-component matrices. Next, in MSCA-PF2, the variances of the component scores may differ across individuals, but the correlations are restricted to be the same. MSCA-IND is even more restrictive in that the correlations of the component scores must be zero for each individual. Finally, MSCA-ECP leaves no room for individual differences in the variances or correlations of the within-component scores. To understand how these restrictions shed light on the individual differences in the underlying mechanisms, it is instructive to consider a study in which subjects are asked to indicate which emotions they experience at a number of time points. If one assumes that emotions can be organized in a two-dimensional Valence-Arousal space, applying MSCA-P implies that one expects that people vary in how stable their emotions are across time (i.e., the variances vary across people): whereas some people always feel happy or sad, others are less stable. Moreover, with MSCA-P, the correlation between the valence and arousal dimensions may differ across subjects: whereas for some people feeling more positive implies that they are more aroused, for others it is the other way around. In contrast, fitting MSCA-ECP would imply that one assumes that all subjects are equally stable across time and are characterized by identical valence–arousal relations. For a more extensive discussion of the interpretation of these four MSCA variants we refer to Timmerman and Kiers [12] and to Timmerman et al. [9].

Just as in MCA, the between-components of an MSCA solution can be freely rotated. Whether or not the within-components can be rotated depends on the particular MSCA variant: Whereas the within-loading matrices $\mathbf{B}^w$ of MSCA-P and MSCA-ECP solutions have transformational freedom, the within-loading matrices of MSCA-PF2 and MSCA-IND solutions are essentially unique, implying that the within-components can be permuted and reflected only (see [12], for uniqueness conditions).

2.3. Fitting MCA and MSCA models

To obtain a multilevel component solution with given numbers of between- and within- components for a data matrix $\mathbf{X}$, one may use the algorithms that were proposed by Timmerman [1]. These algorithms minimize the sum of squares of the residual matrices $\mathbf{E}_i$ across the I subjects ($i = 1,\ldots,I$) in Eqs. (1) and (4). As proven in [1], the between- and within-model estimation problems can be solved independently, because the between- and within-parts of the model are mutually orthogonal. Specifically, the parameters of the between- and within-models can be estimated by performing a regular PCA on $\mathbf{X}^b$ and simultaneous component analysis (SCA) on $\mathbf{X}^w$, where the $\mathbf{X}_i^b$ and $\mathbf{X}_i^w$ matrices of subject i are defined as $\mathbf{X}_i^b = \mathbf{1}_{K_i}\mathbf{m}_i'$ and $\mathbf{X}_i^w = \mathbf{X}_i - \mathbf{1}_{K_i}\mathbf{m}_i'$, with $\mathbf{m}_i$ containing the J variable means of subject i.

The fit of an estimated model to the observed data can be expressed as the percentage of variance of the observed data that is accounted for, called *VAF* in the following. The *VAF* can be computed as follows:

$$VAF = 100\left(1 - \frac{\sum_{i=1}^{I}\|\mathbf{E}_i\|^2}{\sum_{i=1}^{I}\|\mathbf{X}_i\|^2}\right). \quad (5)$$

Moreover, the between- and the within-parts of the model being orthogonal, a further distinction can be made between the percentage of variance of the between-part of the data that is accounted for by the between-model, called VAF^b, and analogously the percentage of variance of the within-part that is accounted for, called VAF^w [7]. Specifically, VAF^b and VAF^w can be computed as

$$VAF^b = 100\left(\frac{\sum_{i=1}^{I}\|\mathbf{1}_{K_i}\mathbf{f}_i^b\mathbf{B}^{b'}\|^2}{\sum_{i=1}^{I}\|\mathbf{X}_i^b\|^2}\right) \quad (6)$$

and

$$VAF^w = 100\left(\frac{\sum_{i=1}^{I}\|\mathbf{F}_i^w\mathbf{B}^{w\prime}\|^2}{\sum_{i=1}^{I}\|\mathbf{X}_i^w\|^2}\right). \quad (7)$$

3. The CHull model selection heuristic

In this section, we first recapitulate the general principle of the CHull model selection heuristic, which formalizes the visual inspection based model selection procedure proposed by Kroonenberg [13,14]. Subsequently, we discuss how this CHull heuristic can be used to select among multilevel component solutions that differ with respect to variant used, and the numbers of between- and within-components. Because the between- and within-parts of the model are estimated independently, the appropriate models for the between- and within-parts can be determined independently. We will first explain how the CHull heuristic can be used to decide upon the appropriate number of between-components. Next, it will be discussed how to select the appropriate model for the within-part of the data, that is, the model variant and the number of within-components.

3.1. General principle

The CHull heuristic [2,15] is based on the same principle as the scree test [11], namely that a model should have an optimal balance of fit and complexity: Considering a scree-like plot with on the Y-axis a measure of the goodness-of-fit (e.g., *VAF*) of the solutions amongst which one wants to choose, and on the X-axis a measure of their complexity (e.g., degrees of freedom or number of free parameters), solutions that are on or close to an elbow in the higher boundary of the convex hull of this plot are favoured (see also [13,14]). The CHull

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heuristic has been shown to be a powerful tool for solving diverse complex model selection problems: promising results were reported for hierarchical classes analysis [15], three-mode component analysis [2,3], and two-and three-mode partitioning [16].

Given the complexity-value c and goodness-of-fit-value f of all solutions from which one wants to choose, the CHull method can be summarized in seven steps (see [2] for a more extensive description). The first five steps serve to find the solutions on the higher boundary of the convex hull:

1. If a number of solutions have an identical complexity-value c, retain only the best fitting solution.
2. Sort the n retained solutions by their complexity values c from least to most complex and denote them by s_i ($i=1\ldots n$).
3. Exclude all solutions s_i for which a solution s_j ($j<i$) exists such that $f_j>f_i$.
4. Consecutively consider all triplets of adjacent solutions: Exclude the middle solution if its point is located below or on the line connecting its neighbours in a fit-value f versus complexity-value c plot.
5. Repeat Step 4 until no solution can be excluded anymore. The remaining ñ solutions, which are denoted by $\tilde{s}_i$ ($i=1\ldots\tilde{n}$) all lie on the higher boundary of the convex hull.

To find the solution after which the increase in fit levels off, in the sixth step the *st*-values of the obtained 'hull' solutions $\tilde{s}_i$ are computed, with

$$st_i = \frac{f_i - f_{i-1}}{c_i - c_{i-1}} \Big/ \frac{f_{i+1} - f_i}{c_{i+1} - c_i}. \quad (8)$$

As the numerator and denominator of (8) refer to the slope of two adjacent pieces of the higher boundary of the convex hull, a relatively large *st*-value indicates that the solution of complexity c_i fits the data considerably better than the solution of complexity c_{i-1}, whereas the fit values of the solutions of complexity c_i and c_{i+1} differ much less. Finally, in the seventh step, the solution $\tilde{s}_i$ with the highest *st*-value is selected. For this solution, the angle between the two adjacent pieces of the higher boundary of the convex hull is relatively small, but not necessarily the smallest (i.e, small values in the denominator of Eq. (8) will also lead to relatively high *st*-values, even if the corresponding angle is not the smallest). The use of the CHull heuristic will be further illustrated in Section 5.

Note that in practice it is wise to consider models close to the higher boundary as important alternative models, as well as models with a high but not maximal *st*-value [2]. Indeed, the subjects and/or the measurement occasions are often considered to be a random sample from a population; yet, small changes in the data may alter the order of the *st*-values. Moreover, models are often an approximation to, rather than a complete reflection of phenomena present in reality. Hence, when selecting a final model, one should also take substantive considerations into account.

3.2. Fit- and complexity values of MCA and MSCA solutions

To use the CHull heuristic to select among MCA and MSCA solutions, we have to select measures to indicate the goodness-of-fit and the complexity of the between- and within-parts of the solutions under consideration. As a goodness-of-fit measure, we consider the variance accounted for. Specifically, we use VAF^b for the between-part and VAF^w for the within-part. The complexity of the solutions will be quantified by the number of free parameters with a correction for the number of observations involved.

In the following paragraphs, we discuss the number of free parameters in the models for the between- and within-parts and propose three possible strategies for correcting for the number of observations, yielding three complexity definitions for the between-part as well as the within-part.

3.2.1. Three complexity definitions of the between-part of the model

The number of free parameters of the between-part of the multilevel component solutions is denoted as fp^b. Because the between-solutions are regular PCA solutions, one can verify that these fp^b-values amount to $IQ_b + JQ_b - Q_b^2 - Q_b$ (see [17]). Specifically, the total number of parameters is $IQ_b + JQ_b$. From this number we have to subtract Q_b^2, because we may fix a $Q_b \times Q_b$ block of elements in $\mathbf{B}^b$ (i.e., we can always transform the obtained solution without loss of fit into a solution with thus fixed elements) and we have to subtract Q_b because we can always fix Q_b elements in $\mathbf{F}^b$ due to the constraint in Eq. (2).

In the present paper, we further consider three strategies for correcting the number of free parameters for the number of observations, which equals the number of subjects I for the between-part, yielding the following three definitions of complexity:

- c_1: complexity equals the number of free parameters, hence $c_1 = fp^b$
- c_2: complexity equals the number of free parameters, with I replaced by $\min(I,J)$, hence $c_2 = \min(I,J)Q_b + JQ_b - Q_b^2 - Q_b$
- c_3: complexity equals the number of free parameters, with I replaced by $\min(I,\ln(I)J)$, hence $c_3 = \min(I,\ln(I)J)Q_b + JQ_b - Q_b^2 - Q_b$.

The first definition, in which the number of observations is not corrected for, may seem the most obvious one, but for the following reasons, we introduced the other two definitions as well. The second complexity definition is based on the argument that in case the number of subjects I is larger than the number of variables J, the number of free parameters would overstate the complexity of the model. This is so because the data set can be reduced to a smaller data set that can be modeled equally well, in that exactly the same fit values will be obtained. That is, for regular PCA solutions, it can be shown that, if the number of observations I is larger than the number of variables J, the loss function value $\|\mathbf{X} - \mathbf{FB}'\|^2$ is equal to $\|\mathbf{R} - \mathbf{UB}'\|^2$, where $\mathbf{R}$ is the matrix of order $J \times J$ that is obtained from computing the QR decomposition of $\mathbf{X}$, and $\mathbf{U}$ is a matrix of order $J \times Q$. Thus, in such cases a data matrix of order $J \times J$ exists that will lead to exactly the same series of fit values. Therefore, one could say that a better measure for the complexity-value of the model is that in which the size of the data is considered to be $J \times J$. Hence, in our second definition of complexity, I is replaced by $\min(I,J)$.

The rationale for the third complexity definition is as follows. In cases where $I>J$, the second definition completely ignores the number of observations. As is done in the Bayesian Information Criterion literature (BIC, [18]), one might argue however that the complexity of a model always increases when more observations are involved, but slower than linearly. A reasonable choice is then to replace I by $\ln(I)J$. However, if the number of observations I is smaller than $\ln(I)J$, this choice gives more weight to the number of observations rather than correcting for them. Therefore, in the third complexity definition, I is replaced by $\min(I,\ln(I)J)$.

3.2.2. Three complexity definitions of the within-part of the model

Before giving our complexity definitions of the within-part of the model, we first describe the number of free parameters fp^w of the within-part of the multilevel component solutions for the different model variants. We will discuss the different model variants from the least to the most constrained:

- For an MCA solution, the number of free within-parameters fp^w equals $\sum_{i=1}^{I}\left[K_i Q_{wi} + JQ_{wi} - Q_{wi}^2 - Q_{wi}\right]$, where the third term corrects for the transformational freedom of the I within-loading matrices $\mathbf{B}_i^w$ and the fourth term for the restriction on the within-component scores that is imposed by Eq. (3).
- For an MSCA-P solution, the value of fp^w equals $KQ_w + JQ_w - Q_w^2 - IQ_w$, with $K = \sum_{i=1}^{I} K_i$ and with the last two terms accounting for the transformational freedom of the within-loading matrix $\mathbf{B}^w$ and for the restriction in Eq. (3), respectively.

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- For an MSCA-PF2 solution, fp^w amounts to $KQ_w + JQ_w - (I+1)Q_w - (I-1)\frac{Q_w(Q_w-1)}{2}$, where the third term corrects for Eq. (3) and for the restriction that the variances of the within-component scores equal 1; the fourth term corrects for the equality restriction on the correlations of the within-component scores (thus, e.g., the correlations of individual $i=2...I$ have to equal those of the first individual).
- An MSCA-IND solution has fp^w-values of $KQ_w + JQ_w - (I+1)Q_w - I\frac{Q_w(Q_w-1)}{2}$, because for all individuals the correlations of the within-component scores are restricted to equal zero.
- Finally, for MSCA-ECP solutions, the fp^w-values equal $KQ_w + JQ_w - (I-1)Q_w - (I-1)\frac{Q_w(Q_w-1)}{2} - Q_w^2 - IQ$. The third and fourth terms respectively take the equality restrictions on the variances and the correlations of the within-component scores of the individuals into account (i.e., the variances and correlations of individual $i=2...I$ are restricted to equal those of the first individual); the last two terms correct for transformational freedom and for the restriction in Eq. (3), respectively.

In this paper, these numbers of free within-parameters for the different variants are further corrected for the number of observations K_i per subject. Using the same modification strategies as in Section 3.2.1, we obtain the following three definitions of complexity:

- c_1: complexity equals the number of free within-parameters, hence $c_1 = fp^w$
- c_2: complexity equals the number of free within-parameters, with K_i replaced by $\min(K_i J)$
- c_3: complexity equals the number of free within-parameters, with K_i replaced by $\min(K_i, \ln(K_i)J)$

4. Simulation study

To assess how well the proposed CHull procedure succeeds in indicating the correct multilevel component variant and the number of between- and within-components in a range of conditions, a simulation experiment was performed. Moreover, we were interested in which of the three considered CHull strategies (i.e., employing the three discussed complexity definitions) yields the best performance.

4.1. Design

In this study, the population offsets ($\mathbf{m}$) were fixed to zero. Each simulated data matrix $\mathbf{Xsim_i}$ for the i-th subject was created as follows:

$$\mathbf{Xsim}_i = \mathbf{1}_{K_i}\mathbf{f}_i^b\mathbf{B}^{b'} + \mathbf{F}_i^w\mathbf{B}_i^{w'} + \mathbf{E}_i,$$

where the between-component scores in $\mathbf{f}_i^b$ and the residuals in $\mathbf{E}_i$ were sampled from a standard normal distribution and the within-component scores in $\mathbf{F}_i^w$ were sampled from a multivariate normal distribution. The number of variables was fixed to 12. In all but one condition, the between-loadings in $\mathbf{B}^b$ and the within-loadings in $\mathbf{B}_i^w$ were constructed to be optimally simple in terms of the Varimax criterion (see below). For instance, if Q_b equals 3 and Q_w equals two, the MSCA $\mathbf{B}^b$ and $\mathbf{B}^w$ matrices were constructed as follows:

$$\mathbf{B}^b = \begin{bmatrix} c_b & 0 & 0 \\ c_b & 0 & 0 \\ c_b & 0 & 0 \\ c_b & 0 & 0 \\ 0 & c_b & 0 \\ 0 & c_b & 0 \\ 0 & c_b & 0 \\ 0 & c_b & 0 \\ 0 & 0 & c_b \\ 0 & 0 & c_b \\ 0 & 0 & c_b \\ 0 & 0 & c_b \end{bmatrix} \text{ and } \mathbf{B}^w = \begin{bmatrix} c_w & 0 \\ c_w & 0 \\ c_w & 0 \\ c_w & 0 \\ c_w & 0 \\ c_w & 0 \\ 0 & c_w \\ 0 & c_w \\ 0 & c_w \\ 0 & c_w \\ 0 & c_w \\ 0 & c_w \end{bmatrix},$$

where c_b and c_w are constants, chosen such that the proportion of structural variance that is contributed by the between- and within-parts of the simulated data was kept fixed at .20 and .80, respectively.

The following seven factors were fully crossed:

1. the underlying model variant and the specification of the variances and correlations of the within-components, at thirteen levels. Two levels pertain to MCA, one level to MSCA-ECP, two levels to MSCA-IND, four levels to MSCA-PF2, and four levels to MSCA-P.
   - *MCA.* Whereas the within-loading matrices are randomly sampled between −1 and 1 in the first MCA condition, the second MCA condition implies that the subjects fall apart into two equal-sized clusters which are characterized by different within-loading matrices displaying simple structure.
   - *MSCA-IND.* In these two conditions we manipulated the extent to which the variance of the within-component scores differs across the subjects: specifically, the variances of the within-component scores are uniformly sampled between .5 and 1.5 and between .25 and 1.75, respectively.
   - *MSCA-PF2.* The four MSCA-PF2 conditions are obtained by crossing the extent to which the variances of the within-component scores differ across the subjects (see MSCA-IND) with the strength of the correlations between the within-component scores; these correlations are set to .25 and .50, respectively.
   - *MSCA-P.* Finally, in the four MSCA-P conditions the variances of the within-component scores are again uniformly sampled between .5 and 1.5 or between .25 and 1.75, and the extent to which the correlations between the within-component scores differ across the subjects is manipulated by uniformly sampling these correlations between −.25 and .25 and between −.50 and .50, respectively.
2. the sampling scheme, at three levels (for an extensive discussion of the implications of the different sampling schemes for the simulated data, see [1]):
   - multilevel, implying that both the level 2 and level 1 elements are considered random
   - multigroup, implying that the level 2 elements are considered fixed and the level 1 elements random
   - multiobservation, implying that the level 2 elements are considered random and the level 1 elements fixed
3. the number of subjects, I, at two levels: 20, 40;
4. the number of measurement occasions per subject, K_i, at four levels: K_i was sampled uniformly between 20 and 30, between 30 and 70, between 80 and 120, and between 180 and 220;
5. the number of between-components Q_b, at three levels: 2, 3, and 4;
6. the number of within-components Q_w, at three levels: 2, 3, and 4;
7. the amount of error, at three levels: 10%, 30%, and 50%

In each cell of the design we had 10 replicates, leading to 84,240 generated data matrices.

Each simulated data matrix was analyzed with MCA and with the four MSCA variants, with the number of between- and within-components varying from one to eight. MSCA-PF2, MSCA-IND and MSCA-ECP solutions were obtained by running the alternating least squares algorithm [1] from a rational start. Subsequently, the complexities and goodness-of-fit-values VAF^b and VAF^w were computed for the between- and within-solutions, using each of the three complexity definitions.

4.2. Results

4.2.1. Overall performance of the CHull method for the three complexity definitions

For each of the three complexity definitions, Table 2 presents how frequently the CHull heuristic selected the correct number of between-components, the correct number of within-components

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Table 2
Percentage of correct selection of the number of between-components Q_b, the number of within-components Q_w and the model variant, using different complexity definitions.

Definition	Q_b	Q_w	Model variant	Q_w + model variant
c_1	98.80	73.19	47.44	44.02
c_2	98.85	30.46	24.99	10.51
c_3	98.80	91.40	60.71	59.13

and the correct model variant. From Table 2, it can be read that the three definitions hardly differ with respect to selecting the number of between-components Q_b, in that Q_b is almost always established correctly. With respect to the number of within-components Q_w and the model variant, it can be concluded that the complexity definitions in which the number of observations are taken into account — c_1 and c_3 — clearly outperform the c_2 definition in which this is not the case. Moreover, the c_3-definition yields the best results, correctly selecting the number of within-components Q_w in 91.40% of the cases and the model variant in 60.71% of the cases; note that in 59.13% of the cases both the number of within-components and the model variant is assessed correctly. The conclusion that the c_3-definition is to be preferred also holds if one considers the correct selection percentages at each level of the manipulated factors.

4.2.2. Dependence on the manipulated data characteristics

To further investigate the extent to which the performance of the CHull heuristic depends on the manipulated factors, two analyses of variance were conducted, only considering the c_3 complexity definition. The dependent variables of these ANOVAs were the frequencies of the correct selection of Q_w and of the model variant, respectively, computed per cell of the design. These frequencies range from 0 to 10, because we had 10 replicates for each cell of the design. The independent variables were underlying model variant, sampling scheme, number of subjects, number of observations, number of within-components, and error level.

Only considering the effects accounting for at least 10% of a dependent variable (i.e., intraclass correlations $\hat{\rho}_I \geq .10$ [19,20]), the analysis of variance for the selection of the number of within-components Q_w yielded a relatively large main effect of error level ($\hat{\rho}_I = .11$): the higher the error level, the harder it is for the model selection strategy to correctly estimate the number of within-components (see Fig. 1). Furthermore, this main effect of error level is qualified by an underlying model variant by error interaction effect ($\hat{\rho}_I = .10$) and an underlying model variant by the number of within-components by error level interaction effect ($\hat{\rho}_I = .16$): from Fig. 1, it can be read that the effect of error level is much stronger for some of the underlying model variants — MCA data in which the loading matrices were generated randomly, MSCA-PF2 data in which the within-components are rather strongly correlated and MSCA-P data in which the correlations of the within-components vary substantially across the subjects — and for higher numbers of within-components.

The analysis of variance with the frequency of correct selection of the model variant as the dependent variable yielded a main effect of the underlying model variant ($\hat{\omega}_I = .19$): as shown in Fig. 2, some of the multilevel component variants are easy to trace (i.e., MCA), whereas others are quite difficult (i.e., MSCA-PF2). Moreover, the extent to which the within-components are correlated and to which these correlations differ across subjects determines whether the CHULL heuristic can correctly assess MSCA-PF2 and MSCA-P solutions.

In addition, an interaction effect of the underlying model variant and the error level ($\hat{\rho}_I = .18$) was obtained. Unexpectedly, the MSCA-ECP, MSCA-IND, and some MSCA-PF2 variants are easier to trace when the amount of error increases, whereas the opposite holds for the MCA and MSCA-P variants. The latter effect can be explained as follows: the MSCA-ECP, MSCA-IND, and MSCA-PF2 variants all imply that the within-component scores are equally correlated for each subject. However, in the multilevel and multigroup sampling conditions, the correlations of the simulated component scores will almost always not be equal across subjects due to sampling fluctuations. Yet, when the resulting data are perturbed with a lot of random error these differences in correlations are mitigated, making the underlying model variants easier to trace.

Finally, we explored which model is indicated by the CHULL heuristic for the data sets for which the underlying model variant is

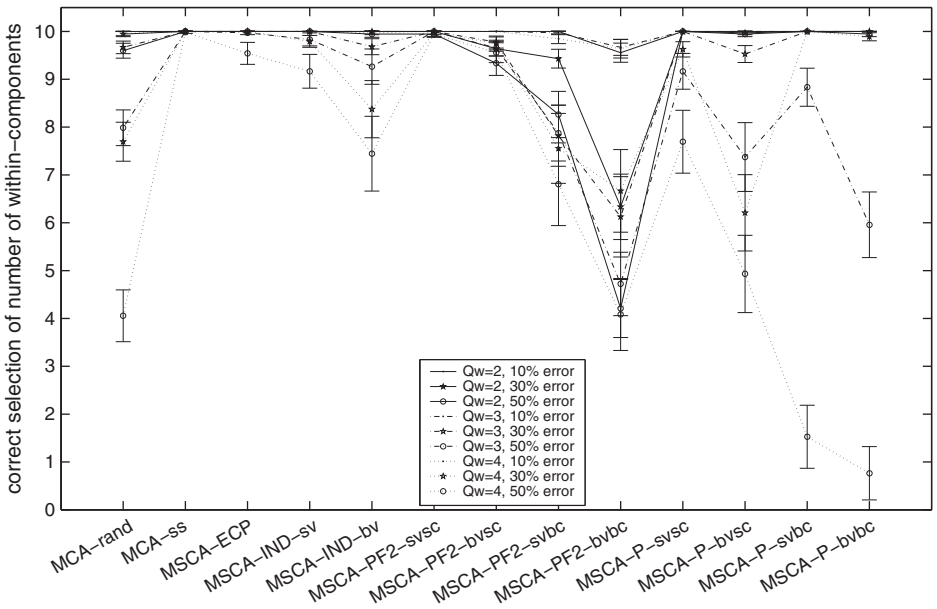

Fig. 1. Mean frequency of correct selection of number of within-components (out of 10) and associated 95% confidence intervals as a function of the underlying model variant, the underlying number of within-components and error level. MCA-rand means that the within-loading matrices are randomly sampled between −1 and 1, and MCA-ss that the within-loading matrices display simple structure. For MSCA-IND, MSCA-PF2 and MSCA-P, 'sv' and 'bv' indicate that the variances of the within-component scores are uniformly sampled between .5 and 1.5 and between .25 and 1.75, respectively. For MSCA-PF2, 'sc'and 'bc' means that the correlations of the within-component scores are set to .25 and .50, respectively, whereas for MSCA-P, 'sc' and 'bc' indicate that these correlations are uniformly sampled between −.25 and .25 and between −.50 and .50, respectively.

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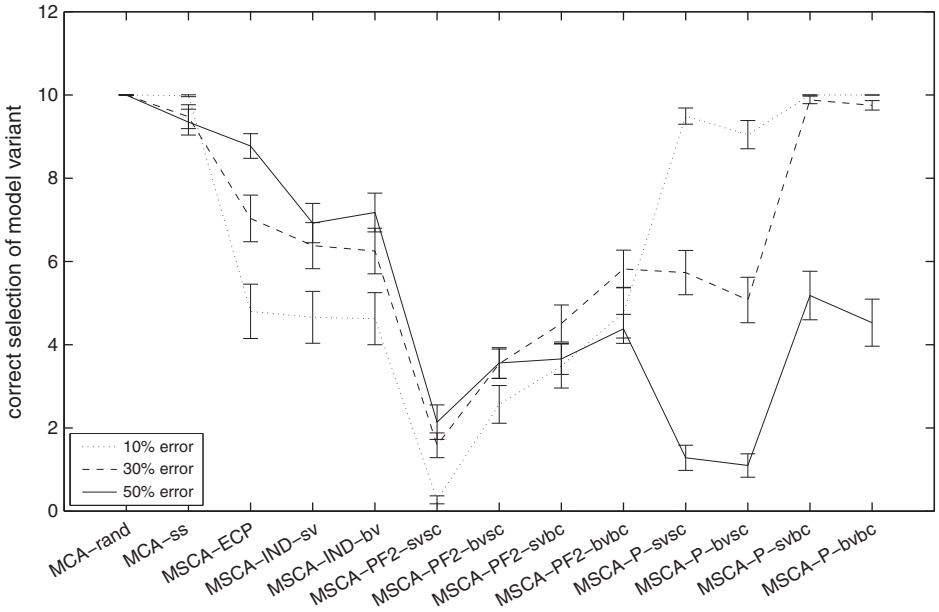

Fig. 2. Mean frequency of correct model selection (out of 10) and associated 95% confidence intervals as a function of the underlying model variant and error level. MCA-rand means that the within-loading matrices are randomly sampled between −1 and 1, and MCA-ss that the within-loading matrices display simple structure. For MSCA-IND, MSCA-PF2 and MSCA-P, 'sv' and 'bv' indicate that the variances of the within-component scores are uniformly sampled between .5 and 1.5 and between .25 and 1.75, respectively. For MSCA-PF2, 'sc'and 'bc' means that the correlations of the within-component scores are set to .25 and .50, respectively, whereas for MSCA-P, 'sc' and 'bc' indicate that these correlations are uniformly sampled between −.25 and .25 and between −.50 and .50, respectively.

not correctly assessed. From Table 3, it can be read that for MSCA-ECP and MSCA-IND data sometimes an MSCA-P solution seems indicated. MSCA-PF2 data are often mistakenly seen as MSCA-IND or MSCA-P data. In turn, for MSCA-P data sometimes an MSCA-IND solution is suggested. All these results imply that the precise correlational structure of the within-components is sometimes difficult to trace.

5. Illustrative application

To illustrate the use of the CHull heuristic, we apply it to sensory profiling data. In a study on cream cheese, 8 panelists were asked to rate 3 samples of 10 cream cheeses on 23 descriptors. For a detailed description of the study, we refer to Bro et al. [4]. The resulting data can be organized into a two-level data matrix **X** by concatenating the 30 samples by 23 descriptors data matrices $\mathbf{X}_i$ ($i=1...8$) of the 8 panelists. To eliminate arbitrary differences between descriptors in variability across panelist–sample combinations, the variance of each of the 23 descriptors across panelists and across samples was set to 1 in **X**.

Table 3
Percentage of selection of the five multilevel component variants as a function of the underlying model. Percentages pertaining to correctly indicated models are printed in bold face. MCA-rand means that the within-loading matrices are randomly sampled between -1 and 1, and MCA-ss that the within-loading matrices display simple structure. For MSCA-IND, MSCA-PF2 and MSCA-P, 'sv' and 'bv' indicate that the variances of the within-component scores are uniformly sampled between .5 and 1.5 and between .25 and 1.75, respectively. For MSCA-PF2, 'sc' and 'bc' means that the correlations of the within-component scores are set to .25 and .50, respectively, whereas for MSCA-P, 'sc' and 'bc' indicate that these correlations are uniformly sampled between −.25 and .25 and between −.50 and .50, respectively.

Underlying model	Selected multilevel component variant				
	MCA	MSCA-ECP	MSCA-IND	MSCA-PF2	MSCA-P
MCA-random	**99.97**	0	0	.02	.02
MCA-ss	**96.02**	3.84	.08	.03	.03
MSCA-ECP	.54	**68.69**	1.33	4.17	25.28
MSCA-IND-sv	1.34	3.21	**59.86**	8.66	26.93
MSCA-IND-bv	5.85	.05	**60.17**	7.76	26.17
MSCA-PF2-svsc	0	2.15	53.26	**13.32**	31.28
MSCA-PF2-bvsc	.40	0	38.19	**32.22**	29.18
MSCA-PF2-svbc	.31	1	30.11	**38.84**	29.74
MSCA-PF2-bvbc	.83	0	22.61	**49.89**	26.67
MSCA-P-svsc	3.90	3.01	27.36	10.71	**55.02**
MSCA-P-bvsc	13.32	0	27.89	8.07	**50.73**
MSCA-P-svbc	10.71	1.31	1.36	3.09	**83.53**
MSCA-P-bvbc	14.88	0	1.20	2.99	**80.93**

The data matrix **X** was analyzed with the five multilevel component analysis variants that were discussed in Section 2. Specifically, each of these model variants was fitted with the number of between-components varying from 1 to 6 and the number of within-components varying from 1 to 8. Because, for a given number of between-components Q_b, the between-parts of the MCA and MSCA solutions are identical, this yields 6 solutions for the between-part of the data.

For the within-part of the data, we obtain 8 solutions for each of the five considered variants, resulting in $5\times8=40$ solutions. For MSCA-PF2, MSCA-IND and MSCA-ECP, the iterative algorithm was run 6 times, with 5 random starts and 1 rational start, and the best fitting solution was taken. Subsequently, the complexities (using definition c_3) and goodness-of-fit-values VAF^b and VAF^w for the 6 between-solutions and the 40 within-solutions were computed.

Fig. 3 displays a plot of the VAF^b and c_3 values of the six between-solutions. Applying the CHull procedure reveals that five of the six solutions lie on the higher boundary of the hull (i.e., all solutions except for the one with complexity $c_3=125$). Furthermore, the CHull heuristic indicates the selection of a between-solution with four components, as can be verified from the *st*-values of these solutions presented in Table 4. Inspection of the solution revealed interpretable between-components.

In Fig. 4, a VAF^w versus c_3 plot of the 40 within-solutions is shown. The CHull procedure revealed that 9 solutions lie on the higher boundary of the hull; the associated *st*-values are given in Table 5. It can be verified from Table 5 that the CHull heuristic indicates the selection of an MSCA-PF2 solution with two components. However, this MSCA-PF2 solution appears to be degenerate, in that the correlation between the within-component scores equals .9875. Therefore, we decided to retain the MSCA-IND solution with two

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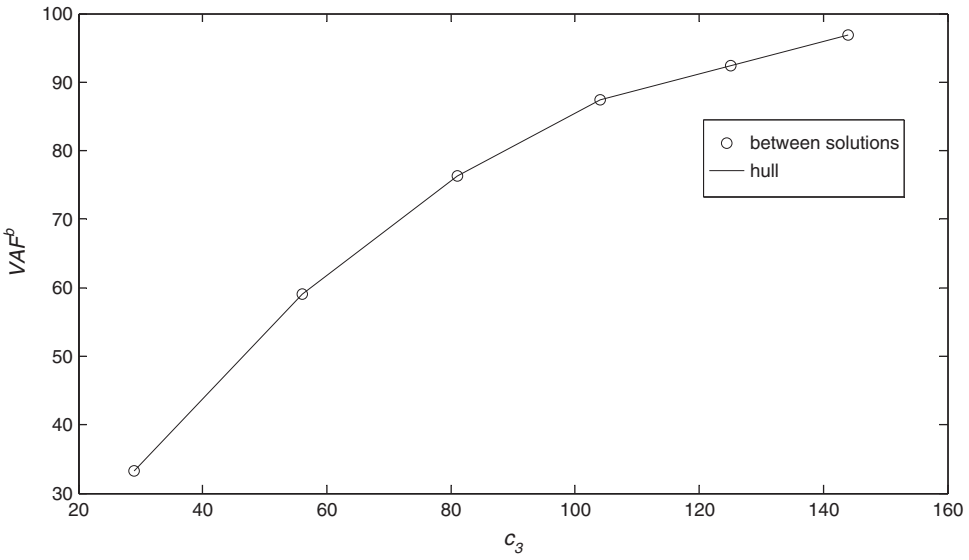

Fig. 3. Plot of VAF^b versus c_3-values for the six between-solutions for the cream cheese data, with the line representing the higher boundary of the convex hull.

Table 4
Goodness-of-fit-values VAF^b, complexity values c_3, and scree test-values st of the five between-solutions on the higher boundary of the convex hull of Fig. 3.

Q_b	c_3	VAF^b	st
1	29	33.29	–
2	56	59.02	1.37
3	81	76.36	1.44
4	104	87.45	2.04
6	144	96.90	–

components, which lies very close to the MSCA-PF2 solution in Fig. 4. It is interesting to note that Bro et al. [4] conducted PARAFAC analyses [21,22] on the within-part of the cream cheese data and also selected a solution with two components. A comparison of the within-loadings of the PARAFAC and the MSCA-IND solutions revealed that they are very similar, and lead to an identical interpretation of the components. However, the MSCA-IND solution yields more insight into the individual differences between the panelists than the PARAFAC solution, because it does not restrict the component scores of the cheese samples to be equal across the panelists.

6. Discussion

In this paper, we have presented a CHull heuristic for selecting among different multilevel component model variants and for establishing the number of between- and within-components. Simulation results show that this heuristic performs almost perfectly when assessing the number of between-components. The CHull heuristic also succeeds very well in determining the number of within-components. Only for high error levels and higher numbers of within-components the performance deteriorates for some of the considered types of MCA, MSCA-PF2 and MSCA-P data. In all these

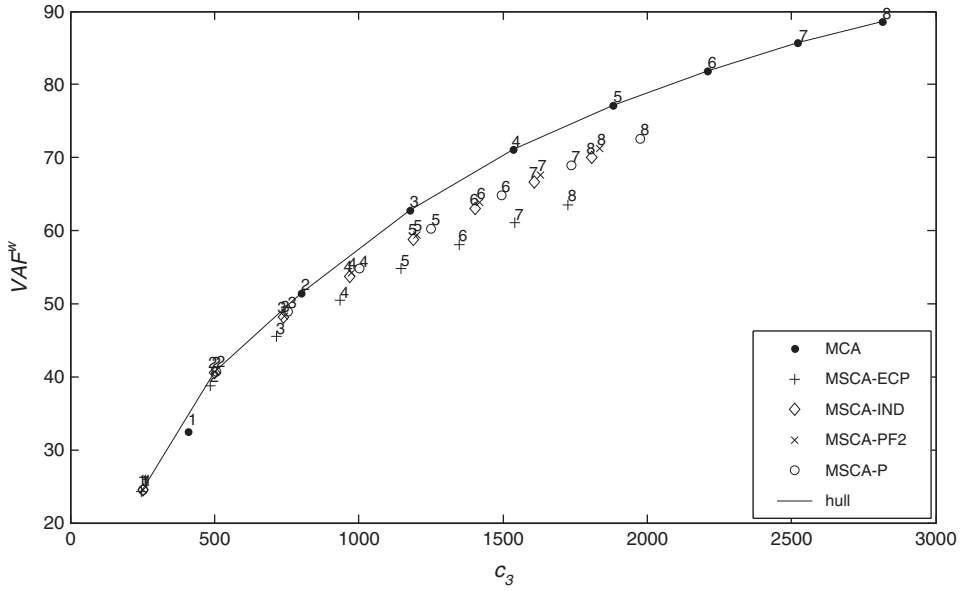

Fig. 4. Plot of VAF^w versus c_3-values for the forty within-solutions for the cream cheese data, with the line representing the higher boundary of the convex hull. The numbers indicate the number of within-components of the corresponding solutions.

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Table 5
Goodness-of-fit-values VAF^w, complexity values c_3, and scree test-values st of the nine within-solutions on the higher boundary of the convex hull of Fig. 4.

Variant	Q_w	c_3	VAF^w	*st*
MSCA-ECP	1	247	24.23	–
MSCA-PF2	2	501	40.68	1.81
MCA	2	800	51.38	1.18
MCA	3	1176	62.81	1.32
MCA	4	1536	71.10	1.30
MCA	5	1880	77.19	1.26
MCA	6	2208	81.81	1.14
MCA	7	2520	85.66	1.23
MCA	8	2816	88.63	–

data types, the within-components are correlated, which may lead to an underestimation of the number of within-components. Indeed, in only seven (less than .01%) of the cases in which the number of within-components is not assessed correctly, a solution with a higher number of within-components was selected.

Tracing the underlying model variant proved to be a harder model selection problem, however. Whether or not the CHull heuristic detects the multilevel component variant correctly mostly depends on the variant under study: Whereas differences in within-loading matrices and differences in variances are very easy to detect, the precise correlational structure of the within-components appears much harder to trace. This makes sense as these differences in correlational structure are much more subtle. Indeed, if the number of measurement occasions in a multilevel or multigroup sampling scheme is small, the population structure might not be reflected adequately in the sample data. Some evidence for this conjecture is found by further inspecting the simulation results, which revealed that the performance of the CHull heuristic improves if the multi-observation sampling scheme is used (implying that the level 1 elements are considered fixed) or when the number of measurement occasions for each subject is large.

A more fundamental issue that remains unsolved, is what the best definition of the complexity of multilevel component solutions is. In this paper, three different definitions were employed, and the use of c_3 led to the best selection results. Although this c_3-definition bears relations to the BIC [18], a solid theoretical rationale that explains this result is lacking. Note that the c_3 definition was not used when evaluating the performance of the CHull procedure in three-mode component analysis [2]. Therefore, it may be worthwhile to explore whether the c_3 definition may be useful in that context too. However, based on the results reported in [2], the multiway model selection problem seems to be less difficult than its multilevel counterpart; therefore, for multiway models, the performance of CHull is expected to depend less on the complexity measure used than for multilevel component models.

Defining the complexity is a ubiquitous problem for many more or less complex models, however. Even for regular PCA models, various conflicting proposals for complexity (or the related notion of the number of degrees of freedom) have been published (for an overview, see [17]; for earlier discussions, see [23–25]). As a way out, it has been proposed to define generalized or pseudo degrees of freedom by examining the extent to which the estimation results are sensitive to small perturbations in the data [26,27]. For future research, it may be worthwhile to investigate whether concepts like generalized or pseudo degrees of freedom are useful in the framework of multilevel component analysis.

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