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Uncovering and Treating Unobserved Heterogeneity with FIMIX-PLS: Which Model Selection Criterion Provides an Appropriate Number of Segments?

Abstract

Since its first introduction in the Schmalenbach Business Review, Hahn et al.'s (2002) finite mixture partial least squares (FIMIX-PLS) approach to response-based segmentation in variance-based structural equation modeling has received much attention from the marketing and management disciplines. When applying FIMIX-PLS to uncover unobserved heterogeneity, the actual number of segments is usually unknown. As in any clustering procedure, retaining a suitable number of segments is crucial, since many managerial decisions are based on this result. In empirical research, applications of FIMIX-PLS rely on information and classification criteria to select an appropriate number of segments to retain from the data. However, the performance and robustness of these criteria in determining an adequate number of segments has not yet been investigated scientifically in the context of FIMIX-PLS. By conducting computational experiments, this study provides an evaluation of several model selection criteria's performance and of different data characteristics' influence on the robustness of the criteria. The results engender key recommendations and identify appropriate model selection criteria for FIMIX-PLS. The study's findings enhance the applicability of FIMIX-PLS in both theory and practice.

JEL-Classification: C39, M31.

Keywords: FIMIX-PLS; Finite Mixture Modeling; Model Selection; Partial Least Squares (PLS); Segmentation; Structural Equation Modeling.

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1 Introduction

Structural equation models are widely used in business research to model relations between unobserved constructs and manifest variables. Most applications assume that data come from a homogeneous population. However, this assumption of homogeneity is unrealistic, since individuals are likely to differ in their perceptions and evaluations of latent constructs (Ansari, Jedidi, and Jagpal (2000)). To account for heterogeneity, researchers frequently use sequential procedures in which homogeneous subgroups are formed by means of a-priori information, or else they revert to the application of cluster analysis techniques. However, none of these approaches is considered satisfactory, because observable characteristics often gloss over the true sources of heterogeneity (Wedel and Kamakura (2000)). Conversely, the application of traditional cluster analysis techniques suffers from conceptual shortcomings and cannot account for heterogeneity in the relations between latent variables. These weaknesses have been broadly recognized in the prior literature; consequently, research efforts have been devoted to the development of model-based clustering methods (e.g., Jedidi, Jagpal, and DeSarbo (1997a)).

Uncovering unobserved heterogeneity in covariance-based structural equation modeling (CBSEM) has been studied for several years (Arminger and Stein (1997); Jedidi, Jagpal, and DeSarbo (1997a); Dolan and van der Maas (1998); Muthén (2008)). Nevertheless, only recently has research interest focused on this problem in the context of partial least squares (PLS) path modeling (Wold (1982); Lohmöller (1989)), which is a complementary modeling approach to the widely used covariance-based methods (Jöreskog and Wold (1982); Hair, Ringle, and Sarstedt (2011)). Currently, researchers have proposed different approaches to latent class detection that hold considerable promise for segmentation tasks in PLS path modeling. Sarstedt (2008a) presents a theoretical review of available procedures and concludes that finite mixture PLS (FIMIX-PLS) is now the primary choice for segmentation tasks within a PLS context.

Hahn et al. (2002) introduced the FIMIX-PLS technique for latent class detection. The technique was later advanced by Ringle, Sarstedt, and Mooi (2010) and Ringle, Wende, and Will (2010), and implemented in the software application SmartPLS 2.0 (M3) (Ringle, Wende, and Will (2005)). The method allows the simultaneous estimation of model parameters and segment affiliations of observations. Simulation studies (e.g., Esposito Vinzi et al. (2007); Ringle, Sarstedt, and Schlittgen (2010)) and numerical comparisons (Sarstedt and Ringle (2010)) underline favorable capabilities of this approach compared to those of alternative segmentation methods. Furthermore, empirical studies (e.g., Hahn et al. (2002); Becker (2004); Conze (2007); Scheer (2008); Sarstedt, Schwaiger, and Ringle (2009)) also reveal that FIMIX-PLS has advantageous features for further differentiating and specifying the findings and interpretation of PLS path modeling analyses.

However, an unresolved problem in the application of FIMIX-PLS is the issue of model selection (i.e., determining of the number of segments underlying the data; Esposito Vinzi et al. (2008)). As in any clustering procedure, retaining a suitable number of segments is crucial, since many managerial decisions are based on this result. A misspecification can result in an under- or over-segmentation, thus leading to flawed management decisions on, for example, customer targeting, product positioning, or determining the optimal marketing mix (Andrews and Currim (2003a)). If the number of segments is over-specified, marketers risk treating audience segments separately, even though dealing with them as a group would be more effective. But if a market is under-segmented, marketers might fail to identify distinct segments that could be addressed separately, enabling the marketer to more precisely satisfy customers' varying wants. Since companies may spend millions of dollars developing and targeting market segments, the costs of over-specifying the appropriate number of segments are significant. Moreover, the problem of revenue losses, which is associated with under-segmenting a market and not targeting potentially lucrative niche segments, is a highly relevant issue (Boone and Roehm (2002)).

Unlike other segmentation procedures in PLS path modeling, the FIMIX-PLS algorithm allows the researcher to compute several statistical model selection criteria that are well-known from finite mixture modeling literature (Sarstedt (2008a)). Correspondingly, in empirical research, applications of FIMIX-PLS rely on criteria such as Akaike's information criterion (AIC, Akaike (1973)), Bayesian information criterion (BIC, Schwarz (1978)), consistent AIC (CAIC, Bozdogan (1987)), and normed entropy criterion (EN, Ramaswamy, DeSarbo, and Reibstein (1993)) to determine the number of data segments that should be retained. Since these applications use real-world data in which the number of segments is unknown, it is not clear whether these criteria are effective. This fact is problematic, since previous studies have shown that analytical deviations cannot predict the relative performance of model selection criteria (Lin and Dayton (1997)).

The common approach to this problem is to evaluate the efficacy of the criteria in detecting segments by means of simulated data. However, likelihood-based fit criteria are frequently not comparable across segmentation approaches (Andrews and Currim (2003b)) and classes of finite mixture models (Yang and Yang (2007)). Consequently, their performance has been evaluated in different contexts, such as mixtures of univariate normal distributions (e.g., Bozodgan (1994); Celeux and Soromenho (1996); Biernacki and Govaert (1997)), multivariate normal distributions (Bozodogan (1994); Biernacki, Celeux, and Govaert (2000)), mixture regression models (Andrews and Currim (2003c); Sarstedt (2008b)), and mixture logit models (Andrews and Currim (2003a)).

These simulation studies provide evidence that different criteria are particularly effective for specific segmentation approaches. Hence, prior research can provide only limited guidance on the criteria's performance in a FIMIX-PLS context. Since fitting mixture models to large "full-blown" path models, which is often done against the background of PLS' properties (Henseler , Ringle, and Sinkovics (2009)), quickly exhausts degrees of freedom (Henson, Reise, and Kim (2007)), an explicit analysis in the context of FIMIX-PLS is necessary. Despite the fundamental relevance, no simulation has yet determined an accurate model selection criterion for the FIMIX-PLS method. This lacuna in research is particularly critical, because FIMIX-PLS continues to grow in popularity. Further, recent publications have demanded that FIMIX-PLS should be routinely carried out when evaluating any PLS path model (Albers (2010); Ringle, Sarstedt, and Mooi (2010)).

In this paper we contribute to the knowledge on PLS path modeling and FIMIX-PLS segmentation by conducting computational experiments that allow the researcher to examine the performance and robustness of alternative model selection criteria. There are many studies on computational experiments that evaluate estimators in the context of structural equation modeling. Even though analytical statistical theory can address some research questions, the finite sample properties of structural equation model estimators are often beyond the reach of established asymptotic theory. Similarly, distributions of the statistical measures of fit indexes, such as model selection criteria, are not even asymptotically known. In such situations, computational experiments and Monte Carlo studies provide an excellent method for evaluating estimators and goodness-of-fit statistics under a variety of conditions (Paxton et al. (2001)). This kind of approach allows the researcher to evaluate performance of the criteria against the background of diverse factors, such as sample size, number of segments, or the path model's complexity. By providing recommendations on the selection of an appropriate model selection criterion, our paper answers the call of previous studies (Esposito Vinzi et al. (2007); Sarstedt (2008a)) and contributes to the body of knowledge in PLS path modeling.

The remainder of this paper is organized as follows. After a brief introduction of the FIMIX-PLS method in Section 2, we discuss the model selection problem in the context of FIMIX-PLS in Section 3. We describe the experimental design and present the analysis results in Section 4. Lastly, in Section 5, we summarize the findings and discuss potential limitations as well as opportunities for further research.

2 The FIMIX-PLS Approach

The FIMIX-PLS method (Hahn et al. (2002)) combines the strengths of the PLS method with the advantages of classifying market segments according to finite mixture models (e.g., Everitt and Hand (1981); McLachlan and Basford (1988)). Based on this concept, FIMIX-PLS simultaneously estimates the structural model parameters and ascertains the data structure's heterogeneity within a PLS path modeling framework.

Initially, a path model is estimated by using the PLS algorithm and empirical data on the aggregate data level. This implies that the perceptions of the constructs are homogeneous in the outer measurement model. Thereafter, the resulting latent variable scores in the structural model are employed to run the FIMIX-PLS algorithm. The path model's segment-specific heterogeneity is concentrated in the parameters of the estimated relations between latent variables. FIMIX-PLS captures this heterogeneity and calculates the probability of the observations' segment memberships, so that they fit into each of the predetermined S numbers of segments. Assuming that each endogenous latent variable η_i is distributed as a finite mixture of conditional multivariate normal densities $f_{i|s}(\cdot)$, the segment-specific distributional function is defined as follows:

$$\boldsymbol{\eta}_i \sim \sum_{s=1}^{S} \rho_s f_{i|s}(\boldsymbol{\eta}_i | \boldsymbol{\xi}_i, \boldsymbol{B}_s, \boldsymbol{\Gamma}_s, \boldsymbol{\Psi}_s), \tag{1}$$

where ξ_i is an exogenous variable vector in the inner model regarding observation i, B_s is the path coefficient matrix of the endogenous variables, and Γ_s the exogenous latent variables. Ψ_s depicts the matrix of each segment's regression variances of the inner model on the diagonal, zero else. The mixture proportion ρ_s determines the relative size of segment s $(s = 1, \ldots, S)$ with $\rho_s > 0 \; \forall s$ and $\sum_{s=1}^{S} \rho_s = 1$.

Substituting $f_{i|s}(\boldsymbol{\eta}_i | \boldsymbol{\xi}_i, \boldsymbol{B}_s, \boldsymbol{\Gamma}_s, \boldsymbol{\Psi}_s)$ results in:

$$\boldsymbol{\eta}_i = \sum_{s=1}^{S} \rho_s \left[\frac{1}{(2\pi)^{Q/2}\sqrt{|\boldsymbol{\Psi}_s|}} \right] exp\left\{ -\frac{1}{2}((I - \boldsymbol{B}_s)\boldsymbol{\eta}_i + (-\boldsymbol{\Gamma}_s)\boldsymbol{\xi}_i)' \, \boldsymbol{\Psi}_s^{-1}((I - \boldsymbol{B}_s)\eta_i + (-\boldsymbol{\Gamma}_s)\boldsymbol{\xi}_i) \right\}, \tag{2}$$

where Q depicts the number of endogenous latent variables in the inner model and I the identity matrix[1]. We use an EM formulation of the FIMIX-PLS algorithm for statistical computations to maximize the log-likelihood of equation (2).

Conceptually, FIMIX-PLS is equivalent to a mixture regression approach. However, the main difference is that the structural model can comprise a multitude of (interrelated) endogenous latent variables. The specification of such a system of linear equations cannot be realized with conventional mixture regressions (Hahn (2002)).

3 Model Selection in FIMIX-PLS

When applying FIMIX-PLS to empirical data, the actual number of segments S is usually unknown. As a result of problems that arise when using hypothesis tests in a finite mixture model framework (Aitkin and Rubin (1985)), researchers frequently revert to a heuristic approach. For example, they do so by building on model selection criteria that can be categorized into information and classification criteria (McLachlan and Peel (2000)). Information criteria are based on a penalized form of the likelihood, since they simultaneously take into account a model's goodness-of-fit (likelihood) and the number of parameters used to achieve that fit. Therefore, they correspond to a penalized likelihood function, that is, two times the negative log-likelihood plus a penalty term that increases with the number of parameters and/or the number of observations. Information criteria generally favor models with a large log-likelihood and few parameters, and are scaled so that a lower value represents a better fit. Operationally, the researcher examines several competing models with alternating numbers of segments, picking the model that minimizes a particular information criterion. However, in line with substantive theory, researchers usually use a combination of criteria to guide this decision in their applications (Sarstedt (2008b)).

1 We note that this presentation differs from Hahn et al.'s (2002) original presentation, which requires additional descriptions and clarifications in some instances (see *Table A4* in the appendix). Even though these modifications do not significantly affect FIMIX-PLS' capability to accurately recover parameters, they have noticeable effects on the development of log-likelihood values. We have implemented corresponding changes in the experimental version of SmartPLS that will be made available in the software version that will follow release M3.

Although the preceding heuristics account for overparametrization through the integration of a penalty term, they do not ensure that the segments are sufficiently separated in the selected solution. Since the targeting of markets requires segments to be differentiable – that is, that the segments are conceptually distinguishable and respond differently to different marketing-mix elements and programs (Mooi and Sarstedt (2011)) – this point is of great practical interest. Based on an entropy statistic that indicates the degree of separation between the segments, classification criteria can help assess whether the analysis produces well-separated clusters (Wedel and Kamakura (2000)). These classification criteria include combinations of log-likelihood and entropy-based concepts, such as the integrated completed likelihood BIC (ICL-BIC, Biernacki, Celeux, and Govaert (2000)) and classification likelihood criterion (CLC, Biernacki and Govaert (1997)).

In the past, many different information and classification criteria were developed to assess the number of segments, all of which have different theoretical underpinnings and statistical properties (McLachlan and Peel (2000)). The applicability of these model selection criteria is one of the most important features of FIMIX-PLS, since alternative approaches to response-based segmentation in PLS path modeling do not provide any guidance on model selection (Sarstedt (2008a)).

To date, only limited research has addressed statistical criteria's performance concerning model selection in finite mixture SEMs. The problem of testing for the number of segments is only briefly addressed, if at all, in simulation studies that test newly proposed segmentation algorithms in a CBSEM context (Jedidi, Jagpal, and DeSarbo (1997a); Arminger, Stein, and Wittenberg (1999)). However, it is important to note that these approaches to CBSEM are based on different statistical features than its FIMIX-PLS adaption by Hahn et al. (2002). Since FIMIX-PLS is essentially based on a mixture regression concept (Hahn et al. (2002)), previous studies in this context can provide some guidance regarding model selection criteria's performance.

While some studies focus on the influence of specific data constellations (e.g., Oliveira-Brochado and Martins (2006); Sarstedt (2008b); Becker et al. (2010)), only two studies present a comprehensive evaluation of data characteristics' influence on model selection criteria's performance in mixture regression models. In their primary study, Hawkins, Allen, and Stromberg (2001) assess the performance of different criteria in determining the number of segments in mixtures of linear regression models. In their simulation study, these authors provide a comparison of 12 criteria and multiple approximations of these, taking into account three data characteristics: the number of segments, degree of pairwise separation between the segments, and relative segment sizes. Hawkins, Allen, and Stromberg (2001) compare the percentages of data sets in which each criterion identifies the true number of segments (i.e., the success rate). Based on the analysis results, the authors conclude that BIC is the recommended criterion for choosing between one- and two-segment mixtures of linear regression models. None of the measures outperforms the others across the simulation runs for three and four segments, but all the criteria perform poorly for four segments, showing success rates of less than 50%.

Andrews and Currim (2003c) investigate the performance of seven model selection criteria used with mixture regression models. These authors evaluate eight data characteristics that would potentially affect the criteria's performance, including the number of segments, the mean separation between segment coefficients, sample size, and relative segment sizes. Their study shows that because it has the highest success rate, the modified AIC with a penalty factor of three (AIC_3, Bozdogan (1994)) is clearly the best criterion to use across a wide variety of model specifications and data configurations.

Although these studies provide important insights into the performance of the criteria, no previous study has evaluated their efficacy in the context of FIMIX-PLS, which has become an important analysis context in marketing (Rigdon, Ringle, and Sarstedt (2010)). In the light of this gap in the academic literature and the importance of choosing the correct number of segments in marketing studies, an evaluation of commonly used model selection criteria in FIMIX-PLS by means of computational experiments is particularly valuable from both a research and practice perspective.

4 Computational Experiments

4.1 Design

The study of computational experiments analyzes the performance and robustness of the following model selection criteria, frequently used for model selection in finite mixture modeling (McLachlan and Peel (2000); Sarstedt (2008b))[2]:

- Information criteria: AIC (Akaike (1973)), AIC_3 (Bozdogan (1994)), AIC_4 (Bozdogan (1994)), AIC_c (Hurvich and Tsai (1989)), BIC (Schwarz (1978)), CAIC (Bozdogan (1987)), MDL_2, MDL_5, (both, Liang, Jaszczak, and Coleman (1992)), and HQ (Hannan and Quinn (1979)).
- Classification criteria: $\ln L_c$ (Dempster, Laird, and Rubin (1977)), NEC (Celeux and Soromenho (1996)), ICL-BIC (Biernacki, Celeux, and Govaert (2000)), PC (Bezdek (1981)), NFI (Roubens (1978)), NPE (Bezdek (1981)), AWE (Banfield and Raftery (1993)), CLC (Biernacki and Govaert (1997)), and EN (Ramaswamy, DeSarbo, and Reibstein (1993)).

In this study, we manipulate six data characteristics (factors). Our choice of the factors and their levels draws primarily on related research conducted by Hawkins, Allen, and Stromberg (2001), and Andrews and Currim (2003a; 2003c), as well as previous empirical analyses using FIMIX-PLS:

Factor 1: Number of segments [2, 4].

Analyzing a two- and four-segment solution is consistent with the range of segments found in Hawkins, Allen, and Stromberg's (2001) primary study on the performance of

2 *Table A1* in the appendix includes the formal definitions of the criteria. The reader is referred to the references cited below for detailed discussions of these criteria's theoretical underpinnings.

model selection criteria in the context of mixtures of linear models. Furthermore, these factor levels have been evaluated in numerical FIMIX-PLS experiments (e.g., Ringle, Wende, and Will (2005a); Esposito Vinzi et al. (2007); Rigdon, Ringle, and Sarstedt (2010)). The selected factor levels also cover findings from FIMIX-PLS studies using real data (e.g., Becker (2004); Scheer (2008); Sarstedt, Schwaiger, and Ringle (2009)). In light of the increased complexity of the analysis task, we expect an inferior performance from the model selection criteria when we consider a higher number of segments.

Factor 2: Number of observations [100, 400].
This factor includes two different levels. We choose sample sizes of 100 and 400 because similar levels have been reported in related simulation studies (Andrews and Currim (2003a; 2003c); Sarstedt (2008b)), as well as in PLS path modeling (e.g., Sarstedt and Schloderer (2010); Wagner, Henning-Thurau, and Rudolph (2009)) and FIMIX-PLS applications (Sarstedt and Ringle (2010)). In partial accordance with the consistency at large issue for PLS path modeling (e.g., Hui and Wold (1982); Henseler, Ringle, and Sinkovics (2009); Hair, Ringle, and Sarstedt (2011)), we expect a better performance from the model selection criteria when the number of observations increases.

Factor 3: Disturbance term of the endogenous latent variables [10%, 25%].
Past research has identified the level of endogenous latent variables' disturbance term as a key standard for clear-cut segmentation (e.g., Ringle and Schlittgen (2007)). In line with prior research on response-based segmentation techniques' performance in PLS path modeling (Becker, Ringle, and Völckner (2009); Ringle, Sarstedt, and Schlittgen (2010)), we choose two levels of disturbance terms. A higher level disturbance term complicates the segment identification. Thus, we expect the model selection criteria to perform poorly if there is an increase in the endogenous latent variables' error variance and, hence, in the manifest variables.

Factor 4: Distance between segment-specific path coefficients [0.25, 0.75].
Past studies support the assertion that similar segments are harder to detect (Hawkins, Allen, and Stromberg (2001); Andrews and Currim (2003a; 2003c)). Andrews and Currim (2003c) account for very high levels of mean separation between segment coefficients (0.5, 1.0, and 1.5), but we choose smaller deviations, as they more adequately reflect the results of actual applications (e.g., Conze (2007); Sarstedt, Schwaiger, and Ringle (2009)). Hence, in this study, we change the prespecified path coefficients' absolute difference between segments. We assume that the model selection criteria show an increased performance when segments' distinctiveness increases in terms of the distance between the segment-specific path coefficients.

Factor 5: Model complexity [low, high].
Previous simulation studies often account for different model complexities. For example, in the context of mixture logit models, Andrews and Currim (2003a) vary the number of choice alternatives. In their follow-up study on mixture regression models, these authors use a varying number of predictors to account for different levels of model complexity (Andrews and Currim (2003c)). Following this notion, we utilize two models, one with low complexity and another with high.

The PLS path model with lower complexity (*Figure A2*, Appendix) uses four exogenous latent variables (ξ_1, ξ_2, ξ_3, and ξ_4), all of which relate to a single endogenous variable (η_1). Thus, there are four relations with coefficients γ_{11}, γ_{21}, γ_{31}, and γ_{41} in the structural model. In the data simulation, the prespecification of the path coefficients uses a higher γ_{11} value and lower values for γ_{21}, γ_{31}, and γ_{41} for the first group of data. For the second group, γ_{21} is at a higher level, but all the remaining path coefficients consistently remain at a lower level. Depending on the segment under consideration, the same logic holds for four segments, when the path coefficients are increased in turn.

Since the size of the coefficients is not important but their distinctiveness is, we focus on their alternative levels of difference in the inner path model (factor 4). We use five manifest variables for construct measurement and all loadings exhibit the same level. This kind of structural equation model has previously been reported in FIMIX-PLS studies (e.g., Ringle (2006)), and in covariance-based finite mixture structural equation modeling (Jedidi, Jagpal, and DeSarbo (1997b)).

The complex model (*Figure A3*, Appendix) uses three exogenous latent variables (ξ_1, ξ_2, and ξ_3), three endogenous latent variables (η_1, η_2, and η_3), and six inner model path relations (with coefficients γ_{11}, γ_{21}, γ_{22}, γ_{32}, β_{13}, and β_{23}). The parameter prespecification to generate the experimental data is analogous to the previous model. A specific group of data has a few specifically strong relations in the inner model, but all other paths remain at a lower level. Since the number of free parameters in the complex model increases considerably compared to those of the less complex structural equation model, we expect lower success rates in the complex model.

Factor 6: Relative segment sizes [balanced, unbalanced].
In past simulation studies, researchers evaluated the effect of segment sizes on criteria performance (Hawkins, Allen, and Stromberg (2001); Andrews and Currim (2003a; 2003c); Sarstedt (2008a)). This factor is critically important for PLS segmentation methods, since Esposito Vinzi et al. (2007) show that the other prominent approach to response-based segmentation in PLS, PLS-TPM, which has been further developed into REBUS-PLS (Esposito Vinzi et al. (2008)), cannot handle unbalanced segments. FIMIX-PLS however performs as expected in almost all data constellations. We choose two factor levels, balanced and unbalanced. The balanced factor level is connected with equally sized segments (50%/50% in the case of two segments; 25%/25%/25%/25% in the case of four segments). The unbalanced factor level characterizes the existence of one segment that is considerably larger than the other segments (80%/20% in the case of two segments; 55%/15%/15%/15% in the case of four segments). Hawkins, Allen, and Stromberg (2001) and Sarstedt (2008b) evaluate similar situations in their simulation studies. Further, several empirical studies (e.g., Scheer (2008); Sarstedt and Ringle (2010)) report these conditions. Although previous studies account for a minimum segment size of 5% for the smallest segment (Andrews and Currim (2003a; 2003c)), this level is not feasible in our study, because the smallest sample size of 100 would not produce sufficiently large niche segments to successfully apply the FIMIX-PLS algorithm. In

the light of Esposito Vinzi et al.'s (2007) findings, we assume that the performance of the criteria only declines slightly, if at all, with unbalanced relative segments sizes than with balanced segment sizes.

We generate data sets for each possible combination of factor levels. Since there are six factors with two levels, this adds up to $2^6 = 64$ factor level combinations.

Computational experiments on structural equation models require the generation of data for indicator variables. After estimating the model, these data meet both the relations' pre-specified parameters in the structural model and in the measurement models. In covariance structure analysis, there are two different approaches that are appropriate for obtaining such data. One approach calculates the indicator variables' implied covariance matrix for given values of the parameters in the model and generates data from a multivariate distribution that fits this covariance matrix. The second approach requires the latent variables' scores in keeping with the specified relations in the structural model, after which data are generated for the observed variables in accordance with the measurement models' pre-specified parameters. The latter approach allows the researcher to obtain data with certain distributional characteristics, as implied by the model (Mattson (1997)). Only a few Monte Carlo simulation studies and computational experiments, which require artificial data for pre-specified parameters, have been presented for PLS path modeling thus far (e.g., Chin, Marcolin, and Newsted (2003); Reinartz, Haenlein, and Henseler (2009); Ringle, Sarstedt, and Schlittgen (2009); Henseler and Chin (2010)). All of these studies use the second CBSEM data generation approach, which we also apply in this research[3].

4.2 Model Estimation and Evaluation

This study applies the FIMIX-PLS method by using the software application SmartPLS 2.0 (M3) (Ringle, Wende, and Will (2005b)). To identify the appropriate number of segments, we test alternative segment number solutions for each factor constellation. If the set of artificially generated data consists of two (four) segments, then in this analysis we draw on FIMIX-PLS solutions for one through six (one through eight) segments. We save the results for the FIMIX-PLS runs with different numbers of segments per factor constellation.

Owing to the possible convergence of the EM algorithm in local optimum solutions (Wu (1983)), each FIMIX-PLS analysis uses 30 replications. To avoid premature convergence, we only truncate the FIMIX-PLS algorithm when the improvement δ of the log-likelihood is under the threshold value of $1 \cdot 10^{-15}$, or the maximum number of 30,000 iterations is attained. In all cases, the δ criterion terminates the algorithm, indicating that the stop criterion parameter has been set at a sufficiently low level, as demanded by Wedel and Kamakura (2000). Moreover, to ensure the robustness of the

3 The authors would like to thank Rainer Schlittgen (Institute of Statistics and Econometrics, University of Hamburg, Von-Melle-Park 5, 20146 Hamburg, Germany, rainer.schlittgen@uni-hamburg.de) for sharing his GAUSS programs for PLS data generation (Ringle and Schlittgen (2007)) with them.

results in this study, we include an analysis of 30 different artificially generated sets of data for each of the 64 factor-level combinations.

Testing alternative numbers of latent classes with 30 replications each requires two kinds of evaluation to determine a FIMIX-PLS solution. First, we select the best solution in terms of the 30 replications' log-likelihood values. Second, we compare the model selection criteria for these best FIMIX-PLS solutions across the one through six (one through eight) alternative segment solutions per factor constellation. We conduct this procedure for all 30 alternative artificially generated sets per factor constellation that become part of the final results presentation. Finally, for each criterion, we compute the percentages of data sets, identifying the true number of segments (i.e., the success rate; *Table 1*). In total, we draw on 32 x 6 x 30 x 30 (two segments) + 32 x 8 x 30 x 30 (four segments) = 403,200 FIMIX-PLS runs. The best solution for each of the 18 FIMIX-PLS selection criteria from 30 replications becomes part of the results presentation of this study's computational experiments. Consequently, this study includes 403,200 / 30 x 18 = 241,920 model selections.

4.3 Results Analysis and Discussion

The results in *Table 1* illustrate the average success rates (S) for each criterion and the rates for underfitting (U) and overfitting (O) (Andrews and Currim (2003a; 2003c)). For example, BIC identifies the true number of segments in 47% of all simulation runs in which the sample size is held constant at $N = 100$ and all other factors are varied according to the factor levels described above. At this factor level, BIC overestimates (underestimates) the true number of segments in 6% (47%) of all simulation runs (e.g., the criterion pointed at the three- to six-segment solution where $S = 2$ and at the five- to eight-segment-solution where $S = 4$).

The results show that AIC_4 is the best information criterion to use with a large variety of data configurations. With an overall success rate of 58%, AIC_4 proves to be advantageous, particularly in more complex model set-ups (74%). BIC also performs well (overall success rate, 57%), especially when analyzing models using a higher number of observations (73%) and more distinct segment-specific path coefficients (88%). Similarly, CAIC and HQ perform favorably with success rates of 55%. PE, PC, AIC_3, NFI, and MDL_2 achieve significantly lower overall success rates between 39% and 45%. All other criteria (AIC, AIC_c, MDL_5, lnL_c, NEC, ICL-BIC, AWE, CLC, and EN) exhibit very unsatisfactory success rates of 28% and lower. AIC achieved the worst performance of only 6%.

With overfitting quotas of more than 80%, the three criteria AIC, AIC_c, and EN have a propensity to overestimate the true number of segments. In contrast to this finding, MDL_5, lnL_c, ICL-BIC, and AWE exhibit a strong tendency to underestimate the prespecified number of segments with underfitting quotas of at least 77%. Consequently, these criteria should be used in cases in which an overestimation must be avoided at all costs.

Of the criteria with the highest success rates, BIC and CAIC show a clear-cut underfitting tendency, while AIC_4 and HQ provide results in both over- and underfitting directions. Only AIC_3 has a relatively high success rate (43%) and a very strong overfitting tendency. *Tables 2* and *3* provide a detailed analysis of these criteria, separated into a one- through six-segment solution (for $S = 2$; *Table 2*) and a one- through eight-segment solution (for $S = 4$; *Table 3*), respectively[4]. The results indicate that for $S = 4$ (*Table 3*), both BIC and CAIC either match or clearly underestimate the correct number of segments. In contrast, AIC_3 either matches the prespecified number of segments or tends to strongly overestimate the correct number of segments. Finally, AIC_4 and HQ show a more or less equal distribution in the number of segments with which this criterion over- and underfits the correct number of segment.

In view of these findings, we combine the criteria with high success rates and pronounced tendencies to over- and underestimate the correct number of segments. In about one third (31%) of all cases, AIC_3 and CAIC simultaneously indicate the correct number of segments. Likewise, in 6% of all cases, both criteria indicate the same, incorrect, number of segments. Thus, whenever AIC_3 and CAIC indicate the same number of segments, this result meets the correct number of segments in 84% of all cases. Alternatively, a joint consideration of AIC_3 and BIC appears promising, because this combination yields the true number of segments in 82% of all cases where both criteria indicate the same number of segments.

Overall, the success rates of the criteria generally increase with lower numbers of segments, more observations, higher differences between the segment-specific path coefficients, and smaller disturbance terms. Even though we would expect the model selection criteria's performance to decline with unbalanced relative segment sizes, the performance remains at levels that are similar to those in situations of equally sized segments. This result provides support for FIMIX-PLS' exceptionally high degree of robustness in respect of this factor (Esposito Vinzi et al. (2007)). Furthermore, although we might suppose that more complex path models would lead to a decline in performance, the results of the computational experiments clearly show that the model selection criteria perform better in the more complex path model constellation. Andrews and Currim (2003a) report a similar result in their study on mixture logit models and surmise that less complex models provide a better fit, thus leaving less opportunity for improvement in fit by increasing the number of segments. The same reason holds in our study. A detailed analysis shows that for $S = 1$, the lnL value computed across all the factor levels is almost three times higher in the complex model than in the simple model. This difference is also more pronounced in a one-segment solution than in higher-segment solutions in the complex model.

To further examine the results of this study, we determine the effects of the simulation design's factors on the criteria success rates. Therefore, we meta-analyze the results of the criteria by fitting multinomial logistic regression models to the success

4 The remaining criteria's detailed analysis results are available online at http://www.smartpls.de/sbr-app1.pdf.

Table 1: Success (S), underfitting (U) and overfitting (O) rates of the criteria

		AIC			AIC_3		
		U	**S**	O	U	**S**	O
Factor 1:	2	0%	**8%**	92%	5%	**49%**	46%
# segments	4	0%	**5%**	95%	8%	**38%**	54%
Factor 2:	100	0%	**6%**	94%	6%	**36%**	57%
# observations	400	0%	**6%**	94%	7%	**48%**	46%
Factor 3:	10%	0%	**5%**	95%	3%	**48%**	49%
Disturbance term	25%	0%	**7%**	92%	10%	**39%**	51%
Factor 4:	0.75	0%	**8%**	92%	0%	**51%**	49%
Path distance	0.25	0%	**5%**	95%	14%	**36%**	50%
Factor 5:	simple	0%	**3%**	97%	6%	**22%**	71%
Model complexity	complex	0%	**10%**	90%	8%	**64%**	28%
Factor 6:	balanced	0%	**6%**	94%	7%	**42%**	51%
Segment sizes	unbalanced	0%	**7%**	93%	7%	**46%**	46%
Overall		0%	**6%**	93%	7%	**43%**	50%
		HQ			**MDL_2**		
		U	**S**	O	U	**S**	O
Factor 1:	2	11%	**61%**	29%	44%	**54%**	2%
# segments	4	30%	**50%**	20%	76%	**24%**	0%
Factor 2:	100	20%	**43%**	37%	74%	**24%**	2%
# observations	400	18%	**66%**	16%	44%	**56%**	0%
Factor 3:	10%	14%	**62%**	23%	49%	**49%**	1%
Disturbance term	25%	26%	**48%**	26%	71%	**28%**	1%
Factor 4:	0.75	0%	**74%**	26%	30%	**69%**	1%
Path distance	0.25	40%	**37%**	23%	90%	**9%**	1%
Factor 5:	simple	24%	**37%**	39%	71%	**29%**	0%
Model complexity	complex	17%	**74%**	10%	49%	**49%**	2%
Factor 6:	balanced	19%	**55%**	26%	59%	**40%**	1%
Segment sizes	unbalanced	23%	**56%**	21%	62%	**37%**	1%
Overall		20%	**55%**	24%	60%	**39%**	1%
		PC*			**NFI***		
		U	**S**	O	U	**S**	O
Factor 1:	2	0%	**85%**	15%	0%	**79%**	21%
# segments	4	91%	**2%**	7%	89%	**3%**	8%
Factor 2:	100	44%	**39%**	17%	42%	**34%**	23%
# observations	400	49%	**47%**	5%	48%	**43%**	9%
Factor 3:	10%	47%	**45%**	7%	47%	**42%**	11%
Disturbance term	25%	44%	**42%**	14%	42%	**40%**	18%
Factor 4:	0.75	50%	**47%**	3%	49%	**45%**	6%
Path distance	0.25	41%	**40%**	18%	40%	**37%**	24%
Factor 5:	simple	43%	**42%**	15%	42%	**38%**	20%
Model complexity	complex	48%	**46%**	6%	47%	**44%**	9%
Factor 6:	balanced	46%	**43%**	11%	45%	**39%**	16%
Segment sizes	unbalanced	44%	**46%**	10%	43%	**45%**	12%
Overall		46%	**44%**	11%	44%	**41%**	15%

	AIC_4			**AIC_c**			**BIC**			**CAIC**	
U	**S**	O	U	**S**	O	U	**S**	O	U	**S**	O
17%	**65%**	18%	1%	**20%**	79%	27%	**69%**	4%	30%	**68%**	2%
35%	**50%**	14%	1%	**12%**	87%	53%	**45%**	2%	56%	**42%**	2%
31%	**47%**	22%	1%	**22%**	77%	47%	**47%**	6%	50%	**46%**	4%
20%	**69%**	11%	1%	**10%**	89%	26%	**73%**	1%	28%	**72%**	1%
18%	**66%**	16%	0%	**15%**	85%	29%	**68%**	3%	31%	**67%**	2%
34%	**49%**	16%	2%	**17%**	81%	51%	**46%**	3%	54%	**44%**	2%
1%	**80%**	19%	0%	**19%**	81%	9%	**88%**	4%	11%	**87%**	2%
51%	**35%**	14%	2%	**14%**	85%	71%	**26%**	3%	75%	**23%**	2%
32%	**41%**	26%	1%	**5%**	94%	53%	**44%**	3%	55%	**43%**	2%
20%	**74%**	6%	1%	**27%**	73%	27%	**70%**	3%	30%	**67%**	3%
26%	**58%**	16%	1%	**16%**	83%	37%	**60%**	4%	39%	**59%**	2%
27%	**56%**	17%	1%	**16%**	84%	47%	**51%**	2%	50%	**48%**	2%
26%	**58%**	16%	1%	**16%**	83%	40%	**57%**	3%	43%	**55%**	2%
	MDL_5			**lnL_c**			**NEC***			**ICL-BIC**	
U	**S**	O	U	**S**	O	U	**S**	O	U	**S**	O
61%	**39%**	0%	49%	**22%**	28%	0%	**45%**	55%	74%	**25%**	1%
93%	**7%**	0%	61%	**5%**	34%	25%	**11%**	64%	88%	**11%**	1%
89%	**11%**	0%	36%	**5%**	58%	6%	**18%**	76%	80%	**17%**	2%
61%	**39%**	0%	75%	**16%**	9%	17%	**34%**	49%	81%	**19%**	0%
69%	**31%**	0%	46%	**18%**	36%	14%	**36%**	50%	75%	**24%**	1%
84%	**16%**	0%	64%	**9%**	27%	11%	**19%**	69%	87%	**12%**	1%
56%	**44%**	0%	41%	**23%**	37%	19%	**45%**	36%	63%	**35%**	2%
97%	**3%**	0%	70%	**5%**	26%	6%	**10%**	84%	100%	**0%**	0%
85%	**15%**	0%	68%	**8%**	24%	3%	**19%**	78%	99%	**0%**	0%
68%	**32%**	0%	43%	**19%**	38%	22%	**36%**	42%	63%	**35%**	2%
75%	**25%**	0%	56%	**11%**	33%	12%	**26%**	62%	81%	**18%**	1%
81%	**19%**	0%	54%	**19%**	27%	15%	**31%**	55%	82%	**17%**	1%
77%	**23%**	0%	55%	**14%**	31%	13%	**28%**	60%	81%	**18%**	1%
	PE*			**AWE**			**CLC**			**EN***	
U	**S**	O	U	**S**	O	U	**S**	O	U	**S**	O
0%	**89%**	11%	67%	**33%**	0%	50%	**22%**	28%	0%	**15%**	85%
93%	**2%**	5%	95%	**3%**	1%	79%	**7%**	14%	6%	**5%**	89%
45%	**41%**	13%	87%	**12%**	0%	55%	**4%**	41%	4%	**6%**	90%
49%	**48%**	3%	75%	**23%**	2%	74%	**19%**	7%	3%	**5%**	91%
48%	**47%**	5%	75%	**24%**	2%	53%	**20%**	27%	3%	**12%**	85%
45%	**44%**	11%	87%	**12%**	0%	75%	**9%**	16%	3%	**8%**	88%
50%	**48%**	3%	63%	**36%**	2%	41%	**26%**	33%	2%	**13%**	85%
43%	**43%**	14%	100%	**0%**	0%	87%	**3%**	10%	4%	**7%**	88%
44%	**43%**	12%	92%	**8%**	0%	81%	**7%**	11%	5%	**8%**	87%
49%	**47%**	4%	70%	**28%**	2%	47%	**22%**	31%	2%	**12%**	86%
47%	**45%**	8%	81%	**18%**	1%	65%	**11%**	24%	3%	**6%**	91%
46%	**47%**	8%	81%	**19%**	0%	63%	**21%**	15%	2%	**19%**	79%
47%	**45%**	8%	81%	**18%**	1%	64%	**15%**	21%	3%	**10%**	87%

* Factor 1: Number of segments; Factor 2: Number of observations; Factor 3: Disturbance term; Factor 4: Distance between segment-specific path coefficients; Factor 5: Model complexity; Factor 6: Relative segment sizes.
By its formal definition (*Table A1*, Appendix), the criterion does not provide reasonable results for the one-segment solution.

Table 2: Detailed analysis of selected criteria *(S* = 2)

Factor 1: 2 segments		AIC$_3$						AIC$_4$						BIC					
		1	**2**	3	4	5	6	1	**2**	3	4	5	6	1	**2**	3	4	5	6
Factor 2: # observations	100	6%	**46%**	12%	9%	13%	14%	21%	**59%**	9%	3%	4%	4%	34%	**62%**	2%	0%	1%	1%
	400	3%	**55%**	9%	6%	14%	13%	10%	**77%**	4%	3%	4%	3%	15%	**83%**	2%	0%	0%	0%
Factor 3: Disturbance term	10%	1%	**54%**	12%	7%	12%	14%	9%	**73%**	9%	3%	4%	3%	17%	**79%**	2%	1%	1%	1%
	25%	9%	**44%**	10%	9%	14%	14%	26%	**56%**	6%	3%	5%	4%	38%	**58%**	2%	0%	1%	1%
Factor 4: Path distance	0.75	0%	**54%**	13%	7%	13%	13%	0%	**78%**	10%	3%	4%	4%	0%	**94%**	3%	0%	1%	1%
	0.25	11%	**44%**	9%	9%	13%	14%	34%	**51%**	5%	3%	4%	4%	55%	**43%**	0%	0%	1%	1%
Factor 5: Model complexity	simple	8%	**20%**	14%	13%	21%	24%	27%	**43%**	12%	5%	7%	6%	41%	**54%**	3%	1%	1%	1%
	complex	2%	**78%**	8%	3%	5%	4%	7%	**87%**	3%	1%	1%	1%	14%	**84%**	0%	0%	1%	1%
Factor 6: Segment sizes	balanced	5%	**49%**	12%	8%	12%	15%	17%	**64%**	8%	3%	4%	4%	25%	**70%**	3%	0%	1%	1%
	unbalanced	5%	**50%**	10%	9%	14%	13%	17%	**66%**	6%	3%	5%	3%	33%	**66%**	0%	0%	1%	1%
Overall		5%	**49%**	11%	8%	13%	14%	17%	**65%**	7%	3%	4%	4%	27%	**69%**	2%	0%	1%	1%

Factor 1: 2 segments		CAIC						HQ					
		1	**2**	3	4	5	6	1	**2**	3	4	5	6
Factor 2: # observations	100	36%	**61%**	0%	0%	1%	1%	13%	**56%**	11%	6%	7%	7%
	400	17%	**83%**	0%	0%	0%	0%	5%	**70%**	5%	4%	9%	6%
Factor 3: Disturbance term	10%	19%	**79%**	1%	0%	1%	1%	4%	**68%**	11%	5%	7%	6%
	25%	40%	**58%**	0%	0%	1%	1%	17%	**54%**	8%	6%	8%	8%
Factor 4: Path distance	0.75	0%	**98%**	1%	0%	1%	1%	0%	**70%**	11%	5%	8%	6%
	0.25	59%	**39%**	0%	0%	1%	1%	21%	**51%**	8%	5%	7%	8%
Factor 5: Model complexity	simple	44%	**55%**	1%	0%	1%	0%	18%	**34%**	14%	9%	13%	12%
	complex	16%	**82%**	0%	0%	1%	1%	4%	**87%**	4%	1%	2%	2%
Factor 6: Segment sizes	balanced	27%	**71%**	0%	0%	1%	1%	9%	**59%**	11%	6%	7%	7%
	unbalanced	36%	**63%**	0%	0%	1%	1%	14%	**64%**	6%	3%	8%	5%
Overall		30%	**68%**	0%	0%	1%	1%	11%	**61%**	9%	5%	8%	7%

Table 3: Detailed analysis of selected criteria ($S = 4$)

Factor 1: 4 segments		AIC$_3$ 1	2	3	**4**	5	6	7	8	AIC$_4$ 1	2	3	**4**	5	6	7	8	BIC 1	2	3	**4**	5	6	7	8
Factor 2: # observations	100	1%	3%	3%	**36%**	7%	10%	21%	18%	19%	11%	7%	**45%**	5%	4%	5%	4%	39%	18%	4%	**36%**	1%	0%	1%	1%
	400	0%	2%	8%	**41%**	10%	11%	14%	14%	10%	8%	13%	**62%**	3%	2%	2%	0%	23%	12%	1%	**63%**	0%	0%	0%	0%
Factor 3: Disturbance term	10%	1%	0%	4%	**42%**	8%	10%	18%	17%	9%	7%	11%	**59%**	4%	2%	4%	3%	24%	14%	3%	**57%**	1%	0%	1%	1%
	25%	1%	6%	5%	**34%**	9%	11%	19%	16%	23%	13%	7%	**42%**	5%	4%	3%	3%	44%	18%	3%	**33%**	0%	1%	1%	1%
Factor 4: Path distance	0.75	0%	0%	0%	**48%**	9%	11%	16%	16%	0%	1%	1%	**81%**	7%	4%	3%	3%	5%	10%	3%	**81%**	1%	0%	1%	0%
	0.25	2%	6%	9%	**28%**	7%	10%	22%	17%	31%	19%	18%	**20%**	3%	2%	5%	3%	63%	22%	3%	**9%**	0%	1%	1%	1%
Factor 5: Model complexity	simple	1%	1%	1%	**25%**	6%	15%	21%	29%	25%	7%	6%	**40%**	6%	6%	6%	4%	53%	11%	1%	**34%**	1%	1%	0%	1%
	complex	1%	5%	8%	**51%**	10%	6%	16%	4%	6%	14%	13%	**61%**	3%	0%	2%	1%	15%	21%	4%	**56%**	0%	0%	1%	1%
Factor 6: Segment sizes	balanced	1%	3%	4%	**35%**	10%	9%	23%	15%	16%	9%	9%	**53%**	5%	3%	4%	3%	33%	13%	3%	**49%**	0%	0%	1%	1%
	unbalanced	1%	3%	5%	**43%**	5%	12%	11%	20%	14%	13%	10%	**47%**	5%	4%	4%	3%	35%	23%	4%	**36%**	1%	0%	0%	1%
Overall		1%	3%	4%	**38%**	8%	10%	19%	17%	16%	10%	9%	**50%**	5%	3%	4%	3%	34%	16%	3%	**45%**	0%	0%	1%	1%

Factor 1: 4 segments		CAIC 1	2	3	**4**	5	6	7	8	HQ 1	2	3	**4**	5	6	7	8
Factor 2: # observations	100	43%	18%	4%	**33%**	0%	0%	1%	1%	12%	11%	7%	**44%**	7%	5%	9%	6%
	400	26%	9%	3%	**61%**	0%	0%	0%	0%	10%	8%	13%	**62%**	3%	2%	2%	0%
Factor 3: Disturbance term	10%	26%	15%	2%	**55%**	1%	0%	1%	1%	6%	7%	11%	**57%**	5%	3%	7%	3%
	25%	48%	16%	4%	**29%**	0%	1%	1%	1%	16%	13%	7%	**43%**	6%	5%	6%	4%
Factor 4: Path distance	0.75	8%	10%	4%	**77%**	1%	0%	1%	0%	0%	0%	0%	**77%**	8%	5%	6%	4%
	0.25	67%	20%	3%	**8%**	0%	1%	1%	1%	22%	20%	18%	**23%**	4%	3%	8%	4%
Factor 5: Model complexity	simple	56%	10%	1%	**33%**	0%	0%	0%	1%	18%	7%	5%	**40%**	8%	7%	9%	7%
	complex	19%	21%	6%	**52%**	0%	0%	1%	1%	4%	13%	13%	**60%**	3%	1%	5%	1%
Factor 6: Segment sizes	balanced	38%	10%	3%	**47%**	0%	0%	1%	1%	11%	9%	9%	**50%**	6%	3%	8%	4%
	unbalanced	36%	25%	4%	**33%**	0%	0%	0%	1%	10%	13%	9%	**49%**	5%	6%	5%	3%
Overall		37%	15%	3%	**42%**	0%	0%	1%	1%	11%	10%	9%	**50%**	6%	4%	7%	4%

data. We code the dependent variable as –1, the criterion underestimated the correct number of segments; 0, the criterion identified the correct number of segments (reference category); and 1, the criterion overestimated the correct number of segments. Following Andrews and Currim (2003a) and Andrews and Currim (2003c), we fit separate logistic models to the data of each of the criteria. *Table 4* shows the resulting parameter estimates for the five criteria AIC_3, AIC_4, BIC, CAIC, and HQ, discussed above[5]. The results indicate whether the explanatory variables increase or decrease the log odds of underestimating (dependent equals –1) or overestimating (dependent equals 1) the correct number of segments.

For example, in the case of AIC_4, increasing the error variance – that is, switching from the reference category (disturbance term = 10%) to the higher category (disturbance term = 25%) – increases the log odds of under- or overestimating the correct number of segments, which is mirrored in the positive β coefficients (1.95 for underestimations and 0.61 for overestimation). Similarly, because both β coefficients are negative, increasing the distance between segment-specific path coefficients from 0.25 (reference category) to 0.75 decreases the log odds of misspecifying the correct number of segments. Overall, increasing the number of observations, the distance between segment-specific path coefficients, or model complexity increases the log odds of estimating the true number of segments. We note that the influence of relative segment size is small (but mostly significant in the case of overestimation), which is also mirrored in the somewhat inconsistent descriptive results of this factor (*Table 1*).

5 Summary and Conclusion

In PLS path modeling applications, uncovering and treating unobserved heterogeneity is critical to the quality of the result presentations and interpretations (Rigdon, Ringle, and Sarstedt (2010)). This important issue should be a matter of concern when evaluating any PLS path modeling results (Ringle, Sarstedt, and Mooi (2010); Sarstedt, Schwaiger, and Ringle (2009); Hair, Ringle, and Sarstedt (2011)). Sarstedt's (2008a) review of approaches to response-based segmentation within a PLS framework reveals that FIMIX-PLS (Hahn et al. (2002)) is the primary method in this respect[6].

Answering the call for a further evaluation of the problematic aspects of the FIMIX-PLS approach when it was initially presented by Hahn et al. (2002), and in subsequent studies on computational experiments and in empirical applications (Esposito Vinzi et al. (2007); Ringle, Sarstedt, and Mooi (2010); Ringle, Wende, and Will (2010); Sarstedt and Ringle (2010); Sarstedt, Schwaiger, and Ringle (2009)), in this paper we address the problem of model selection by providing a comprehensive evaluation of 18 different model selection criteria in the context of FIMIX-PLS. Despite FIMIX-PLS' frequent application in recent research work, the question of how many segments

5 The analysis results of all the remaining criteria are available online at http://www.smartpls.de/sbr-app1.pdf

6 The technique has been implemented in the SmartPLS software application (Ringle, Sarstedt, and Schlittgen (2005b)), and hence, is generally available for PLS path modeling applications.

Table 4: Meta analysis of best-performing criteria: Multinomial logistic regression results

Dependent		Reference category	AIC_3 β	AIC_4 β	BIC β	CAIC β	HQ β
–1 under-estimation	Factor 1: # segments	2	0.84	1.94	4.66	5.08	1.89
	Factor 2: # observations	100	–0.41 ns	–1.71	–4.37	–4.70	–1.00
	Factor 3 : Disturbance term	10%	1.58	1.95	4.10	4.43	1.50
	Factor 4: Path distance	0.25	–24.16	–5.89	–9.29	–9.58	–6.51
	Factor 5: Model complexity	low	–1.07	–2.14	–4.94	–4.62	–1.80
	Factor 6: Segment sizes	un-balanced	0.25 ns	0.68	0.38 ns	0.21 ns	0.22 ns
	Intercept		–1.66	–0.15 ns	2.20	2.66	–0.43 ns
1 over-estimation	Factor 1: # segments	2	0.55	0.27 ns	0.95 ns	2.63	0.02 ns
	Factor 2: # observations	100	–0.67	–1.43	–2.85	–4.24	–1.63
	Factor 3 : Disturbance term	10%	0.35	0.61	1.35	2.28	0.58
	Factor 4: Path distance	0.25	–0.49	–1.17	–2.81	–5.02	–1.03
	Factor 5: Model complexity	low	–2.08	–2.34	–1.81	–1.83	–2.42
	Factor 6: Segment sizes	un-balanced	0.59	0.57	1.37	1.01 ns	1.05
	Intercept		0.87	0.08 ns	–1.30	–1.08 ns	0.32 ns
	-2 logL		403.27	448.53	333.11	293.10	452.69
	%correct		68.3	76.6	94.8	95.1	71.6

ns = nonsignificant; all others are significant at $p \leq 0.01$.
Factor 1: Number of segments; Factor 2: Number of observations; Factor 3: Disturbance term; Factor 4: Distance between segment-specific path coefficients; Factor 5: Model complexity; Factor 6: Relative segment sizes.

should be retained from the data has hitherto not been investigated scientifically in this context.

In the overall results, AIC_4 shows the highest overall success rate of 58% for model selection in FIMIX-PLS, followed by BIC (57%), CAIC (55%), and HQ (55%). A detailed result analysis shows that a joint consideration of AIC_3 and CAIC is very promising, because these criteria indicate the correct number of segments in 84% of all cases in which both criteria indicate the same number of segments.

Furthermore, the results show the tendency of several criteria to under- and overfit. Although researchers usually conclude that such criteria are inappropriate for model selection (e.g., Andrews and Currim (2003a; 2003c); Henson, Reise, and Kim (2007)), we believe that these performances yield important implications. For example, if AIC indicates more segments than competing criteria, then due to its overfitting tendency, researchers should conclude that the appropriate number of segments to retain is lower than actually indicated by AIC. The same holds for underfitting, for example, for AWE or ICL-BIC. However, because of their low overall success rate, these criteria should not be directly used for model selection, as was common in past research studies that considered AIC, amongst others, in the course of their analysis (e.g., Hahn et al. (2002); Ringle (2006); Ringle et al. (2009); Sarstedt, Schwaiger, and Ringle (2009)).

In view of all the classification criteria's overall weak performance, the entropy concept does not appear promising for model selection in FIMIX-PLS path modeling. By basing the model selection decision primarily on entropy-based statistics, researchers may misspecify the number of segments, thus jeopardizing the validity of their results (e.g., the analyses by Conze (2007) and Scheer (2008) explicitly rely on Ramaswamy, DeSarbo, and Reibstein's (1993) entropy criterion). However, the entropy concept should not be disregarded per se, since it indicates the degree of separation between the segments. This criterion is critical to assessing whether the analysis produces well-separated clusters, which is important for deriving management implications from any analysis. Thus, researchers may revert to EN when its levels show relatively high disparity, while there are relatively few differences in the information criterion outcomes of two to three consecutive segments that lie at the minimum level of all the different numbers of analyzed segments' results. Nevertheless, researchers should rely primarily on information criteria when deciding on the number of segments in FIMIX-PLS. In summary, our key finding and decision rule are to use AIC_3 and CAIC jointly when evaluating FIMX-PLS results.

Our study's results match the findings of Andrews and Currim's (2003c) study in several regards. Both BIC and CAIC exhibit similar underfitting rates (38% | 40%), as well as success (61% | 58%) and overfitting rates (1% | 1%) compared to those of our study (40% | 43%, 57% | 55%, and 3% | 2%). However, although AIC_3 performed best overall in Andrews and Currim's (2003c) study, its performance is only average in our study. Further, AIC performs much worse in our study, which more closely resembles the results reported by Hawkins, Allen, and Stromberg (2001) and Sarstedt (2008b).

Compared to those of Andrews and Currim (2003c), the success rates in our study are generally lower and show a greater variance across the criteria. This result is due to the factor levels chosen, the FIMIX-PLS method's different properties and because in our study we consider a greater number of criteria. When we more closely compare the two studies' simulation designs, the reason for this divergence becomes obvious. Andrews and Currim (2003c) choose extremely high levels of mean separation between segment-specific parameters, but these levels do not reflect actual applications of regression-based mixture models well. In line with prior applications of FIMIX-PLS, in our research we use a minimum path coefficient separation level of 0.25, which strongly influences the criteria's overall performance. The average success rate of the criteria at this factor level is a mere 18% our study, compared to 47% in that of Andrews and Currim (2003c), who specify a minimum mean separation level of 0.5.

Our study investigates only the ability of the criteria to determine the correct number of segments, but it does not consider the quality of the parameter recovery. However, we could argue that in a situation with an increased number of segments in which the majority of observations are classified correctly and which includes a favorable parameter recovery in some segments, is preferable to a second situation in which the number of segments is correct but the parameters are biased. This conflict between segment and parameter recovery has not yet been thoroughly addressed in the academic literature and a preference for either one or another aspect depends on the researcher's subjective considerations.

Future research should continue to search for better model selection criteria. Research in this field requires additional elaborations to integrate the costs of a wrong model selection decision into the measures by fitting a penalty function. Following Andrews and Currim's (2003a) argument, managers must be enabled to consider the costs and benefits (in monetary units) of under- or overestimating the true number of segments. Research should also evaluate the role of additional data characteristics commonly encountered in empirical studies, such as missing values and multicollinearity. Further assessments of the data characteristics' influence on model selection criteria performance would prove valuable for developing new criteria specifically suited for the application of FIMIX-PLS in specific data constellations.

6 Appendix

Table A1: Information and classification criteria considered in the study

Criterion	Description	Reference
Information Criteria		
Akaike Information Criterion	$AIC = -2 \cdot lnL + 2 \cdot N_s$	Akaike (1973)
Small Sample AIC	$AIC_c = AIC + [2 \cdot (N_s + 1) \cdot (N_s + 2)]/(N - N_s - 1)$	Hurvich and Tsai (1989)
Modified AIC 3	$AIC_3 = -2 \cdot lnL + 3 \cdot N_s$	Bozdogan (1994)
Modified AIC 4	$AIC_4 = -2 \cdot lnL + 4 \cdot N_s$	Bozdogan (1994)
Bayes Information Criterion	$BIC = -2 \cdot lnL + ln(N) \cdot N_s$	Schwarz (1978)
Consistent AIC	$CAIC = -2 \cdot lnL + [ln(N) + 1] \cdot N_s$	Bozdogan (1987)
Minimum Description Length 2	$MDL_2 = -2 \cdot lnL + 2 \cdot ln(N) \cdot N_s$	Liang, Jaszczak and Coleman (1992)
Minimum Description Length 5	$MDL_2 = -2 \cdot lnL + 5 \cdot ln(N) \cdot N_s$	Liang, Jaszczak and Coleman (1992)
Hannan-Quinn Criterion	$HQ = -2 \cdot lnL + 2\, ln[ln(N)] \cdot N_s$	Hannan and Quinn (1979)
Classification Criteria		
Complete Log-Likelihood	$lnL_c = \sum_{i=1}^{N}\sum_{s=1}^{N} z_{is} ln(f(\eta_i \mid \xi_i, B_s, \Gamma_s, \Psi_s)) + \sum_{i=1}^{N}\sum_{s=1}^{N} z_{is} ln(\rho_s)$	Dempster, Laird, and Rubin (1977)
Normalized Entropy Criterion	$NEC = E(S) / [ln(S) - ln(1)]$	Celeux and Soromenho (1996)
Integrated Completed Likelihood-*BIC*	$ICL - BIC = -2 \cdot lnL + [ln(N)] \cdot N_s + 2 \cdot E(S)$	Biernacki, Celeux, and Govaert (2000)
Partition Coefficient	$PC = \sum_{i=1}^{N}\sum_{s=1}^{N} p_{is}^2 / N$	Bezdek (1981)
Non-Fuzzy Index	$NFI = \left[S\left(\sum_{i=1}^{N}\sum_{s=1}^{S} p_{is}^2\right) - N\right] \Big/ N \cdot (S-1)$	Roubens (1978)
Partition Entropy	$PE = -\left[\sum_{i=1}^{N}\sum_{s=1}^{S} p_{is} \cdot ln\, p_{is}\right] \Big/ N$	Bezdek (1981)
Approximate Weight of Evidence	$AWE = -2 \cdot lnL_c + 2 \cdot N_s \cdot [1{,}5 + ln(N)]$	Banfield and Raftery (1993)
Classification Likelihood Criterion	$CLC = -2 \cdot lnL + 2 \cdot E(S)$	Biernacki and Govaert (1997)
Entropy Criterion	$EN = 1 - \left[\sum_{i=1}^{N}\sum_{s=1}^{S} - p_{is} \cdot ln\, p_{is}\right] \Big/ N lnS$	Ramaswamy, DeSarbo, and Reibstein (1993)

Note: *lnL* describes the log-likelihood of the model, N_s is the number of parameters required to estimate the model with *S* segments, *N* is the sample size, p_{is} is the a-posteriori probability of observation *i* belonging to segment *s*, z_{is} is a 0/1 assignment variable of observation *i* to segment *s*, *E(S)* the estimated entropy for a model with *S* segments defined as $E(S) = -\sum_{i=1}^{N}\sum_{s=1}^{S} p_{is}\, ln\,(p_{is})$.

Figure A2: Simple PLS path model

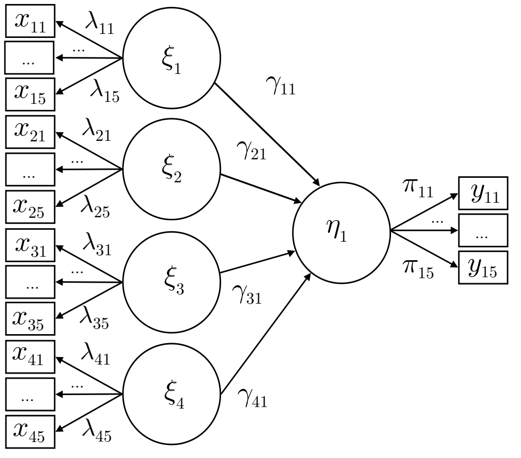

Figure A3: Complex PLS path model

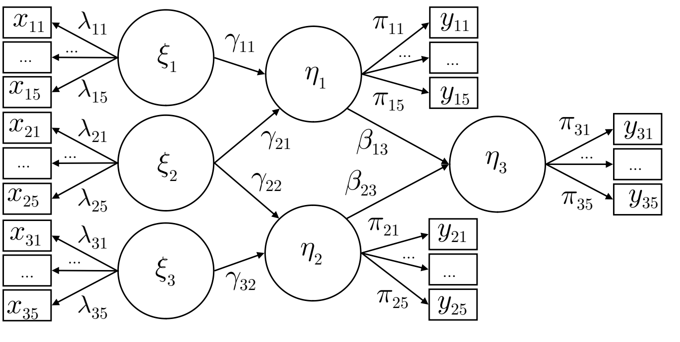

Table A4: FIMIX-PLS extensions

(1) The calculation of the distribution values as presented by Hahn et al. (2002) requires additional clarification, especially for the somewhat inconsistent (and confusing) namingof variables Equation 4 in the paper by Hahn et al. (2002, p. 249) presents the calculation of the distribution values as follows:

$$\eta_i = \sum_{s=1}^{S} \rho_s \left[\frac{|B_s|}{(2\pi)^{Q/2}\sqrt{|\Psi_s|}} \right] exp\left\{ -\frac{1}{2}(B_s\eta_i + \Gamma_s \xi_i)' \, \Psi_s^{-1}(B_s\eta_i + \Gamma_s\xi_i) \right\}, \tag{3}$$

This equation requires accounting for Equation 1 in Hahn et al.'s paper (2002, p. 248) and footnote 23 on the same page. Here, the authors explain that the inner relations of the PLS path model can be expressed by:

$$B\eta_i + \Gamma\xi_i = \zeta_i, \quad \text{with } B = I - B_s \wedge \Gamma = -\Gamma_s. \tag{4}$$

However, the vector of residuals ζ_i must be used when calculating the distribution values. Hence, the original presentation of Equation 4 in the paper by Hahn et al. (2002, p. 249) requires the following clarification:

$$\eta_i = \sum_{s=1}^{S} \rho_k \left[\frac{1}{(2\pi)^{Q/2}\sqrt{|\Psi_s|}} \right] exp\left\{ -\frac{1}{2}((I - B_s)\eta_i + (-\Gamma_s)\xi_i)' \, \Psi_s^{-1}(I - B_s)\eta_i + (-\Gamma_s)\xi_i) \right\}, \tag{5}$$

with $|B| = |I - B_s| = 1$.

(2) For a pre-specified number of S segments, the E-step in the FIMIX-PLS EM algorithm computation of results needs, as provisional estimates, the weighted least squares regressions of the previous M-step. The (S-) weighted least squares computation in the M-step of the FIMIX-PLS EM algorithm, as presented by Hahn et al. (2002, p. 253) in equations 14 and 15, is erroneous. The original presentation of these equations is given as follows:

$$\tau_{ms} = \left[\sum_{i=1}^{N} p_{is}(X'_{mi}X_{mi}) \right]^{-1} \left[\sum_{i=1}^{N} p_{is}(X'_{mi}Y_{mi}) \right] \tag{6}$$

$$\omega_{ms} = \left[\sum_{i=1}^{N} p_{is}(Y_{mi} - X_{mi}\,\tau_{ms})(Y_{mi} - X_{mi}\,\tau_{ms})' \Big/ I\rho_s \right] \tag{7}$$

However, this presentation must be corrected as follows:

$$\tau_{ms} = [(X'_m P_s X_m]^{-1} \, [X'_m P_s Y_m] \tag{8}$$

$$\omega_{ms} = [Y_m - X_m\,\tau_{ms})'(Y_m - X_m\tau_{ms})']P_s] \Big/ I\rho_s \tag{9}$$

Thus, the equations follow the normal weighted least squares procedure.

(3) An important issue in mixture models is the differentiation between the likelihood of the model from the observed data and the likelihood of the complete data problem that is used for solving the optimization problem in the EM algorithm. The likelihood of the observed data is given by Equation 5 in the paper by Hahn et al. (2002, p. 250):

$$L = \prod_{i=1}^{N}\left[\sum_{s=1}^{S} \rho_k\left[\frac{|B_s|}{(2\pi)^{Q/2}\sqrt{|\Psi_s|}} exp\left\{-\frac{1}{2}(B_s\eta_i + \Gamma_s \xi_i)' \Psi_s^{-1}(B_s\eta_i + \Gamma_s\xi_i)\right\}\right]\right]. \quad (10)$$

A simplified presentation of this equation is as follows

$$L = \prod_{i=1}^{N}\left(\sum_{s=1}^{S} \rho_s(f(\eta_i|\xi_i, B_s, \Gamma_s, \Psi_s))\right). \quad (11)$$

Following from this description, the log-likelihood of the model is

$$LnL = \sum_{i=1}^{N} ln\left(\sum_{s=1}^{S} \rho_s(f(\eta_i|\xi_i, B_s, \Gamma_s, \Psi_s))\right). \quad (12)$$

This log-likelihood presentation must be used to compute the information criteria for the model selection. Conversely, the complete log-likelihood function lnL_c (e.g., Dempster, Laird, and Rubin (1977)) must be used for optimization using the EM algorithm which takes the following form (cp. Equation 9 in Hahn et al. (2002, p. 251)):

$$LnL_C = \sum_{i=1}^{N}\sum_{s=1}^{S} z_{is} ln(f(\eta_i|\xi_i, B_s, \Gamma_s, \Psi_s)) + \sum_{i=1}^{N}\sum_{s=1}^{S} z_{is} ln(\rho_s). \quad (13)$$

Thus, a potential uncertainty about these two different versions of the log-likelihood may be avoided in the paper by Hahn et al. (2002). In fact, the FIMIX-PLS module in the current version of the SmartPLS software application (Ringle, Wende, and Will (2005b)) uses lnL_c from the EM algorithm for calculating both the final segmentation results and the information criteria outcomes, but the regular lnL computation should be used for the latter.

A5: Explanation of symbols

A_m	Number of exogenous latent variables in the inner path model as independent variables in regression m
a_m	Exogenous variable a_m with $a_m = 1,\ldots, A_m$
B_m	Number of endogenous latent variables in the inner path model as independent variables in regression m
b_m	Endogenous variable b_m with $b_m = 1,\ldots, B_m$
$\gamma_{a_m ms}$	Regression coefficient of a_m in regression m for segment s
$\beta_{b_m ms}$	Regression coefficient of b_m in regression m for segment s
τ_{ms}	$((\gamma_{a_m ms}),(\beta_{b_m ms})'$ vector of the regression coefficients
ω_{ms}	Cell(m x m) of Ψ_s
δ	Improvement of log-likelihood value
N	Number of observations $(i = 1,\ldots, N)$
S	Number of segments $(s = 1,\ldots, S)$
Q	Number of endogenous latent variables $(m = 1,\ldots, Q)$
I	Identity matrix
N_s	$N_s = (S - 1) + S \cdot R + S \cdot Q$ degrees of freedom for solutions with S segments
p_{is}	A-posteriori probability of membership of observation i and segment s
P_s	Vector of a posteriori probabilities of segment s
R	Number of predictors for all regressions in the structural model
X_m	Case values of the independent variable for regression m
Y_m	Case values of the dependent variable for regression m
z_{is}	0/1 assignment variable of observation i to segment s
	Distribution function of segment s
B_s	Matrix of path coefficients between endogenous latent variables in segment s
Γ_s	Matrix of path coefficients between exogenous and endogenous latent variables in segment s
ζ_i	Vector for endogenous latent variables' residuals of observation i
	Vector for endogenous latent variables' scores of observation i
	Vector for exogenous latent variables' scores of observation i
ρ_s	Relative size of segment s
ψ_s	Matrix with variances of the regressions in the structural model on the diagonal, zero else

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