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On the Use of Formative Measurement Specifications in Structural Equation Modeling: A Monte Carlo Simulation Study to Compare Covariance-Based and Partial Least Squares Model Estimation Methodologies

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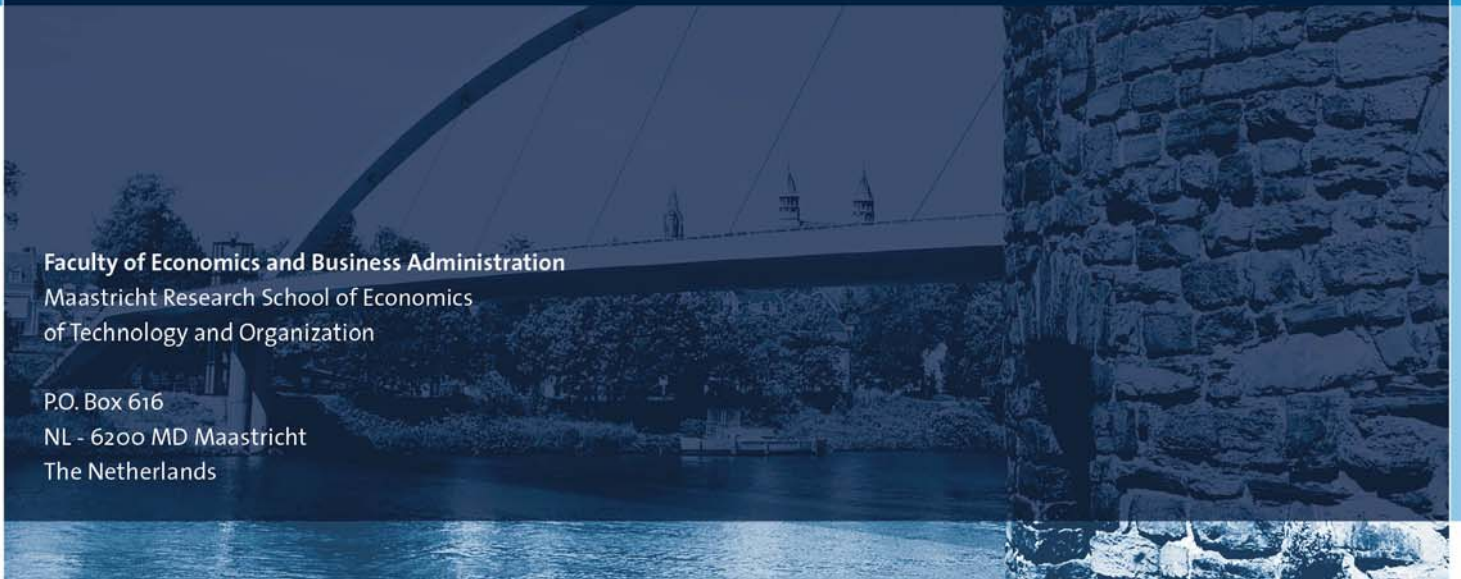
On the Use of Formative Measurement Specifications in Structural Equation Modeling: A Monte Carlo Simulation Study to Compare Covariance-Based and Partial Least Squares Model Estimation Methodologies

Abstract

The broader goal of this paper is to provide social researchers with some analytical guidelines when investigating structural equation models (SEM) with predominantly a formative specification. This research is the first to investigate the robustness and precision of parameter estimates of a formative SEM specification. Two distinctive scenarios (normal and non-normal data scenarios) are compared with the aid of a Monte Carlo simulation study for various covariance-based structural equation modeling (CBSEM) estimators and various partial least squares path modeling (PLS-PM) weighting schemes. Thus, this research is also one of the first to compare CBSEM and PLS-PM within the same simulation study. We establish that the maximum likelihood (ML) covariance-based discrepancy function provides accurate and robust parameter estimates for the formative SEM model under investigation when the methodological assumptions are met (e.g., adequate sample size, distributional assumptions, etc.). Under these conditions, ML-CBSEM outperforms PLS-PM. We also demonstrate that the accuracy and robustness of CBSEM decreases considerably when methodological requirements are violated, whereas PLS-PM results remain comparatively robust, e.g. irrespective of the data distribution. These findings are important for researchers and practitioners when having to choose between CBSEM and PLS-PM methodologies to estimate formative SEM in their particular research situation.

Introduction

Structural Equation Modeling (SEM) with latent variables is becoming increasingly popular in social and behavioral science (Boomsma, 2000) . The literature on SEM distinguishes between two different operationalizations of the relationships between latent variables and their observed indicators: the reflective (principal factor) and the formative (composite index) measurement models of latent variable. Numerous studies have by default or erroneously by design incorrectly specified their items as reflective when they should have used a formative measurement model operationalization (Jarvis, MacKenzie, & Podsakoff, 2003). This is somewhat surprising considering the fact that the understanding of formative indicator orientation is not new (Blalock, 1971) and previous research has focused on the nature, identification, and validation issues of formative indicators (Bollen & Lennox, 1991; Diamantopoulos & Winklhofer, 2001; Edwards & Bagozzi, 2000; MacCallum & Browne, 1993).

There are two statistical methodologies for estimating SEM with latent variables incorporating formative measurement models: the covariance-based (CBSEM) and the partial least squares path modeling (PLS-PM). A common misunderstanding found in the literature is that only PLS-PM allows the estimation of SEM that includes formative measurement models. Even though it has often been neglected, CBSEM is also capable of handling formative specifications, but requires that the model's identification be guaranteed and, thus, that certain model specification rules are followed. These CBSEM specification issues have been thoroughly addressed by MacCallum & Browne (1993).

Despite the broad discussion and establishment of the formative measurement model operationalization as a reasonable alternative to the reflective SEM mode, little attention has

so far been devoted to the conditions under which formative measures and their estimation method lead to precise and robust coefficients for the population sample (Browne, 1984). Some CBSEM estimators require the observed variables to be multivariate normally distributed. Violation of this assumption may distort the standard error of the path coefficient and parameters of the measurement models. However, the majority of data collected in behavioral research do not follow multivariate normal distributions (Micceri, 1989). This property is exacerbated with the use of formative indicators. It would be unreasonable to expect the observed data to follow a multivariate normal distribution in the population when using formative indicators.

Consequently, it is important to fully understand the effects of non-normality with respect to the accuracy and robustness of formative indicators in SEM. Our research is positioned to fill this gap in the literature, and this paper aims to contribute to the body of knowledge on the structural equation model specifications with formative (cause) indicators. The uniqueness of this study is twofold. It is the first one to investigate a model that primarily consists of formative measurement models by conducting a Monte Carlo simulation study to investigate the use of formative measurement model operationalization. Secondly, it is also the first one to compare the robustness and performance of CBSEM with respect to different estimator discrepancy functions, in concert with PLS-PM and its' different path weighting schemes. In this paper, we are mindful of the advice of Boomsma & Hoogland (2001) who, referring to a CBSEM context, stated that:

> The key objective of robustness research is to offer practical guidelines for applied work, so as to prevent non-robust analyses that would inevitably lead to wrong substantive inferences. Within that framework, a predominant question is: if structural models are to be analyzed, what estimation methods have to be preferred under what conditions? (p. 22)

Therefore, the objectives of this research are: (a) to demonstrate the implications of formative measurement model use in SEM, (b) to systematically and empirically test the accuracy and robustness of SEM methods with formative measurement models by using Monte Carlo simulations, and (c) to provide recommendations regarding the appropriate selection of SEM methods, given their specific research requirements.

This paper is organized as follows: We outline issues relevant to the operationalizing of formative measurement models and then address the methodological aspects of CBSEM and PLS-PM with regard to estimating formative relationships within SEM. Building on the findings of a literature review, we explain the design of our primary Monte Carlo simulation study on estimating a SEM that predominantly involves formative measurement model operationalizations by the means of the CBSEM and PLS-PM methodologies. Then, we highlight the pertinent results for each method and present a comparison of these analytical outcomes. Finally, we discuss the substantive implications of our findings for SEM applications and suggest future avenues for further research.

Formative Measurement Model Operationalization

Structural equation modeling applications often involve latent constructs with multiple indicators. The measurement or outer model specifies the relationship between observable variables (i.e., indicators) and latent variables. The direction of relationships and their causality is either in an effect (reflective) or a cause (formative) mode (Bollen, 1989; MacCallum & Browne, 1993). When discussing the nature and direction of relationships between constructs and observed measures, the literature on construct validity and associated measurement issues primarily emphasizes the reflective mode. The reflective measurement model has its roots in traditional test theory and psychometrics (Nunnally & Bernstein, 1994).

Each indicator represents an error-afflicted measurement of the latent variable. The direction of causality is from the construct to the indicators and observed measures are assumed to *reflect* variation in latent constructs. Altering the construct is therefore expected to manifest in changes in all the multi-item scale indicators.

Research on SEM recognizes that in the early stages of model development and in some situations, it is appropriate to determine causality from the measures to the construct, rather than vice versa (Blalock, 1971). Therefore, formative constructs have to be modeled as a (usually linear) combination of their indicators plus a disturbance term (Diamantopoulos, 2006). A frequently cited example of formative measurement is socio-economic status (SES), which is viewed as a composite of social and economic indicators such as occupation, education, residence, and income. If any one of these measures decreases, SES would decline. Figure 1 clarifies this issue: the arrows either point from the construct to the (reflective mode) indicators, or in the opposite direction.

Insert Figure 1 about here

Some researchers provide a conceptual discussion of the differences between formative and reflective measurement models (Bollen & Lennox, 1991; Diamantopoulos & Winklhofer, 2001; Edwards & Bagozzi, 2000) and design rules for determining the specific type of measurement model (Jarvis, MacKenzie, & Podsakoff, 2003). Based on these studies, the decision to use formative measurement models in SEM has specific implications for researchers.

One implication of the direction of causality is that omitting one indicator could omit a unique part of the formative measurement model and change the meaning of the variable (Diamantopoulos & Winklhofer, 2001). Thus, some researchers maintain that a formative measurement model requires a census of all indicators that determine the construct (Jarvis, MacKenzie, & Podsakoff, 2003). It is therefore quite obvious that formative indicators frequently do not follow a multinormal distribution. The response profile of our previous example leads to non-normal item distribution curves with varying degrees of skewness and kurtosis. This violation of multivariate normality can invalidate statistical hypothesis testing and strongly influence the choice of SEM estimations (Browne, 1984). It is clear that this area requires more research attention. Consequently, simulation studies need to investigate the different CBSEM and PLS-PM statistical estimation techniques to compare their relative performance in situations involving non-normal formative indicators. This type of research will lead to a better understanding of each method's robustness and precision in this specific research situation.

Formative Structural Equation Modeling Techniques

Two main approaches have been used to estimate formative measurement models within structural models: the CBSEM and the PLS-PM methods. Both methods have distinctive statistical characteristics (Fornell & Bookstein, 1982; Schneeweiß, 1991) and selecting an approach to SEM depends on the particular research situation. CBSEM is the method of choice for theory testing, while PLS-PM is appropriate for prognosis-oriented applications (Wold 1982b).

In CBSEM (see Rigdon, 1998), the parameter estimation of a given model minimizes the difference between the implied covariance matrix and the sample covariance matrix, with the

final result permitting the appropriate model fit to be determined. There are alternative CBSEM estimation techniques available to the researcher. The most commonly used approaches include: maximum likelihood (ML), generalized least squares (GLS), unweighted least squares (ULS), and asymptotic distribution free (ADF) estimation (Marcoulides & Hershberger, 1997). These CBSEM methods vary in their particular minimization of the discrepancy function, thereby including specific assumptions, for example, regarding sample size or the multivariate

(non-) normality of data.

The inclusion of formative measures in CBSEM has been well documented by Jöreskog & Sörbom (2001) and Jöreskog & Goldberger (1975). Williams, Edwards, & Vandenberg (2003) point out that formative indicators could be modeled in CBSEM by respecifying the formative indicators as latent exogenous variables with single indicators, fixed unit loadings, and a fixed measurement error. MacCallum & Brown (1993) illustrate various other formative model specifications that have adequate model identification. Consequently, if the hypothesized structural and measurement model is correct in the sense that it explains the covariance of all the indicators under the given assumption of different estimation methods, it is believed that the covariance-based methods should provide optimal estimates of the model parameters.

Instead of using the model to explain the covariance of all the indicators, the PLS-PM methodology (Wold, 1973, 1974, 1982a, 1982b) maximizes the variance of all dependent variables. Thus, parameter estimates are obtained based on the ability to minimize the residual variances of dependent (latent and observed) variables. To obtain the weights and subsequent loadings and structural estimates, the PLS-PM approach uses a two-stage

estimation algorithm (Lohmöller, 1989). In the first stage, after an initial, rather arbitrary, estimation of the latent variables, the process iteratively switches between the measurement and the structural model approximation by means of simple and/or multiple regressions until the parameter estimates converge into a set of weights used for estimating the latent variable scores. The PLS algorithm thereby aims at minimizing the residual variance of latent endogenous variables. The second stage involves a non-iterative application of ordinary least squares regression to obtain the loadings, weights, structural estimates, mean scores, and location parameters of the latent and observed variables. Three different kinds of weighting schemes have been used in this context: centroid, factor, and path weighting. Lohmöller (1989) and Tenenhaus, Vinzi, Chatelin, & Lauro (2005), for instance, present a general descriptions of the PLS methodology, particularly of the estimation of formative measurement models, whilst Chin (1998) presents a catalog of non-parametric model PLS-PM evaluation criteria as this statistical approach does not offer global goodness of fit criteria as CBSEM does.

In respect of a comparison of CBSEM and PLS (see Lohmöller, 1989), McDonald (1996) points out that Wold's (1980) (reflective) PLS Mode-A algorithm, like the ULS Method in CBSEM, maximizes the sum of the covariances of directly connected composites (subject to normalized weights). It furthermore allocates a (generally under-identified) rank one approximation to the individual correlations across the connected blocks of latent variables and their respective measurement models. On the other hand, Wold's (1980) (formative) PLS Mode-B algorithm maximizes the sum of correlations between connected blocks. It has no exact counterpart in CBSEM and McDonald (1996) conjectures that it would be difficult to empirically find or construct cases in which the results of PLS Mode-B and certain CBSEM methods (other than ULS) differ notably. Hence, we designed a simulation study and

conducted computational experiments to provide both researchers and practitioners with additional confidence regarding their decision to select an appropriate estimation technique for SEM incorporating formative measurement models.

Literature Review

A substantial number of simulation studies on CBSEM (e.g. Boomsma, 1983; Boomsma & Hoogland, 2001; Paxton, Curran, Bollen, Kirby, & Chen, 2001; Satorra, 1990; Stephenson & Holbert, 2003) primarily compare alternative CBSEM discrepancy functions and investigate their estimation bias, accuracy, and robustness with respect to sample size, and third and fourth-order data moments. Paxton, Curran, Bollen, Kirby, & Chen (2001), for example, provide an introduction to the design and implementation of a Monte Carlo simulation within the SEM area. These authors also present a comparison of the maximum likelihood and two-stage least squares with regard to different sample sizes and misspecifications. Boomsma & Hoogland (2001) conclude that there are non-convergence problems and improper CBSEM solutions in small samples (200 and less). Furthermore, under various non-normal conditions, maximum likelihood estimators in respect of large models have relatively good statistical properties compared to other CBSEM estimators. Satorra (1990) indicates that generally maximum likelihood and weighted least squares are robust against the violation of distributional assumptions. We do not intend to review the whole plethora of CBSEM robustness studies (especially those with reflective specifications) as this knowledge is assumed of the reader. Instead, focus is given to the discussion of previous study results centered on formative model specifications. Even a cursory review will reveal that the majority of analyses have been presented with models dominant in reflective specifications.

With respect to PLS-PM, it is difficult to find published robustness studies compared with the vast work already completed in the CBSEM realm. There are only a few publications utilizing PLS-PM that follow this line of research. Cassel, Hackl, & Westlund (1999) have performed a robustness simulation study on PLS-PM estimates by concentrating on varying the skewness of reflective indicators and having multicollinearity between latent variables and an artificial model misspecification. Their simulation results indicate that PLS-PM based on reflective measurement models is quite robust against skewness, as well as against multicollinearity between latent variables and misspecification due to the omission of a latent variable in the structural model. In respect to inner model coefficients, substantial effects are only observed on the estimates of extremely skewed data and for the erroneous omission of a highly relevant exogenous latent variable.

Chin & Newsted (1999) employ a Monte Carlo simulation for their analysis on PLS-PM with small samples. They find that the PLS approach can provide information about the appropriateness of indicators at sample size as low as 20. This study confirms the consistency at large (Jöreskog & Wold, 1982) in that the PLS-PM estimates will be asymptotically correct under the joint conditions of consistency: large sample size and large number of indicators per latent variable. Moreover, Chin, Marcolin, & Newsted (2003) employ a PLS-PM Monte Carlo simulation for an interactions effect model for varied sample sizes, altered numbers of indicators, and for the loading structure of manifest variables in respect of each of the constructs in their model. They finally provide a comparison of the SEM that incorporates latent variables with a summated scales approach. The authors provide evidence that increasing the number of reflective indicators will have a stronger impact on consistent estimations than increasing the sample size will have. This also holds for higher loadings and the associated reliabilities.

To date, there are only a handful of studies that compare the parameter estimates of both CBSEM and PLS-PM methods. Tenenhaus, Vinzi, Chatelin, & Lauro (2005) analyze a European customer satisfaction index (ECSI) model by means of reflective measures to compare CBSEM and PLS-PM estimates. They find that the outcomes of both methods are at comparable levels, but that CBSEM provides higher R^2 outcomes for the latent endogenous variables and that PLS-PM exhibits higher correlations between indicators and their associated latent variable. The latter is due to the PLS-PM estimation being more data driven and being more substantially influenced by the manifest variables.

The Hsu, Chen, & Hsieh (2006) article features robustness testing of a reflective measurement model orientation. They compare various estimators, including a more recent artificial neural network-based (ANN) SEM technique, PLS-PM, and CBSEM estimations of 200 simulated samples in respect of various scenario designs (e.g., skewness of data). The simulated model only consists of reflective measures and is based on a simple ECSI model structure. Hsu, Chen, & Hsieh (2006) find that the ANN-based SEM technique is similar to PLS-PM and conclude that all SEM techniques offer a certain robustness with respect to skewness of data. The results from this study confirm that PLS-PM underestimates structural path coefficients and that CBSEM is more sensitive to small sample size problems that experience larger deviations.

Our literature review reveals that PLS-PM overestimates the outer loadings of latent constructs and provides more conservative estimates of the inner model than ML-CBSEM. Furthermore, compared to symmetrical data, PLS-PM and ML-CBSEM estimates that incorporate reflective measurement models are negligibly influenced by skewness. CBSEM

methods are also more sensitive to small sample sizes than PLS-PM. It can thus be concluded that research on formative measures is still in its early stages regarding the precision and robustness of coefficients. The review of the literature supports our premise that there has been a dearth of robustness studies undertaken specifically comparing CBSEM and PLS-PM with a formative model specification.

Design of the Simulation Study

As we have previously outlined, a researcher has the choice of utilizing CBSEM and PLS-PM when investigating formative SEMs. This raises the question of which approach to select for SEM applications containing formative measurement models of the latent exogenous variables. A Monte Carlo simulation study (Paxton, Curran, Bollen, Kirby, & Chen, 2001) allows us to address this critical question. Our Monte Carlo design allows us to systematically study the bias, accuracy, and robustness for both the CBSEM and PLS-PM techniques' parameter estimates. The SEM underpinning our design and subsequent analyses (Figure 2) consists of three latent exogenous variables (ξ_1, ξ_2 and ξ_3) and two latent endogenous variables (η_1 and η_2). The manifest variables in the measurement models of the latent exogenous variables are formatively operationalized, while the latent endogenous variables are measured reflectively. This simple design specification has been selected for our simulation for an unambiguous investigation of the effects of non-normality by means of different SEM methods.

Insert Figure 2 about here

Researchers have to ensure that their CBSEM has been identified to indicate that the model fit is indeed a reasonable presentation of the phenomena under investigation. Approaches to

test identification (Rigdon, 1995) include following certain rules but also resolving algebraic solutions, analyzing the information matrix, and evaluating the augmented Jacobian matrix. The model presented in Figure 2 has been identified, because there are more equations describing the model than unknown parameters. However, MacCallum & Browne (1993) address the issue of model identification in CBSEM when formative measurement models are involved. In keeping with their rules – especially with respect to the formative latent exogenous variables ξ_1 and ξ_3, which have only one relationship to a latent endogenous variable – the variance values of the latent endogenous variables η_1 and η_2 need to be set to one in addition to applying the usual reflective CBSEM parameter constraints (Rigdon, 1998). The model in Figure 2 is also appropriate for PLS-PM. Besides other aspects, the model is recursive, latent variables are estimated by non-overlapping blocks of manifest variables, and the model operationalization fits the PLS-PM-specific assumptions of predictor specification (Chin, 1998; Lohmöller, 1989; Tenenhaus, Esposito Vinzi, Chatelin, & Lauro, 2005).

The underlying correlation matrix (Table 5 in the Appendix) of the data generation procedure has some unique characteristics that are important to note for this study. The manifest variables x_1, x_2, and x_3 are slightly to moderately correlated, while x_4 and x_5 have very low correlations with other manifest variables in the ξ_1 measurement model. However, x_4 and x_5 are strongly correlated with the indicators of the latent variables η_1 and η_2, while this does not hold for x_1, x_2, and x_3. The manifest variables x_6, x_7, and x_8 in the measurement model of the latent exogenous variable ξ_2 are poorly correlated. Here, only x_6 and x_7 have significant correlations with the η_1 and η_2 indicators. The manifest variables x_9 to x_{13} in the ξ_3 measurement model are slightly to moderately correlated. All five manifest variables have significant correlations with the indicators of the latent endogenous variable η_2. Finally, the

manifest variables y_1, y_2, and y_3 in the measurement model of the latent endogenous η_1 exhibit strong correlations. The same pattern holds for the η_2 indicators. The information on the correlation pattern is important for analyzing the simulation results.

Insert Table 1 about here

In this study, we pre-specify the relationships in the SEM according to Table 1 and then simulate data for the given parameters. The data generation process is consistent with the procedure described by Chin, Marcolin, & Newsted (2003) for a Monte Carlo PLS-SEM study. We developed a STATISTICA 7.1 (StatSoft, 2005) macro implementation to perform this type of approach in two studies: one on multivariate normal data and one on extremely non-normal data.

The first Monte Carlo simulation study includes the generation of 1000 sets of multivariate normal data that meet – in an evaluation of data simulation (Boomsma & Hoogland, 2001) – the expected raw data characteristics, impart convergence of CBSEM estimations, as well as proper solutions for the structural model regarding the positive sign of variances. Each data set consists of 300 cases, which is a large enough number for model estimation, as well as matching the average sample size of SEM simulation studies presented in academic literature (Stephenson & Holbert, 2003). Although simulation studies on CBSEM (e.g. Curran, Bollen, Paxton, Kirby, & Chen, 2002; Hu & Bentler, 1999; Marcoulides & Saunders, 2006; Satorra & Bentler, 2001) and PLS-PM (e.g. Cassel, Hackl, & Westlund, 1999; Chin, Marcolin, & Newsted, 2003) present varying sample sizes to answer specific methodological research questions, we do not add this level of complexity, which would also require systematic alteration of the number of indicators in the measurement models. In this study, we

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concentrate on CBSEM and PLS-PM comparisons for formative indicator specification. Previous simulation studies on reflective CBSEM indicate that 300 cases are sufficient to provide robust estimations, at least for ML-CBSEM estimation (Boomsma & Hoogland, 2001).

The second Monte Carlo simulation study undertaken in this investigation includes the same analytical design for non-normal data. The non-normal data specification has a skewness of two and kurtosis of eight, whereby the generation of non-normal multivariate random parameter values follows the Vale & Maurelli (1983) procedure implemented in the STATISTICA 7.1 program. This method is an extension of Fleishman's (1978) approach and, in comparison to other methods, fits our non-normal data generation purposes better (Reinartz, Echambadi, & Chin, 2002). The Vale & Maurelli (1983) technique can be used to generate adequate multivariate random numbers with pre-specified intercorrelations and univariate means, variances, skews, and kurtosis as efficiently as possible.

Both approaches, CBSEM and PLS-PM, are applied on the SEM in Figure 2 and on each set of data in the normal, as well as in the non-normal data scenario. This is undertaken contrasting CBSEM standard estimators (ML, GLS, ADF and ULS) and PLS-PM weighting schemes (centroid, factor, and path). The CBSEM computational results are also obtained via STATISTICA 7.1 software by employing a macro program that the authors designed for this study. In addition, a batch computing module was developed to process the simulated data by means of the SmartPLS 2.0 (Ringle, Wende, & Will, 2005) software to obtain PLS-PM results.

Results of the Monte Carlo Simulation Study

The Monte Carlo simulation presented in this study generates normal and non-normal data for a SEM incorporating formative operationalization of latent exogenous variables. These data are used to compare the model parameter estimations of the four main CBSEM discrepancy function procedures. Furthermore, our simulation study evaluates PLS-PM estimations that employ the different centroid, factor, and path inner model weighting schemes (Tenenhaus, Esposito Vinzi, Chatelin, & Lauro, 2005). Finally, we compare the CBSEM and PLS-PM results of the normal and non-normal data scenarios.

Comparison of Alternative CBSEM Model Estimation Techniques

In CBSEM, the parameters of a proposed model are estimated by minimizing the discrepancy between the empirical covariance matrix and a covariance matrix implied by the model. The common methods to measure this discrepancy are ML, GLS and ULS. The ADF/WLS method is a generalization of the other three CBSEM discrepancy functions that use a weight matrix based on a direct estimation of the residuals' fourth-order moments (Satorra & Bentler, 2001). When comparing the average formative model CBSEM estimates of the 1000 sets of normal and non-normal data, we find that the ML (Tables 2 and 3), GLS, and the ADF/WLS procedure exhibit roughly the same results pattern (Tables 6 to 9 in the Appendix).

ML and GLS perform at almost comparable levels. The only exception is the robustness of the formative measurement model estimates in the non-normal data scenario, with ML providing significantly better outcomes. ADF/WLS performs considerably weaker than the other two methods do. This study's results of the formative CBSEM model estimator performance are consistent with Boomsma & Hoogland's (2001) findings with regard to

reflective measurement models and the same selected number of cases. Our results are therefore in line with our expectations regarding the methodological characteristics of the discrepancy functions. The GLS and especially the ADF/WLS model estimation techniques usually require a high number of observations (several thousand) to provide robust outcomes. Consequently, the GLS and ADF/WLS results of small and medium-sized samples should also be interpreted with caution in formative SEM.

The ADF/WLS or ULS for model estimation relaxes the hard assumptions regarding the multivariate normality of the data when utilizing the ML or GLS estimator. ULS is a special ADF/WLS case and these methods do not automatically reveal standard errors or an overall chi-square fit statistic, but provide consistent estimates that are comparable to ML and seem relatively robust (Satorra, 1990). However, in our analysis, ULS does not fit the results pattern of the other CBSEM techniques. The average parameter estimations differ strongly from the given relationships and exhibit elevated deviations and relatively high outliers. McDonald (1996) confirms that ULS is equivalent to the reflective PLS-PM model estimation and is thus, ideally, not suited for our study of formative SEM measurement model operationalization. Consequently, it appears that in respect of the simulated scenarios that we investigated, ML provides the most appropriate CBSEM estimates, especially with regard to the moderate study sample size and specified formative model.

Comparison of Alternative PLS Model Estimation Techniques

The next analysis compares the outcomes of the centroid, factor, and path inner model PLS weighting schemes (Chin, 1998; Lohmöller, 1989; Tenenhaus, Esposito Vinzi, Chatelin, & Lauro, 2005). Applications of PLS illustrate that the alternative inner model weighting schemes only lead to marginal differences in the PLS-PM model estimates. Our simulation

study confirms this observation (Lohmöller, 1989; Tenenhaus, Esposito Vinzi, Chatelin, & Lauro, 2005). On average, the alternative weighting schemes provide the same parameter estimates for the model under investigation (Table 10 in the Appendix).

Comparison of CBSEM and PLS-PM

In our last analysis, we compare CBSEM and PLS-PM estimates for normal (Table 2) and non-normal (Table 3) data scenarios. This comparison for the cause-effect model employs ML, which offers the most suitable CBSEM parameter estimations in this simulation study. Our previous results illustrate that alternative PLS-PM inner weighting schemes provide almost identical results; we therefore only present PLS results for the path-weighting scheme as it is most frequently used in PLS-PM applications (Chin, 1998). In our computational experiments for normal and non-normal data constellations, the comparison of CBSEM and PLS-PM parameter estimates includes their bias (mean deviation), accuracy (mean absolute deviation), and robustness (mean squared error).

Insert Table 2 about here

Mean Deviation. Based on the mean deviation, the simulation study reveals that the ML-CBSEM estimation has a tendency to overestimate the true parameter values, while the PLS-PM has the reverse tendency, i.e. underestimating parameters in formative measurement models (for both normal and non-normal scenarios). It is notable that a bias in the opposite direction holds in respect of reflective outer measurement models, whereas ML-CBSEM has a tendency to underestimate and PLS-PM to overestimate the true values (for both simulations). Finally, ML-CBSEM tends to overestimate the inner relationships in the normal data scenario and exhibits both directions – overestimation and underestimation of

parameters – in the non-normal data scenario, while PLS-PM completely underestimates those parameters in both simulation scenarios.

Insert Table 3 about here

Mean Absolute Deviation. In the formative outer model, ML-CBSEM outperforms PLS-PM in all parameter estimations regarding accuracy in terms of the mean absolute deviation (MAD). It is important to note that both methods perform considerably better in the formative measurement model of latent exogenous variable ξ_3 compared to ξ_1 and ξ_2. The formative indicators of the latter two latent variables consist of a heterogeneous correlation pattern, while those of the manifest variables in the ξ_3 measurement model are relatively homogenous. In the inner model, ML-CBSEM and PLS-PM perform with great precision regarding the relationship between the latent endogenous variables η_1 and η_2. The MAD for the relationships between the latent exogenous ξ_1, ξ_2 and ξ_3 variables and the latent η_1 endogenous variable has a weaker outcome– especially in the case of PLS-PM, which is considerably less accurate in these relationships than ML-CBSEM – although this outcome is still at a relatively high level. The highest estimation precision is found in the reflective measurement models where the MAD for both methods is at a comparable level. Both procedures reveal two indicators with a significantly higher MAD: With regard to ML-CBSEM, both of these relationships are in the outer model of η_1 (paths to y_1 and y_3), while PLS-PM has one indicator with a higher MAD in each of the reflective measurement models (paths from η_1 to y_2 and η_2 to y_4). The accuracy of ML-CBSEM estimates decrease significantly with regard to the non-normal data scenario in all model relationships, whereas PLS-PM performs very well and only experiences a slight decrease in deviation with regard to the formative outer models (Table 4).

Insert Table 4 about here

Mean Squared Error. The mean squared error (MSE) provides additional information about the robustness of ML-CBSEM and PLS-PM parameter estimates. In the formative measurement model and in accordance with the MAD, we find that in the normal data example both methods have the lowest MSE of the parameter estimates for the latent variable ξ_3, which has indicators with a homogenous correlation pattern. Here, the difference between the maximum and minimum MSE is 0.005 for ML-CBSEM and 0.005 for PLS-PM, revealing the high robustness of the computations within the measurement model. In contrast, the MSE is substantially higher in the outer relationships of the latent variables ξ_1 and ξ_2. It is important to note that ML-CBSEM produces many estimates that deviate strongly from the true constrained population parameters, resulting in an increased MSE. This is most apparent with those manifest variables that have a high correlation pattern with the indicators of the latent endogenous variables and, consequently, a high pre-specified outer relationship. The difference between the maximum and minimum MSE is 0.186 in respect of the outer relationships of ξ_1 and 0.063 for ξ_2, indicating a reduced robustness of the ML-CBSEM parameter estimates. We did not find any comparable patterns in respect of the MSE of the measurement models estimated with PLS-PM in the normal data scenario. Here, the difference between the maximum and minimum MSE is 0.011 for the outer relationships of ξ_1 and 0.020 for ξ_2, representing a loss of robustness within the measurement model in comparison to ξ_3, but a much better result compared to the ML-CBSEM estimation.

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We find that ML-CBSEM tends to generate more erratic results– which are associated with high estimation errors (the difference between the estimated and expected path coefficients) – in respect of some indicators, while computations for others in the same, critical latent variable measurement model are robust. On the other hand, PLS-PM exhibits an equal and slight level of volatility regarding estimation errors in respect of all indicators and, consequently, a higher robustness for the estimated ξ_1 and ξ_2 outer relationships. In contrast, the MSE is considerably lower in the reflective outer models and principally performs at comparable levels in respect of ML-CBSEM and PLS-PM. Finally, the simulation study's inner model estimates provide MSE findings that are similar to those described in respect of the MAD.

A comparison of the normal data with the non-normal data scenario of these analytical results provides evidence that ML-CBSEM estimates increase their MSE considerably and, thus, decrease their robustness in all model relationships (Table 4). In contrast, PLS-PM only exhibits a slight MSE increase in respect of the formative measurement models, whereas the robustness of the parameter estimation does not substantially change in respect of the outer reflective and inner model relationships.

Summary and Conclusion

Researchers in the social sciences disciplines are swiftly moving towards using formative constructs within their SEM analyses. CBSEM and PLS-PM are two distinctive statistical techniques with which to estimate these types of models. Furthermore, the decision to apply the one or the other on a SEM depends on the particular research situation: CBSEM is the method of choice for theory testing, while PLS-PM is appropriate for prediction-oriented applications. Nevertheless, there is wide uncertainty about the applicability and behavior of

formative measurement model operationalizations when selecting and applying these techniques. Simulation studies can provide researchers with the confidence they need to support the application of this kind of SEM. However, the available simulation studies focus primarily on reflective model specifications. Our contribution is unique in that it is the first Monte Carlo simulation study to compare CBSEM and PLS-PM results containing formative indicators. Our five main findings are:

First, the CBSEM and PLS-PM estimates of the simulated sets of data are very close to the population parameters when averaged. A comparison of CBSEM discrepancy functions reveals that in our simulations study, ML provides the most appropriate estimates in respect of a SEM with formative latent exogenous and reflective latent endogenous variables. In accordance with reflective CBSEM simulation studies, we assume that alternative discrepancy functions require a greater number of cases than has been used in this study. In contrast, simulation results of the centroid, factor, and path model weighting schemes provide evidence that these alternatives for computing the inner PLS model relationships produce exactly the same results on average. Moreover, other simulation studies indicate that PLS-PM results are also robust regarding varying sample sizes.

Second, ML-CBSEM has a tendency to overestimate, while PLS-PM has tendency to underestimate parameters in the formative measurement model. In the formative outer model, ML-CBSEM outperforms PLS-PM in terms of accuracy of estimates. It is important to note that both methods perform considerably better in the formative measurement model with a homogenous correlation pattern than the two with the manifest variables with heterogeneous correlation patterns. These findings also hold for the robustness of estimates in formative measurement models.

Third, ML-CBSEM has a tendency to underestimate and PLS-PM to overestimate parameters in reflective outer models. Both methods present similar level outcomes. Compared to the formative outer models and the inner path model, we observe the highest accuracy and robustness regarding parameter estimations in the reflective measurement models.

Fourth, ML-CBSEM overestimates inner relationships data, while PLS-PM underestimates those parameters. We find that ML-CBSEM and PLS-PM perform particularly well in terms of accuracy and robustness where there is a relationship between the latent endogenous variables measured by reflective indicators. The accuracy in respect of inner relationships between latent exogenous and latent endogenous variables with different kinds of measurement models (formative exogenous and reflective endogenous) has a considerably weaker outcome, especially regarding PLS-PM. The same finding holds for the robustness of parameter estimations.

Fifth, CBSEM estimates in the formative measurement and the structural model decrease significantly regarding accuracy and robustness when data are non-normal, while the performance regarding reflective measurement models is not affected by changed data characteristics. We demonstrate the same type of results regarding PLS-PM, but the decrease in accuracy and robustness is far less.

In conclusion, formative CBSEM provides accurate and robust parameter estimates that are to some degree superior compared to PLS-PM. In keeping with their analytical goals and when their particular data situation meets CBSEM requirements, researchers should choose CBSEM rather than PLS-PM. However, if the premises for the applications of CBSEM are

violated, for example, regarding the required minimum number of observations for robust model estimations, or the multivariate normality assumption in ML-CBSEM, PLS-PM is a viable alternative. This technique's results are extremely robust irrespective of sample size and data distributions. Consequently, PLS-PM provides a viable approximation of model parameters when the prerequisites for CBSEM are not met. This kind of situation often occurs in formative scales, which incorporate all independent cause indicators that are relevant for explaining the latent variable. In, for example, success factor analyses (Lee & Tsang, 2001; Thatcher, Stepina, & Boyle; Wixom & Watson, 2001) or customer satisfaction studies (Westlund, Cassel, Eklof, & Hackl, 2001), manifest variables often exhibit non-normal distribution curves with varying degrees of skewness and kurtosis. PLS-PM should be the methodology of choice with this particular kind of data and model specification.

Our study is clearly not without limitations. As a first simulation study on formative indicators, it does not verify the generality of our findings. We emphasize that this work is intended to represent only a first step in this direction of comprehension. From the complexity of the estimation procedures, it is clear that the robustness of the model estimators can hardly be assessed in analytic form. The simulation study which is presented in this paper gives some insight into the effects of incorporating formative constructs in SEM. Furthermore, the standard methods of generating non-normal data according to correlation matrices are limited in terms of the levels of skewness and kurtosis that may be achieved (e.g., Vale & Maurelli, 1983). Future extensions of the simulation study should focus on more complex model structures with varied correlation pattern within the formative measurement model and samples sizes, and should incorporate other methods to generate data that may reach extremely high levels of skewness and kurtosis. These extensions should provide an additional basis for generalizing the reported findings to a broader extend.

The simulation study provides essential contributions on the body of knowledge for deciding whether to choose CBSEM or PLS-PM to estimate cause-effect relationship models. We share the view of Marcoulides and Sounders (2006) that most arguments for selecting PLS-PM against CBSEM in empirical applications are false or at least dubious. This paper reviews a key argument that formative measurement models must entail the use of PLS-PM (e.g. Chin 1998). Future research must continue in this direction and provide additional theoretical and empirical substantiation for a comparison of both methodologies. The results of existing and yet to come research must be consolidated in order to provide profound advices for researcher and practitioners to choose an appropriate multivariate analysis method for causal modeling that fits the goals of their particular analysis under certain model and/or data constellations.

Appendix

Insert Table 5 about here

Insert Table 6 about here

Insert Table 7 about here

Insert Table 8 about here

Insert Table 9 about here

Insert Table 10 about here

Tables

Table 1: A-priori specification of relationships in the SEM

Formative Measurement Models		
$[x_1]$-{0.1}->(Ksi_1)	$[x_6]$-{0.4}->(Ksi_2)	$[x_9]$-{0.4}->(Ksi_3)
$[x_2]$-{0.2}->(Ksi_1)	$[x_7]$-{0.6}->(Ksi_2)	$[x_{10}]$-{0.3}->(Ksi_3)
$[x_3]$-{0.1}->(Ksi_1)	$[x_8]$-{0.1}->(Ksi_2)	$[x_{11}]$-{0.2}->(Ksi_3)
$[x_4]$-{0.6}->(Ksi_1)		$[x_{12}]$-{0.2}->(Ksi_3)
$[x_5]$-{0.4}->(Ksi_1)		$[x_{13}]$-{0.4}->(Ksi_3)

Reflective Measurement Models	
(Eta_1)-{0.8}->$[y_1]$	(Eta_2)-{0.8}->$[y_4]$
(Eta_1)-{0.7}->$[y_2]$	(Eta_2)-{0.7}->$[y_5]$
(Eta_1)-{0.8}->$[y_3]$	(Eta_2)-{0.8}->$[y_6]$

Inner Model
(Ksi_1)-{0.4}->(Eta_1)
(Ksi_2)-{0.5}->(Eta_1)
(Ksi_3)-{0.6}->(Eta_1)
(Eta_1)-{0.6}->(Eta_2)

Table 2: Simulation results in respect of normal data

	Mean Value		Mean Deviation		Mean Absolute Deviation		Mean Squared Error	
Outer Model (Formative)	ML	PLS	ML	PLS	ML	PLS	ML	PLS
$[x_1]$-$\{0.1\}$->(Ksi_1)	0.107	0.085	0.008	-0.018	0.135	0.226	0.034	0.080
$[x_2]$-$\{0.2\}$->(Ksi_1)	0.210	0.177	0.010	-0.026	0.142	0.236	0.046	0.085
$[x_3]$-$\{0.1\}$->(Ksi_1)	0.105	0.084	-0.004	-0.023	0.137	0.230	0.053	0.079
$[x_4]$-$\{0.6\}$->(Ksi_1)	0.610	0.452	-0.003	-0.137	0.156	0.234	0.195	0.090
$[x_5]$-$\{0.4\}$->(Ksi_1)	0.421	0.308	-0.000	-0.078	0.151	0.222	0.220	0.081
$[x_6]$-$\{0.4\}$->(Ksi_2)	0.433	0.413	0.024	0.020	0.113	0.210	0.081	0.068
$[x_7]$-$\{0.6\}$->(Ksi_2)	0.649	0.600	0.040	0.000	0.144	0.179	0.112	0.052
$[x_8]$-$\{0.1\}$->(Ksi_2)	0.102	0.098	0.001	0.001	0.103	0.213	0.018	0.072
$[x_9]$-$\{0.4\}$->(Ksi_3)	0.408	0.329	0.006	-0.075	0.088	0.154	0.015	0.038
$[x_{10}]$-$\{0.3\}$->(Ksi_3)	0.300	0.244	-0.003	-0.057	0.089	0.150	0.015	0.036
$[x_{11}]$-$\{0.2\}$->(Ksi_3)	0.199	0.160	0.001	-0.035	0.085	0.146	0.013	0.033
$[x_{12}]$-$\{0.2\}$->(Ksi_3)	0.203	0.166	0.003	-0.030	0.093	0.145	0.015	0.033
$[x_{13}]$-$\{0.4\}$->(Ksi_3)	0.407	0.321	0.008	-0.073	0.095	0.148	0.018	0.035
Average(abs)			0.008	0.044	0.118	0.192	0.064	0.060
Outer Model (Reflective)								
(Eta_1)-$\{0.8\}$->$[y_1]$	0.682	0.841	-0.115	0.041	0.125	0.041	0.019	0.002
(Eta_1)-$\{0.7\}$->$[y_2]$	0.648	0.816	-0.049	0.117	0.072	0.117	0.008	0.014
(Eta_1)-$\{0.8\}$->$[y_3]$	0.682	0.842	-0.114	0.042	0.124	0.042	0.019	0.002
(Eta_2)-$\{0.8\}$->$[y_4]$	0.765	0.871	-0.038	0.071	0.064	0.071	0.007	0.005
(Eta_2)-$\{0.7\}$->$[y_5]$	0.720	0.851	0.017	0.151	0.050	0.151	0.005	0.023
(Eta_2)-$\{0.8\}$->$[y_6]$	0.766	0.871	-0.036	0.072	0.062	0.072	0.006	0.005
Average(abs)			0.062	0.082	0.083	0.082	0.011	0.009
Inner Model								
(Ksi_1)-$\{0.4\}$->(Eta_1)	0.398	0.249	-0.001	-0.025	0.048	0.151	0.007	0.025
(Ksi_2)-$\{0.5\}$->(Eta_1)	0.509	0.254	0.005	-0.064	0.072	0.250	0.015	0.064
(Ksi_3)-$\{0.6\}$->(Eta_1)	0.607	0.382	0.002	-0.051	0.057	0.221	0.008	0.051
(Eta_1)-$\{0.6\}$->(Eta_2)	0.597	0.580	0.001	-0.002	0.038	0.035	0.004	0.002
Average(abs)			0.002	0.036	0.054	0.164	0.009	0.036

$$\text{Mean Value} = \frac{1}{n}\sum_{i=1}^{n}\hat{\theta}_i \; ; \quad \text{Mean Deviation} = \frac{1}{n}\sum_{i=1}^{n}\hat{\theta}_i - \theta \; ; \quad \text{Mean Absolute Deviation} = \frac{1}{n}\sum_{i=1}^{n}\left|\hat{\theta}_i - \theta\right| \; ;$$

$$\text{Mean Squared Error} = \frac{1}{n}\sum_{i=1}^{n}\left(\hat{\theta}_i - \theta\right)^2 \; ; \quad i = 1,...,1000 \; ; \quad \hat{\theta} = \text{Parameter Estimation} \; ; \quad \theta = \text{Population Parameter}$$

Table 3: Simulation results in respect of non-normal data

Outer Model (Formative)	Mean Value		Mean Deviation		Mean Absolute Deviation		Mean Squared Error	
	ML	PLS	ML	PLS	ML	PLS	ML	PLS
$[x_1]$-{0.1}->(Ksi$_1$)	0.104	0.084	0.004	-0.016	0.163	0.245	0.052	0.093
$[x_2]$-{0.2}->(Ksi$_1$)	0.215	0.178	0.015	-0.022	0.168	0.248	0.070	0.096
$[x_3]$-{0.1}->(Ksi$_1$)	0.110	0.084	0.010	-0.016	0.154	0.238	0.045	0.085
$[x_4]$-{0.6}->(Ksi$_1$)	0.612	0.453	0.012	-0.147	0.196	0.247	0.310	0.098
$[x_5]$-{0.4}->(Ksi$_1$)	0.418	0.307	0.018	-0.093	0.168	0.248	0.088	0.097
$[x_6]$-{0.4}->(Ksi$_2$)	0.445	0.412	0.045	0.012	0.150	0.229	0.264	0.084
$[x_7]$-{0.6}->(Ksi$_2$)	0.655	0.602	0.055	0.002	0.185	0.204	0.260	0.065
$[x_8]$-{0.1}->(Ksi$_2$)	0.103	0.095	0.003	-0.005	0.120	0.225	0.027	0.080
$[x_9]$-{0.4}->(Ksi$_3$)	0.418	0.329	0.018	-0.071	0.115	0.172	0.030	0.047
$[x_{10}]$-{0.3}->(Ksi$_3$)	0.307	0.243	0.007	-0.057	0.111	0.168	0.024	0.044
$[x_{11}]$-{0.2}->(Ksi$_3$)	0.203	0.159	0.003	-0.041	0.112	0.164	0.022	0.042
$[x_{12}]$-{0.2}->(Ksi$_3$)	0.211	0.167	0.011	-0.033	0.121	0.165	0.025	0.042
$[x_{13}]$-{0.4}->(Ksi$_3$)	0.413	0.318	0.013	-0.082	0.118	0.172	0.032	0.047
Average(abs)			0.016	0.046	0.145	0.210	0.096	0.071
Outer Model (Reflective)								
(Eta$_1$)-{0.8}->[y$_1$]	0.682	0.842	-0.118	0.042	0.132	0.044	0.023	0.002
(Eta$_1$)-{0.7}->[y$_2$]	0.648	0.817	-0.052	0.117	0.083	0.117	0.011	0.014
(Eta$_1$)-{0.8}->[y$_3$]	0.682	0.842	-0.118	0.042	0.132	0.044	0.023	0.002
(Eta$_2$)-{0.8}->[y$_4$]	0.766	0.872	-0.034	0.072	0.074	0.072	0.010	0.006
(Eta$_2$)-{0.7}->[y$_5$]	0.720	0.851	0.020	0.151	0.066	0.151	0.008	0.023
(Eta$_2$)-{0.8}->[y$_6$]	0.767	0.871	-0.033	0.071	0.074	0.071	0.009	0.005
Average(abs)			0.063	0.082	0.094	0.083	0.014	0.009
Inner Model								
(Ksi$_1$)-{0.4}->(Eta$_1$)	0.397	0.250	-0.003	-0.025	0.058	0.150	0.009	0.025
(Ksi$_2$)-{0.5}->(Eta$_1$)	0.503	0.255	0.003	-0.063	0.082	0.245	0.020	0.063
(Ksi$_3$)-{0.6}->(Eta$_1$)	0.601	0.384	0.001	-0.050	0.077	0.216	0.014	0.050
(Eta$_1$)-{0.6}->(Eta$_2$)	0.596	0.582	-0.004	-0.002	0.048	0.039	0.007	0.002
Average(abs)			0.003	0.035	0.066	0.162	0.012	0.035

Mean Value $= \frac{1}{n}\sum_{i=1}^{n}\hat{\theta}_i$; Mean Deviation $= \frac{1}{n}\sum_{i=1}^{n}\hat{\theta}_i - \theta$; Mean Absolute Deviation $= \frac{1}{n}\sum_{i=1}^{n}\left|\hat{\theta}_i - \theta\right|$;

Mean Squared Error $= \frac{1}{n}\sum_{i=1}^{n}\left(\hat{\theta}_i - \theta\right)^2$; $i = 1,...,1000$; $\hat{\theta}$ = Parameter Estimation ; θ = Population Parameter

Table 4: Comparison of simulation results in respect of normal and non-normal data

| | Relative Absolute Changes between Normal and Non-Normal Parameter Estimations | | | |
| | Mean Absolute Deviation | | Mean Squared Error | |
	ML	PLS	ML	PLS
Outer Model (Formative)	0.228	0.093	0.495	0.178
Outer Model (Reflective)	0.131	0.008	0.311	0.029
Inner Model	0.229	-0.011	0.432	-0.019

$$\text{Relative MAD Change} = \frac{\left|\text{Average MAD}_{normal} - \text{Average MAD}_{nonnormal}\right|}{\text{Average MAD}_{normal}} ;$$

$$\text{Relative MSE Change} = \frac{\left|\text{Average MSE}_{normal} - \text{Average MSE}_{nonnormal}\right|}{\text{Average MSE}_{normal}}$$

Table 5: Correlation matrix of manifest variables

	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}	x_{11}	x_{12}	x_{13}	y_1	y_2	y_3	y_4	y_5	y_6
x_1	1.00																		
x_2	0.71	1.00																	
x_3	0.72	0.65	1.00																
x_4	0.08	0.04	0.09	1.00															
x_5	-0.01	-0.05	-0.02	0.05	1.00														
x_6	0.02	0.03	-0.06	0.06	-0.03	1.00													
x_7	-0.11	-0.12	-0.06	0.00	0.02	-0.01	1.00												
x_8	-0.13	-0.13	-0.09	-0.05	0.01	0.06	0.10	1.00											
x_9	0.02	-0.03	0.00	0.06	0.00	-0.02	0.10	-0.06	1.00										
x_{10}	0.01	0.07	-0.01	0.03	0.12	-0.03	-0.02	-0.01	0.12	1.00									
x_{11}	-0.05	0.04	-0.06	0.07	0.00	0.07	0.01	-0.04	0.24	0.57	1.00								
x_{12}	0.03	0.07	-0.02	0.10	0.06	-0.02	0.02	-0.05	0.29	0.49	0.53	1.00							
x_{13}	0.03	0.05	0.01	-0.01	0.01	0.05	0.00	-0.01	0.13	0.20	0.29	0.27	1.00						
y_1	0.06	0.06	0.05	0.54	0.61	0.15	0.19	0.01	0.08	0.08	0.03	0.06	-0.02	1.00					
y_2	0.00	0.02	0.00	0.54	0.51	0.19	0.16	0.01	0.10	0.04	0.02	0.04	-0.01	0.85	1.00				
y_3	0.08	0.06	0.08	0.54	0.58	0.09	0.15	0.04	0.11	0.01	0.00	0.03	0.00	0.89	0.83	1.00			
y_4	0.06	0.07	0.04	0.33	0.30	0.29	0.36	0.04	0.33	0.37	0.39	0.42	0.32	0.58	0.53	0.55	1.00		
y_5	0.00	0.01	0.01	0.31	0.28	0.26	0.40	0.09	0.29	0.35	0.38	0.35	0.34	0.54	0.51	0.52	0.83	1.00	
y_6	0.05	0.05	0.01	0.35	0.35	0.29	0.40	0.07	0.35	0.37	0.41	0.39	0.36	0.63	0.57	0.58	0.88	0.86	1.00

Table 6: Mean value of alternative CBSEM procedures

	Normal Data				Non-normal Data			
Outer Model (Formative)	ML	GLS	ADF	ULS	ML	GLS	ADF	ULS
$[x_1]$-$\{0.1\}$->(Ksi_1)	0.108	0.106	0.103	0.567	0.104	0.110	0.110	0.599
$[x_2]$-$\{0.2\}$->(Ksi_1)	0.210	0.207	0.206	0.377	0.215	0.229	0.259	0.374
$[x_3]$-$\{0.1\}$->(Ksi_1)	0.096	0.101	0.118	0.376	0.110	0.100	0.153	0.370
$[x_4]$-$\{0.6\}$->(Ksi_1)	0.597	0.592	0.627	0.547	0.612	0.608	0.684	0.563
$[x_5]$-$\{0.4\}$->(Ksi_1)	0.400	0.406	0.410	0.093	0.418	0.430	0.479	0.091
$[x_6]$-$\{0.4\}$->(Ksi_2)	0.424	0.422	0.449	0.388	0.445	0.421	0.433	0.397
$[x_7]$-$\{0.6\}$->(Ksi_2)	0.640	0.631	0.660	0.290	0.655	0.640	0.690	0.300
$[x_8]$-$\{0.1\}$->(Ksi_2)	0.101	0.097	0.101	0.198	0.103	0.097	0.136	0.191
$[x_9]$-$\{0.4\}$->(Ksi_3)	0.406	0.401	0.405	0.198	0.418	0.411	0.413	0.201
$[x_{10}]$-$\{0.3\}$->(Ksi_3)	0.297	0.294	0.297	0.392	0.307	0.300	0.306	0.391
$[x_{11}]$-$\{0.2\}$->(Ksi_3)	0.201	0.200	0.201	0.753	0.203	0.202	0.205	0.752
$[x_{12}]$-$\{0.2\}$->(Ksi_3)	0.203	0.199	0.202	0.717	0.211	0.205	0.210	0.715
$[x_{13}]$-$\{0.4\}$->(Ksi_3)	0.408	0.403	0.412	0.755	0.413	0.407	0.415	0.752
Outer Model (Reflective)								
(Eta_1)-$\{0.8\}$->$[y_1]$	0.682	0.694	0.697	0.792	0.682	0.698	0.697	0.793
(Eta_1)-$\{0.7\}$->$[y_2]$	0.648	0.662	0.663	0.746	0.648	0.666	0.664	0.745
(Eta_1)-$\{0.8\}$->$[y_3]$	0.682	0.695	0.696	0.792	0.682	0.697	0.696	0.792
(Eta_2)-$\{0.8\}$->$[y_4]$	0.765	0.765	0.769	0.389	0.766	0.774	0.771	0.394
(Eta_2)-$\{0.7\}$->$[y_5]$	0.720	0.723	0.729	0.508	0.720	0.730	0.728	0.503
(Eta_2)-$\{0.8\}$->$[y_6]$	0.766	0.767	0.771	0.570	0.767	0.774	0.776	0.575
Inner Model								
(Ksi_1)-$\{0.4\}$->(Eta_1)	0.398	0.407	0.418	0.639	0.397	0.403	0.435	0.640
(Ksi_2)-$\{0.5\}$->(Eta_1)	0.509	0.499	0.499	0.359	0.503	0.506	0.529	0.357
(Ksi_3)-$\{0.6\}$->(Eta_1)	0.607	0.600	0.607	0.419	0.601	0.601	0.624	0.417
(Eta_1)-$\{0.6\}$->(Eta_2)	0.597	0.617	0.619	0.357	0.596	0.619	0.621	0.358

Table 7: Mean deviation of alternative CBSEM procedures

	Normal Data				Non-normal Data			
Outer Model (Formative)	ML	GLS	ADF	ULS	ML	GLS	ADF	ULS
$[x_1]$-$\{0.1\}$->(Ksi_1)	0.008	0.006	0.003	0.467	0.004	0.010	0.010	0.499
$[x_2]$-$\{0.2\}$->(Ksi_1)	0.010	0.007	0.006	0.177	0.015	0.029	0.059	0.174
$[x_3]$-$\{0.1\}$->(Ksi_1)	-0.004	0.001	0.018	0.276	0.010	0.000	0.053	0.270
$[x_4]$-$\{0.6\}$->(Ksi_1)	-0.003	-0.008	0.027	-0.053	0.012	0.008	0.084	-0.037
$[x_5]$-$\{0.4\}$->(Ksi_1)	0.000	0.006	0.010	-0.307	0.018	0.030	0.079	-0.309
$[x_6]$-$\{0.4\}$->(Ksi_2)	0.024	0.022	0.049	-0.012	0.045	0.021	0.033	-0.003
$[x_7]$-$\{0.6\}$->(Ksi_2)	0.040	0.031	0.060	-0.310	0.055	0.040	0.090	-0.300
$[x_8]$-$\{0.1\}$->(Ksi_2)	0.001	-0.003	0.001	0.098	0.003	-0.003	0.036	0.091
$[x_9]$-$\{0.4\}$->(Ksi_3)	0.006	0.001	0.005	-0.202	0.018	0.011	0.013	-0.199
$[x_{10}]$-$\{0.3\}$->(Ksi_3)	-0.003	-0.006	-0.003	0.092	0.007	0.000	0.006	0.091
$[x_{11}]$-$\{0.2\}$->(Ksi_3)	0.001	0.000	0.001	0.553	0.003	0.002	0.005	0.552
$[x_{12}]$-$\{0.2\}$->(Ksi_3)	0.003	-0.001	0.002	0.517	0.011	0.005	0.010	0.515
$[x_{13}]$-$\{0.4\}$->(Ksi_3)	0.008	0.003	0.012	0.355	0.013	0.007	0.015	0.352
Average(abs)	0.008	0.007	0.015	0.263	0.016	0.013	0.038	0.261
Outer Model (Reflective)								
(Eta_1)-$\{0.8\}$->$[y_1]$	-0.115	-0.106	-0.103	-0.008	-0.118	-0.102	-0.103	-0.007
(Eta_1)-$\{0.7\}$->$[y_2]$	-0.049	-0.038	-0.037	0.046	-0.052	-0.034	-0.036	0.045
(Eta_1)-$\{0.8\}$->$[y_3]$	-0.114	-0.105	-0.104	-0.008	-0.118	-0.103	-0.104	-0.008
(Eta_2)-$\{0.8\}$->$[y_4]$	-0.038	-0.035	-0.031	-0.411	-0.034	-0.026	-0.029	-0.406
(Eta_2)-$\{0.7\}$->$[y_5]$	0.017	0.023	0.029	-0.192	0.020	0.030	0.028	-0.197
(Eta_2)-$\{0.8\}$->$[y_6]$	-0.036	-0.033	-0.029	-0.230	-0.033	-0.026	-0.024	-0.225
Average(abs)	0.062	0.057	0.056	0.149	0.063	0.054	0.054	-0.148
Inner Model								
(Ksi_1)-$\{0.4\}$->(Eta_1)	-0.001	0.007	0.018	0.239	-0.003	0.003	0.035	0.240
(Ksi_2)-$\{0.5\}$->(Eta_1)	0.005	-0.001	-0.001	-0.141	0.003	0.006	0.029	-0.143
(Ksi_3)-$\{0.6\}$->(Eta_1)	0.002	-0.000	0.007	-0.181	0.001	0.001	0.024	-0.183
(Eta_1)-$\{0.6\}$->(Eta_2)	0.001	0.017	0.019	-0.243	-0.004	0.019	0.021	-0.242
Average(abs)	0.002	0.006	0.011	0.201	0.003	0.007	0.027	-0.202

Table 8: Mean absolute deviation of alternative CBSEM procedures

	Normal Data				Non-normal Data			
Outer Model (Formative)	ML	GLS	ADF	ULS	ML	GLS	ADF	ULS
$[x_1]-\{0.1\}->(Ksi_1)$	0.135	0.137	0.195	0.474	0.163	0.177	0.251	0.509
$[x_2]-\{0.2\}->(Ksi_1)$	0.142	0.139	0.209	0.229	0.168	0.181	0.266	0.243
$[x_3]-\{0.1\}->(Ksi_1)$	0.137	0.138	0.201	0.283	0.154	0.168	0.266	0.303
$[x_4]-\{0.6\}->(Ksi_1)$	0.156	0.167	0.271	0.140	0.196	0.272	0.404	0.184
$[x_5]-\{0.4\}->(Ksi_1)$	0.151	0.141	0.210	0.312	0.168	0.184	0.309	0.323
$[x_6]-\{0.4\}->(Ksi_2)$	0.113	0.117	0.193	0.106	0.150	0.153	0.241	0.133
$[x_7]-\{0.6\}->(Ksi_2)$	0.144	0.140	0.220	0.319	0.185	0.183	0.306	0.326
$[x_8]-\{0.1\}->(Ksi_2)$	0.103	0.104	0.147	0.134	0.120	0.118	0.190	0.149
$[x_9]-\{0.4\}->(Ksi_3)$	0.088	0.086	0.133	0.220	0.115	0.110	0.169	0.227
$[x_{10}]-\{0.3\}->(Ksi_3)$	0.089	0.089	0.129	0.139	0.111	0.110	0.162	0.157
$[x_{11}]-\{0.2\}->(Ksi_3)$	0.085	0.088	0.127	0.553	0.112	0.115	0.159	0.552
$[x_{12}]-\{0.2\}->(Ksi_3)$	0.093	0.092	0.133	0.517	0.121	0.119	0.156	0.515
$[x_{13}]-\{0.4\}->(Ksi_3)$	0.095	0.095	0.138	0.355	0.118	0.114	0.175	0.352
Average(abs)	0.118	0.118	0.177	0.291	0.145	0.154	0.235	0.306
Outer Model (Reflective)								
$(Eta_1)-\{0.8\}->[y_1]$	0.125	0.118	0.132	0.033	0.132	0.121	0.141	0.041
$(Eta_1)-\{0.7\}->[y_2]$	0.072	0.068	0.094	0.055	0.083	0.078	0.106	0.057
$(Eta_1)-\{0.8\}->[y_3]$	0.124	0.117	0.131	0.035	0.132	0.120	0.140	0.040
$(Eta_2)-\{0.8\}->[y_4]$	0.064	0.073	0.099	0.411	0.074	0.087	0.116	0.407
$(Eta_2)-\{0.7\}->[y_5]$	0.050	0.062	0.090	0.205	0.066	0.080	0.100	0.210
$(Eta_2)-\{0.8\}->[y_6]$	0.062	0.071	0.100	0.233	0.074	0.086	0.113	0.231
Average(abs)	0.083	0.085	0.108	0.162	0.094	0.095	0.119	0.164
Inner Model								
$(Ksi_1)-\{0.4\}->(Eta_1)$	0.048	0.059	0.096	0.239	0.058	0.066	0.136	0.240
$(Ksi_2)-\{0.5\}->(Eta_1)$	0.072	0.066	0.103	0.141	0.082	0.073	0.142	0.144
$(Ksi_3)-\{0.6\}->(Eta_1)$	0.057	0.050	0.086	0.181	0.077	0.066	0.127	0.183
$(Eta_1)-\{0.6\}->(Eta_2)$	0.038	0.037	0.062	0.243	0.048	0.048	0.086	0.242
Average(abs)	0.054	0.053	0.087	0.201	0.066	0.063	0.123	0.202

Table 9: Mean squared error of alternative CBSEM procedures

	Normal Data				Non-normal Data			
Outer Model (Formative)	ML	GLS	ADF	ULS	ML	GLS	ADF	ULS
$[x_1]$-$\{0.1\}$->(Ksi_1)	0.034	0.036	0.069	0.319	0.052	0.174	0.322	0.729
$[x_2]$-$\{0.2\}$->(Ksi_1)	0.046	0.041	0.112	0.091	0.070	0.176	0.297	0.130
$[x_3]$-$\{0.1\}$->(Ksi_1)	0.053	0.042	0.090	0.115	0.045	0.141	0.302	0.268
$[x_4]$-$\{0.6\}$->(Ksi_1)	0.195	0.176	0.460	0.043	0.310	2.757	2.826	0.212
$[x_5]$-$\{0.4\}$->(Ksi_1)	0.220	0.054	0.096	0.120	0.088	0.243	0.703	0.132
$[x_6]$-$\{0.4\}$->(Ksi_2)	0.081	0.086	0.198	0.023	0.264	0.282	0.422	0.044
$[x_7]$-$\{0.6\}$->(Ksi_2)	0.112	0.142	0.225	0.119	0.260	0.446	0.972	0.130
$[x_8]$-$\{0.1\}$->(Ksi_2)	0.018	0.019	0.036	0.031	0.027	0.025	0.145	0.039
$[x_9]$-$\{0.4\}$->(Ksi_3)	0.015	0.015	0.032	0.064	0.030	0.025	0.054	0.071
$[x_{10}]$-$\{0.3\}$->(Ksi_3)	0.015	0.016	0.031	0.037	0.024	0.024	0.049	0.050
$[x_{11}]$-$\{0.2\}$->(Ksi_3)	0.013	0.013	0.027	0.310	0.022	0.025	0.049	0.310
$[x_{12}]$-$\{0.2\}$->(Ksi_3)	0.015	0.015	0.030	0.271	0.025	0.024	0.044	0.269
$[x_{13}]$-$\{0.4\}$->(Ksi_3)	0.018	0.020	0.038	0.130	0.032	0.030	0.065	0.129
Average(abs)	0.064	0.052	0.111	0.129	0.096	0.336	0.481	0.193
Outer Model (Reflective)								
(Eta_1)-$\{0.8\}$->$[y_1]$	0.019	0.019	0.025	0.003	0.023	0.020	0.030	0.004
(Eta_1)-$\{0.7\}$->$[y_2]$	0.008	0.008	0.015	0.006	0.011	0.010	0.019	0.007
(Eta_1)-$\{0.8\}$->$[y_3]$	0.019	0.018	0.025	0.003	0.023	0.020	0.029	0.004
(Eta_2)-$\{0.8\}$->$[y_4]$	0.007	0.009	0.020	0.175	0.010	0.014	0.023	0.175
(Eta_2)-$\{0.7\}$->$[y_5]$	0.005	0.008	0.019	0.050	0.008	0.014	0.021	0.052
(Eta_2)-$\{0.8\}$->$[y_6]$	0.006	0.009	0.020	0.064	0.009	0.014	0.022	0.065
Average(abs)	0.011	0.012	0.021	0.050	0.014	0.016	0.024	0.051
Inner Model								
(Ksi_1)-$\{0.4\}$->(Eta_1)	0.007	0.011	0.020	0.061	0.009	0.015	0.066	0.063
(Ksi_2)-$\{0.5\}$->(Eta_1)	0.015	0.015	0.024	0.022	0.020	0.019	0.050	0.024
(Ksi_3)-$\{0.6\}$->(Eta_1)	0.008	0.008	0.017	0.035	0.014	0.014	0.046	0.037
(Eta_1)-$\{0.6\}$->(Eta_2)	0.004	0.005	0.010	0.061	0.007	0.007	0.015	0.062
Average(abs)	0.009	0.010	0.018	0.045	0.012	0.014	0.045	0.046

Table 10: Comparison of alternative PLS weighting schemes in respect of normal data

	Mean Value			Mean Deviation		
	Centroid	Factor	Path	Centroid	Factor	Path
Outer Model (Formative)						
$[x_1]$-{0.1}->(Ksi_1)	0,093	0,092	0,092	-0,007	-0,008	-0,008
$[x_2]$-{0.2}->(Ksi_1)	0,192	0,191	0,191	-0,008	-0,009	-0,009
$[x_3]$-{0.1}->(Ksi_1)	0,074	0,074	0,074	-0,026	-0,026	-0,026
$[x_4]$-{0.6}->(Ksi_1)	0,446	0,446	0,446	-0,154	-0,154	-0,154
$[x_5]$-{0.4}->(Ksi_1)	0,314	0,314	0,314	-0,086	-0,086	-0,086
$[x_6]$-{0.4}->(Ksi_2)	0,397	0,397	0,397	-0,003	-0,003	-0,003
$[x_7]$-{0.6}->(Ksi_2)	0,608	0,608	0,608	0,008	0,008	0,008
$[x_8]$-{0.1}->(Ksi_2)	0,116	0,116	0,116	0,016	0,016	0,016
$[x_9]$-{0.4}->(Ksi_3)	0,343	0,343	0,343	-0,057	-0,057	-0,057
$[x_{10}]$-{0.3}->(Ksi_3)	0,234	0,234	0,234	-0,066	-0,066	-0,066
$[x_{11}]$-{0.2}->(Ksi_3)	0,157	0,157	0,157	-0,043	-0,043	-0,043
$[x_{12}]$-{0.2}->(Ksi_3)	0,175	0,175	0,175	-0,025	-0,025	-0,025
$[x_{13}]$-{0.4}->(Ksi_3)	0,319	0,319	0,319	-0,081	-0,081	-0,081
Outer Model (Reflective)						
(Eta_1)-{0.8}->$[y_1]$	0,842	0,841	0,841	0,042	0,041	0,041
(Eta_1)-{0.7}->$[y_2]$	0,817	0,817	0,817	0,117	0,117	0,117
(Eta_1)-{0.8}->$[y_3]$	0,842	0,842	0,842	0,042	0,042	0,042
(Eta_2)-{0.8}->$[y_4]$	0,872	0,872	0,872	0,072	0,072	0,072
(Eta_2)-{0.7}->$[y_5]$	0,850	0,850	0,850	0,150	0,150	0,150
(Eta_2)-{0.8}->$[y_6]$	0,872	0,872	0,872	0,072	0,072	0,072
Inner Model						
(Ksi_1)-{0.4}->(Eta_1)	0,248	0,248	0,248	-0,152	-0,152	-0,152
(Ksi_2)-{0.5}->(Eta_1)	0,255	0,254	0,254	-0,245	-0,246	-0,246
(Ksi_3)-{0.6}->(Eta_1)	0,379	0,379	0,379	-0,221	-0,221	-0,221
(Eta_1)-{0.6}->(Eta_2)	0,578	0,578	0,578	-0,022	-0,022	-0,022

Figures

Figure 1: Comparison of reflective and formative measurement models (Diamantopoulos, 2006; Edwards & Bagozzi, 2000)
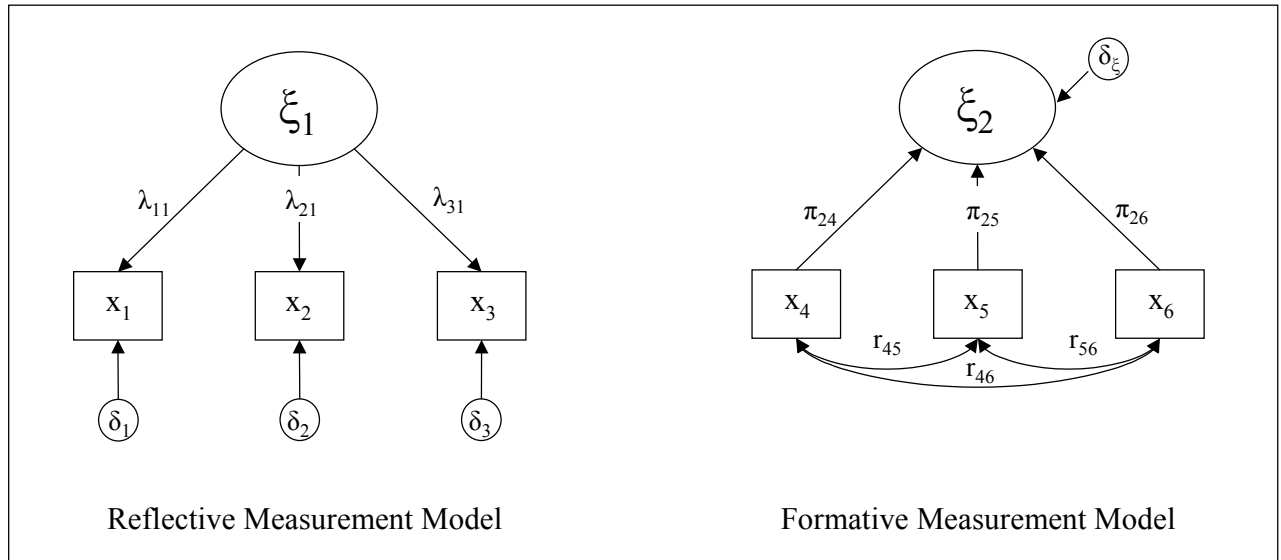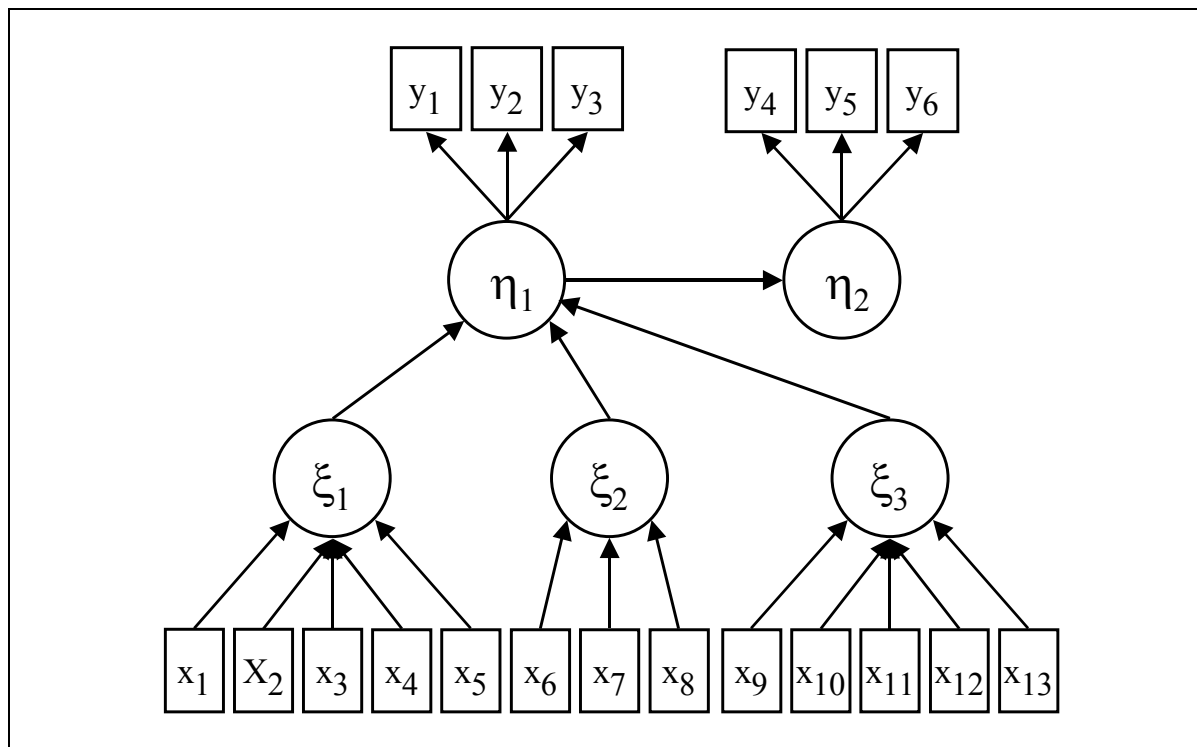
Figure 2: The structural model tested in a simulated study.

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