Composite-based Methods in Structural Equation Modeling

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For my daughter

Marla Louisa.

Zusammenfassung

Die vorliegende Dissertation beschäftigt sich mit kompositenbasierten Schätzverfahren für Strukturgleichungsmodelle mit latenten Variablen sowie deren Weiterentwicklung und einhergehenden Problemen bei deren Verwendung in empirischen Studien.

Die Arbeit umfasst insgesamt fünf Kapitel. Neben einer kurzen Einleitung im ersten Kapitel beinhalten die verbleibenden Kapitel Teile der Ergebnisse meiner Promotion, die in Form von vier, teilweise schon veröffentlichten Aufsätzen präsentiert werden.

Der erste Aufsatz befasst sich mit einer alternativen Modellierungsweise der theoretischen Konstrukte in der Strukturgleichungsmodellierung. Während in den Sozial- und Verhaltenswissenschaften die theoretischen Konstrukte klassischerweise durch sogenannte common factors modelliert werden, stellt dies in manchen Situationen bzw. in anderen Wissenschaftsbereichen eine unplausible Annahme dar. In diesem Teil der Arbeit wird eine abgewandelte Form der konfirmatorischen Faktorenanalyse, die konfirmatorische Kompositenanalyse, vorgestellt, in welcher die theoretischen Konstrukte anstatt durch common factors mit Hilfe von Kompositen modelliert werden. Neben der Ausführung der theoretischen Grundlage wird durch eine Monte Carlo Simulation gezeigt, dass die konfirmatorische Kompositenanalyse geeignet ist, Fehlspezifikationen im zugrundeliegenden Kompositenmodell aufzudecken.

In der zweiten Studie wird die Frage aufgeworfen, wie Parameterunterschiede im Rahmen der partial least squares Pfadmodellierung getestet werden können. Da die Standardfehler des Schätzers keine analytisch-geschlossene Form besitzen, kann der aus der Regressionsanalyse bekannte t- bzw. F-Test nicht direkt für die Beantwortung dieser Frage verwendet werden. Einen Ausweg bietet das Bootstrapping, durch welches

Konfidenzintervalle um den geschätzten Parameterunterschied konstruiert werden können. Mit Hife dieser können statistische Aussagen über den Parameterunterschied in der Grundgesamtheit gemacht werden. Das vorgestellte Verfahren wird anhand eines empirischen Beispiels demonstriert.

Der dritte Aufsatz dieser Arbeit geht der Frage nach, wie ordinale Indikatoren mit festen Kategorien in der partial least squares Pfadmodellierung berücksichtigt werden können. Es wird ein neues, konsistentes Schätzverfahren vorgestellt, das den qualitativen Charakter der ordinalen Variablen mittels der polychorischen Korrelation bei der Schätzung berücksichtigt. Der neue Schätzer trägt den Namen „ordinal consistent partial least squares" und kombiniert die Verfahren consistent partial least squares und ordinal partial least squares. Neben der Darbietung des Schätzverfahrens wird mit Hilfe einer Monte Carlo Simulation gezeigt, dass das Verfahren ordinal consistent partial least squares geeignet ist, Modelle, die ordinale Indikatoren mit festen Kategorien enthalten, zu schätzen. Darüber hinaus wird ein empirisches Beispiel mit ordinal consistent partial least squares geschätzt.

Das letzte Kapitel widmet sich der Schätzung nicht-linearer Strukturgleichungsmodelle mit latenten Variablen, wobei sich die Nichtlinearität auf die latenten Variablen und nicht auf deren Parameter bezieht. In diesem Kontext wird ein neues Schätzverfahren vorgestellt, welches ähnlich wie consistent partial least squares funktioniert und konsistente Parameterschätzungen für rekursive, nicht-lineare Gleichungssysteme liefert. Im Gegensatz zu consistent partial least squares benötigt der vorgestellte Momentenschätzer kein iteratives Verfahren, um die Gewichte für die Bildung der Kompositen zu bestimmen. Es wird mit Hilfe einer Monte Carlo Simulation gezeigt, dass der Schätzer geeignet ist, nicht-lineare Strukturgleichungsmodelle mit latenten Variablen zu schätzen.

Acknowledgment

I wrote this dissertation during my employment as a research and teaching assistant at the Chair of Econometrics at the University of Würzburg. The work at this chair offered a stimulating environment to conduct my research and to learn more about the exciting field of econometrics, in general. Above all, I am deeply grateful to my supervisor, Prof. Dr. Martin Kukuk, who had already stimulated my interest during my Master's studies, and finally, provided me with the chance to delve deeper into the field of econometrics, in particular, structural equation modeling, by offering me an employment at his chair. He patiently encouraged my work, gave me the necessary freedom, and supported all my research activities, e.g., my research visits to the Netherlands or my visits of conferences and workshops during the last five years. Thank you!

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Chapter 1

Introduction

Structural equation modeling with latent variables (SEM) has become an established method, especially in research fields such as social and behavioral sciences. Its capacity to model dependencies between theoretical constructs, take into account various forms of measurement errors, and test entire theories makes it a favorable tool for engagement with a plethora of research problems.

The origin of SEM dates back to the early 20th century (Westland, 2015, Chap. 2), and it combines developments from various fields of methodological research, e.g., psychometrics, econometrics, and biometrics. However, (linear) SEM, as it is known today, was initially developed by Jöreskog (1969), who assumed that latent theoretical constructs are modeled as common factors. This kind of SEM is also named factor-based SEM due to the way in which construct modeling takes place within its purview.[1]

In general, SEM comprises the following two models: structural model and measurement model (see Bollen (1989) for a more detailed overview). The structural model connects the endogenous and exogenous common factors, as seen in the equation below:

$$\boldsymbol{\eta} = \boldsymbol{\Gamma}\boldsymbol{\xi} + \boldsymbol{B}\boldsymbol{\eta} + \boldsymbol{\zeta}, \tag{1.1}$$

where the vectors $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$ contain the endogenous and the exogenous common factors, while the vector $\boldsymbol{\zeta}$ contains the structural error terms. The matrices $\boldsymbol{\Gamma}$ and $\boldsymbol{B}$ contain

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[1]See Rigdon (2012, 2014) for a more detailed explanation of construct modeling in SEM, and how the common factor has reached such a predominant position in SEM.

the path coefficients of the exogenous and the endogenous common factors respectively. The measurement model, which also provides the basis for confirmatory factor analysis (CFA), defines how the latent common factors are connected to the observed indicators, as outlined in the formulas below:

$$\boldsymbol{x} = \boldsymbol{\Lambda}_x \boldsymbol{\xi} + \boldsymbol{\epsilon} \tag{1.2}$$

$$\boldsymbol{y} = \boldsymbol{\Lambda}_y \boldsymbol{\eta} + \boldsymbol{\delta}, \tag{1.3}$$

where the observed indicators are stacked in the vectors $\boldsymbol{x}$ and $\boldsymbol{y}$, and the vectors $\boldsymbol{\epsilon}$ and $\boldsymbol{\delta}$ contain the measurement errors. Thus, in context of factor-based SEM, the variance of an observed indicator can be decomposed into the following two parts: a common variance, which is explained by common factors; and a unique variance, which is explained by some other source captured in the measurement error.

In Chapter 2, the assumption that the underlying construct must be modeled as a common factor is relaxed and the confirmatory composite analysis (CCA) (Henseler et al., 2014) is presented as being analogous to CFA. In CCA, theoretical constructs are modeled as composites instead of as common factors; and therefore, CCA can be used in situations where CFA faces conceptual limitations because of the strict assumptions imposed upon the model due to its insistence upon the use of common factors. Figure 1.1 draws out the contrast between the common factor model and the composite model as different ways of construct modeling.

(a) Common factor model   (b) Composite model
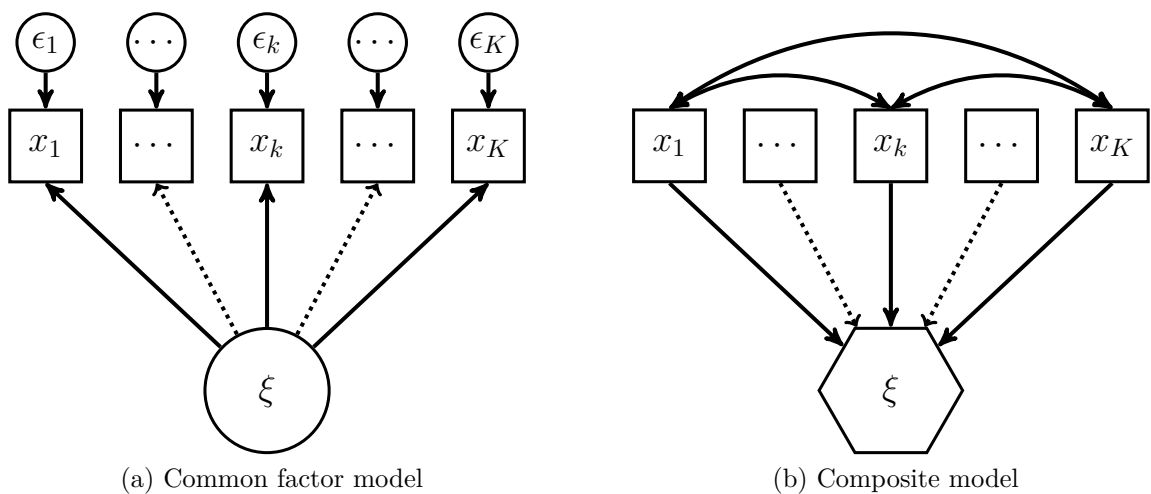
Figure 1.1: Common factor vs. composite

By introducing the CCA, composites are put into a holistic model framework that comprises the same steps as involved in CFA, i.e., model specification, model esti-

mation, model identification, and testing of the overall model fit. Besides providing a description of each step, a Monte Carlo simulation is conducted to investigate the performance of a bootstrap-based procedure to statistically test the overall model fit in CCA. The results of the simulation confirm that various misspecification can be detected and highlight the confirmatory character of CCA.

A consistent estimator for CCA or, more generally, composite-based SEM[2] is partial least squares path modeling (PLS) (Lohmöller, 2013). It is applied across many disciplines, e.g., marketing science (Hair et al., 2012b), information systems (Gefen et al., 2011; Hair et al., 2017), or strategic management (Hair et al., 2012a), and it has been subject to intensive debate highlighting its advantages and its limitations (Aguirre-Urreta and Marakas, 2013, 2014; Henseler et al., 2014; Rigdon et al., 2014; Rönkkö and Evermann, 2013). A secondary benefit of the scientific debate was the introduction of further enhancements of PLS, e.g., the heterotrait-monotrait ratio of common factor correlations as new criterion for discriminant validity (Henseler et al., 2015) or invariance testing of composites using PLS (Henseler et al., 2016b).

However, practitioners often struggle with issues that are of a rather practical relevance. Chapter 3 addresses such an issue and provides a user guideline on how the difference between two parameters in the framework of PLS can be tested. In regression analysis, this is typically done by a so-called t-test. Since the variance of PLS estimates cannot be expressed in a closed-form expression, bootstrap-based approaches are employed to construct confidence intervals around the estimated parameter difference in order to draw conclusions about the population parameter difference. To illustrate this advancement in PLS, a reduced version of the well-established technology acceptance model is used.

As PLS always creates composites as stand-ins for theoretical constructs, even for factor-based SEM, its estimates suffer from attenuation (Cohen, 1988, Chap. 2.10.2) and are, therefore, biased. This is due to the fact that in factor-based SEM, indicators containing measurement error are used to build composites as a weighted linear combination. However, it can be shown that the estimates are "consistent at large"(Schneeweiss, 1993), which, in turn, means that the estimate converges in probability to the true parameter if the sample size as well as the number of indicators converge to infinity. To overcome the drawback of inconsistent parameter estimates in

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[2]SEM where theoretical constructs are modeled as composites.

factor-based SEM, Dijkstra and Henseler (2015a,b) developed consistent partial least squares (PLSc), which uses a correction for attenuation of the composite correlations as well as of the correlations between the composites and the indicators. This makes PLSc an outstanding and appealing estimator for both, composite-based and factor-based SEM and, in particular, for models wherein composites as well as common factors are included.

Chapter 4 provides an extension of PLSc by incorporating the polychoric correlation to deal with ordinal categorical indicators. The approach is called ordinal consistent partial least squares (OrdPLSc) and permits one to estimate structural equation models of composites and common factors if some or all indicators are measured on an ordinal categorical scale. Its performance is evaluated by a Monte Carlo simulation and compared to means and variance adjusted weighted least squares (WLSMV), a covariance-based alternative. Furthermore, three approaches are presented to obtain constructs scores from OrdPLS and OrdPLSc, which can be used, for instance, in importance performance matrix analysis. Finally, the behavior of OrdPLSc is shown on an empirical example and a practical guidance is provided for the assessment of SEMs with ordinal categorical indicators in the context of OrdPLSc.

The last chapter of my dissertation, Chapter 5, proposes an estimator for polynomial factor models similar to PLSc for nonlinear structural equation models containing latent variables (Dijkstra, 2014). In contrast to PLSc, non-iterative weights are used to build composites which are the proxies for the latent variables. The approach is called the non-iterative method-of-moments for polynomial factor models (MoMpoly); and it corrects the moments of the composites in order to consistently estimate the moments of the latent variables that can, in turn, be used to obtain consistent estimates for the parameters of the structural and the measurement model. A Monte Carlo simulation is conducted to examine the performance of MoMpoly and it is compared to latent moderated structural equations (LMS), which is a full information maximum likelihood estimator. In this context, an R package named *MoMpoly* has been developed where the MoMpoly estimator is implemented.

Chapter 2

Confirmatory Composite Analysis

2.1 Introduction[1]

Structural equation modeling with latent variables (SEM) comprises confirmatory factor analysis (CFA) and path analysis, thus combining methodological developments from different disciplines such as psychology, sociology, and economics, while covering a broad variety of traditional multivariate statistical procedures (Bollen, 1989; Muthén, 2002). It is capable of expressing theoretical constructs by means of multiple manifest variables, to connect them via the structural model as well as to account for measurement error. Since SEM allows for statistical testing of the estimated parameters and even entire models, it is an outstanding tool for confirmatory purposes such as for assessing construct validity (Markus and Borsboom, 2013) or for establishing measurement invariance (Van de Schoot et al., 2012). Apart from the original maximum likelihood estimator, robust versions and a number of alternative approaches were also introduced to encounter violations of the original assumptions in empirical work, such as the asymptotic distribution free (Browne, 1984) or the two-stage least squares (2SLS) estimator (Bollen, 2001). Over time, the initial model has been continuously improved upon to account for more complex theories. Consequently, SEM is able to deal with categorical (Muthén, 1984) as well as longitudinal data (Little, 2013)

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[1]This chapter is based on joint work with Jörg Henseler and Theo K. Dijkstra.

and can be used to model non-linear relationships between the constructs (Klein and Moosbrugger, 2000).[2]

Researchers across many streams of science appreciate SEM's versatility. In particular, in behavioral and social sciences, SEM enjoys large popularity, e.g., in marketing (Bagozzi and Yi, 1988; Steenkamp and Baumgartner, 2000), psychology (MacCallum and Austin, 2000), communication science (Holbert and Stephenson, 2002), operations management (Shah and Goldstein, 2006), or information systems (Gefen et al., 2011) – to name a few. Additionally, beyond the realm of behavioral and social sciences, researchers have acknowledged the capabilities of SEM, such as in construction research (Xiong et al., 2015) or neurosciences (McIntosh and Gonzalez-Lima, 1994).

Over the last decades, the conceptualization of the theoretical construct and the common factor has become more and more conflated such that hardly any distinction is made between both the terms (Rigdon, 2012). The common factor, as a way of modeling the underlying construct, dominates SEM and confirmatory factor analysis (CFA) to an extent that both terms are incorrectly used interchangeably. This is unfortunate and misleading because in disciplines besides and even within social and behavioral sciences, the construct under investigation is sometimes represented by a composite rather than by a common factor, e.g., in design research (Henseler, 2017) or in marketing (Edwards and Bagozzi, 2000). At present, the validity of composites models cannot be systematically assessed. Current approaches are limited to assessing the indicators' collinearity (Diamantopoulos and Winklhofer, 2001) and their relations to other variables in the model (Bagozzi, 1994). A rigorous test of composites models in analogy to CFA does not exist so far. Not only does this situation limit the progress of composites models, it also represents an unnecessary weakness of SEM.

For this reason, we introduce the confirmatory composite analysis (CCA) wherein the theoretical construct is modeled as a composite to make SEM accessible to a broader audience. We show that the composites model relaxes the restrictions imposed by the common factor model. However, it still provides testable restrictions, which makes CCA a full-fledged method for confirmatory purposes. In general, it involves the same steps as CFA or SEM, without assuming that the underlying construct is necessarily modeled as a common factor.

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[2]For more details and a comprehensive overview, we referred to the following text books: Hayduk (1988), Bollen (1989), Marcoulides and Schumacker (2001), Raykov and Marcoulides (2006), Kline (2015), and Brown (2015).

There is no exact instruction on how to apply SEM; however, there exists a general consensus that SEM and CFA comprise at least the following four steps: model specification, model identification, model estimation, and model testing (Schumacker and Lomax, 2009, Chap. 4). To be in line with this proceeding, the remainder of the paper is structured as follows: Section 2.2 introduces the composites model providing the theoretical foundation for the CCA and how the same can be specified; Section 2.3 considers the issue of identification in CCA and states the assumptions as being necessary to guarantee the unique solvability of the composites model; Section 2.4 presents one approach that can be used to estimate the model parameters in the framework of CCA; Section 2.5 provides a test for the overall model fit to assess how well the specified model fits the observed data; Section 2.6 assesses the performance of this test in terms of a Monte Carlo simulation and presents the results; and finally the last section discusses them and gives an outlook for future research.

2.2   Specifying composites models

Composites have a long tradition in multivariate data analysis (Pearson, 1901). Originally, they are the outcome of dimension reduction techniques, i.e., the mapping of the data to a lower dimensional space. In this respect, they are designed to capture the most important characteristics of the data as efficiently as possible. Apart from dimension reduction, composites often serve as proxies for theoretical constructs (MacCallum and Browne, 1993). In marketing research, Fornell and Bookstein (1982) recognized that theoretical constructs like marketing mix or population change are not appropriately modeled by common factors. This is because these constructs are rather built than that they constitute latent variables. Thus, they are defined as an aggregate of observable variables forming a new entity. In the recent past, more and more researchers recognized composites as a legit way of construct modeling, e.g., in marketing science (Diamantopoulos and Winklhofer, 2001; Rossiter, 2002), business research (Diamantopoulos, 2008), environmental science (Grace and Bollen, 2008), or in design research (Henseler, 2017). Additionally, the use of composites in SEM is supported by the *concept proxy framework* (Rigdon, 2012).

Since most researchers are used to employing common factors as a way of construct modeling, Table 2.1 contrasts the common factor and the composite as proxies for

theoretical constructs.[3] In social and behavioral sciences, latent constructs are often

Table 2.1: Type of theoretical construct

Criterion:	Latent variable	Artifact
Dominant statistical model:	Common factor model	Composites model
Fundamental scientific question:	Does it exist?	Is it useful?
Scientific paradigm:	Positivist	Pragmatist
Examples:	Abilities, attitudes, traits	Indices, management success factors

understood as ontological entities such as abilities or attitudes, which rests on the assumption that the theoretical construct of interest exists in nature, regardless of whether it is the subject of scientific examination. In contrast, a construct can be conceived as a result of theoretical thinking or as a construction, i.e., as an artifact. This way of thinking has its origin in constructivist epistemology. The epistemological distinction between ontological and constructivist nature of constructs has important implications when modeling the causal relationships among the constructs and their relationships to the observed indicators. While a common factor model seeks to explore whether a certain latent entity exists by testing if collected measures of a construct are consistent with the assumed nature of that construct, a composite is more pragmatic in the sense that it explores whether a formed construct is useful at all.

In the following part, we present the theoretical foundation of the composites model. Although the formal development of the composites model and the *composites factor model* (Henseler et al., 2014) were already laid out by Dijkstra (2013a, 2015), it has not been put into a holistic framework yet. In the following, it is assumed that each theoretical construct is modeled as a composite c_j with $j = 1, \ldots, J$.[4] By definition, a composite is completely determined by a unique block of K_j indicators, $\boldsymbol{x}'_j = \begin{pmatrix} x_{j1} & \ldots & x_{jK_j} \end{pmatrix}$, $c_j = \boldsymbol{w}'_j \boldsymbol{x}_j$. The weights of block j are included in the column vector $\boldsymbol{w}_j$ of length K_j. Usually, each weight vector is scaled to ensure that the composites have unit variance (see also Section 2.3). Here, we assume that each indicator is connected to only one composite. The theoretical covariance matrix $\boldsymbol{\Sigma}$ of the indicators can be expressed as

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[3] For a comparison of composites and common factors, we referred to Rigdon (2016).

[4] In general, models containing common factors and composites are also conceivable but have not been considered here.

partitioned matrix as follows:

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} & \dots & \boldsymbol{\Sigma}_{1J} \\ & \boldsymbol{\Sigma}_{22} & \dots & \boldsymbol{\Sigma}_{2J} \\ & & \ddots & \vdots \\ & & & \boldsymbol{\Sigma}_{JJ} \end{pmatrix}. \tag{2.1}$$

The intra-block covariance matrix $\boldsymbol{\Sigma}_{jj}$ of dimension $K_j \times K_j$ is unconstrained and captures the covariation between the indicators of block j; thus, effectively allowing the indicators of one block to freely covary. Moreover, it can be shown, that the indicator covariance matrix is positive-definite, if and only if the following two conditions hold: (i) all intra-block covariance matrices are positive-definite, and (ii) the covariance matrix of the composite is positive-definite (Dijkstra, 2015, 2018). The covariances between the indicators of block j and l are captured in the inter-block covariance matrix $\boldsymbol{\Sigma}_{jl}$, with $j \neq l$ of dimension $K_j \times K_l$. However, in contrast to the intra-block covariance matrix, the inter-block covariance matrix is constrained, since by assumption, the composites carry all information between the blocks:

$$\boldsymbol{\Sigma}_{jl} = \rho_{jl} \boldsymbol{\Sigma}_{jj} \boldsymbol{w}_j \boldsymbol{w}_l' \boldsymbol{\Sigma}_{ll} = \rho_{jl} \boldsymbol{\lambda}_j \boldsymbol{\lambda}_l', \tag{2.2}$$

where $\rho_{jl} = \boldsymbol{w}_j' \boldsymbol{\Sigma}_{jl} \boldsymbol{w}_l$ equals the correlation between the composites c_j and c_l. The vector $\boldsymbol{\lambda}_j = \boldsymbol{\Sigma}_{jj} \boldsymbol{w}_j$ of length K_j contains the composite loadings, which are defined as the covariances between the composite c_j and the associated indicators $\boldsymbol{x}_j$. Equation 2.2 is highly reminiscent of the corresponding equation where all constructs are modeled as common factors instead of composites. In a common factor model the vector $\boldsymbol{\lambda}_j$ captures the covariances between the indicators and its connected common factor and ρ_{jl} represents the correlation between common factor j and l. Hence, both models show the rank-one structure for the covariances matrices between two indicator blocks.

Although, the intra-block covariance matrices of the indicators, $\boldsymbol{\Sigma}_{jj}$ are not restricted, we emphasize that the composites model is still a model from the point of view of SEM. It assumes that all information between the indicators of two different blocks is conveyed by the composite(s), and therefore, it imposes rank one restrictions on the inter-block covariance matrices of the indicators (see Equation 2.2). These restrictions can be used for testing the overall model fit (see Section 2.5). It is emphasized that the weights $\boldsymbol{w}_j$ producing these matrices are the same across all inter-block covariance matrices $\boldsymbol{\Sigma}_{jl}$ with $l = 1, ..., J$ and $l \neq j$.

Figure 2.1 illustrates a minimal composites model.[5] The composite c is illustrated by a hexagon and the observed indicators are represented by squares. The unconstrained covariance σ_{12} between the indicators of block $\boldsymbol{x}' = \begin{pmatrix} x_1 & x_2 \end{pmatrix}$ forming the composite is highlighted by a double-headed arrow.
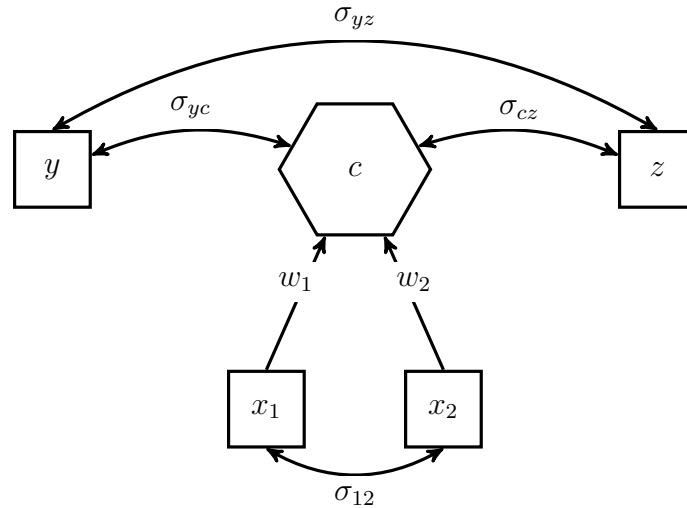
Figure 2.1: Minimal composites model

In contrast, the observed variables y and z do not form the composite; however, they are allowed to freely covary among each other as well as with the composite.

To emphasize upon the difference of the composites model to the model typically used in CFA where constructs are modeled as common factors, we depict the composites model as *composites factor* model (Dijkstra, 2013a; Henseler et al., 2014). Figure 2.2 shows the same model as Figure 2.1 but in terms of a *composite factor* representation. This illustration is advantageous since in it the deduction of the model implied correlations is straightforward.

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[5]The model is still over-identified with one degree of freedom.
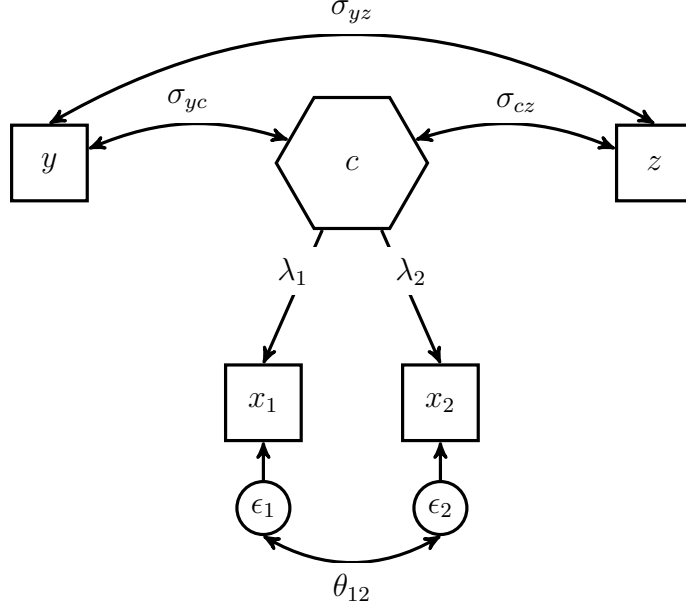
Figure 2.2: Minimal composites model displayed as composites factor model

The composite loading λ_i, $i = 1, 2$ captures the covariance between the indicator x_i and the composite c. In general, the error terms are included in the vector $\boldsymbol{\epsilon}$, explaining the variance of the indicators and the covariances between the indicators of one block, which are not explained by the composite factor. As the composites model does not restrict the covariances between the indicators of one block, the measurement errors are allowed to freely covary. The covariations among the measurement errors as well as their variances are captured in matrix $\boldsymbol{\theta}$. Therefore, the model implied intra-block covariances among the indicators of one block equal the empirical ones. The model implied covariance matrix of the minimal composites model can be displayed as follows:

$$
\boldsymbol{\Sigma} =
\begin{array}{cccc}
\underline{y} & \underline{x_1} & \underline{x_2} & \underline{z}
\end{array}
\left(
\begin{array}{cccc}
\sigma_{yy} & & & \\
\lambda_1 \sigma_{yc} & \sigma_{11} & & \\
\lambda_2 \sigma_{yc} & \lambda_1 \lambda_2 + \theta_{12} & \sigma_{22} & \\
\sigma_{yz} & \lambda_1 \sigma_{cz} & \lambda_2 \sigma_{cz} & \sigma_{zz}
\end{array}
\right). \tag{2.3}
$$

In comparison to the same model using a common factor instead of a composite, the composites model is less restrictive as it allows all error terms of one block to be correlated, which leads to a more general model (Henseler et al., 2014). In fact, the common factors model is always nested in the composites model since it uses the same restriction as the composites model; but additionally, it assumes that (some) covariances between the error terms of one block are restricted (usually to zero). Under

certain conditions, it is possible to rescale the intra- and inter-block covariances of a composites model to match those of a common factors model (Dijkstra, 2013a; Dijkstra and Henseler, 2015a).

2.3   Identifying composites models

Model identification is an important issue in CCA as well as in SEM and CFA. Since practitioners can freely specify their models, it needs be ensured that the model parameters have a unique solution (Bollen, 1989, Chap. 8). Therefore, model identification is necessary to obtain consistent parameter estimates and to reliably interpret them (Marcoulides and Chin, 2013).

In general, the following three states of model identification can be distinguished: under-identified, just-identified, and over-identified. An under-identified model, also known as not-identified model, offers several sets of parameters that are consistent with the model constraints, and thus, no unique solution for the model parameters exist. Therefore, only questionable conclusions can be drawn. In contrast, a just-identified model provides a unique solution for the model parameters and has the same number of free parameters as non-redundant elements of the indicator covariance matrix (degrees of freedom (df) are 0). In empirical analysis such models cannot be used to evaluate the overall model fit, since they perfectly fit the data. An over-identified model also has a unique solution; however, it provides more non-redundant elements of the indicator covariance matrix than model parameters (df > 0). This can be exploited in empirical studies for assessing the overall model fit, as these constraints should hold for a sample within the limits of sampling error if the model is valid.

A necessary condition for ensuring identification is to normalize each weight vector. In doing so, we assume that all composites are scaled to have a unit variance, $\boldsymbol{w}_j' \boldsymbol{\Sigma}_{jj} \boldsymbol{w}_j = 1$.[6] Besides the scaling of the composite, each composite must be connected to at least one composite or one variable not forming a composite. As a result, at least one inter-block covariance matrix $\boldsymbol{\Sigma}_{jl}$, $l = 1, ..., J$ with $l \neq j$ satisfies the rank one condition. Along with the normalization of the weight vector, the model parameters can be uniquely retrieved from the rank one inter-block covariance matrix

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[6]Another way of normalization is to fix one weight of each block to certain value. Furthermore, we ignore trivial regularity assumptions such as weight vectors consisting of zeros only; and similarly, we ignore cases where intra-block covariance matrices are singular.

displayed in Equation 2.2. Otherwise, if a composite c_i is isolated in the nomological network, all inter-block covariances $\mathbf{\Sigma}_{jl}$, $l = 1, ..., J$ with $l \neq j$, belonging to this composite are of rank zero, and thus, the weights forming this composite cannot be uniquely retrieved.

In the following part, we give a description on how the number of degrees of freedom is counted in case of the composites model.[7] It is given by the difference between the number of non-redundant elements of the indicator covariance matrix $\mathbf{\Sigma}$ and the number of free parameters in the model. The number of free model parameters is given by the number of covariances among the composites, the number of covariances between composites and indicators not forming a composite, the number of covariances among indicators not forming a composite, the number of non-redundant off-diagonal elements of each intra-block covariance matrix, and the number of weights. Since we fix composite variances to one, one weight of each block can be expressed by the remaining ones of this block. Hence, we regain as many degrees of freedom as fixed composite variances, i.e., as blocks in the model. Equation 2.4 summarizes the way of determining the number of degrees of freedom of a composites model.

$$
\begin{aligned}
\text{df} = {} & \text{number of non-redundant off-diagonal elements of the indicator covariance matrix} \\
& - \text{number of free correlations among the composites} \\
& - \text{number of free covariances between the composites and indicators not forming a composite} \\
& - \text{number of covariances among the indicators not forming a composite} \\
& - \text{number of free non-redundant off-diagonal elements of each intra-block covariance matrix} \\
& - \text{number of weights} \\
& + \text{number of blocks.}
\end{aligned}
\tag{2.4}
$$

To illustrate the way of calculating the number of degrees of freedom, we consider the minimal composites model presented in Figure 2.1. As described above, the model consists of four (standardized) observed variables, thus the indicator correlation matrix has six non-redundant off-diagonal elements. The number of free model parameters is counted as follows: no correlations among the composites as the models consists of only one composite, two correlations between the composite and the observable variables

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[7]The number of degrees of freedom can be helpful at determining whether or not a model is identified, since an identified model has non-negative number of degrees of freedom.

not forming a composite (σ_{yc} and σ_{cz}), one correlation between the single indicators (σ_{xz}), one non-redundant off-diagonal of the intra-block correlation matrix (σ_{12}), and two weights (w_1 and w_2) minus one, the number of blocks. As a result, we obtain the number of degrees of freedom as follows: $df = 6 - 0 - 2 - 1 - 1 - 2 + 1 = 1$. Once identification of the composites model is ensured, in a next step the model can be estimated.

The existing literature sometimes mentions *empirical under-identification* in the context of model identification (Kenny, 1979). We emphasize that empirical under-identification refers to an issue of estimation rather than to the issue of model identification. Although a model is in principle identified by its structure, model parameters can be undetermined and unstable due to the indicator sample covariance matrix. To exemplify the problem of empirical under-identification, we consider a model with two composites each formed by two standardized indicators: $c_1 = w_1 x_1 + w_2 x_2$ and $c_2 = w_3 x_3 + w_4 x_4$. For normalization, we fix the variance of each composite to one. Moreover, the two composites are allowed to freely correlate. The model implied correlation matrix is given by the following:

$$
\boldsymbol{\Sigma} = \begin{pmatrix} 1 & \sigma_{12} & \boxed{\begin{matrix} \rho\lambda_1\lambda_3 & \rho\lambda_1\lambda_4 \\ \rho\lambda_2\lambda_3 & \rho\lambda_2\lambda_4 \end{matrix}} \\ & 1 & \\ & & 1 & \sigma_{34} \\ & & & 1 \end{pmatrix},
\tag{2.5}
$$

where ρ is the correlation between the two composites c_1 and c_2 and λ_i, with $i = 1, \ldots, 4$, represents the correlation between the indicator x_i and its corresponding composite. Since each composite is connected to at least one variable, the model is identified with one degree of freedom; however, when the inter-block correlation matrix (elements surrounded by a rectangle) are close to zero or even zero in the sample, the estimates may be unstable or cannot be retrieved uniquely from the indicator sample correlation matrix.

2.4 Estimating composites models

The existing literature provides various ways of constructing composites from blocks of indicators. The most common among them are principal component analysis (PCA) (Pearson, 1901), linear discriminant analysis (LDA) (Fisher, 1936), and (generalized)

canonical correlation analysis ((G)CCA) (Hotelling, 1936; Kettenring, 1971). All these approaches seek composites that 'best' explain the data and can be regarded as *prescriptions* for dimension reduction (Dijkstra and Henseler, 2011). Further approaches are partial least squares path modeling (PLS-PM) (Wold, 1975), regularized general canonical correlation analysis (RGCCA) (Tenenhaus and Tenenhaus, 2011), and generalized structural component analysis (GSCA) (Hwang and Takane, 2004). Of course, the use of predefined weights is also possible.

We follow Dijkstra (2010) and apply GCCA in a first step to estimate the correlation between the composites.[8] In the following part, we give a brief description of GCCA. The vector of indicators $\boldsymbol{x}$ of length K is split up into J subvectors $\boldsymbol{x}_j$, so called blocks, each of dimension $(K_j \times 1)$ with $j = 1, \ldots, J$. We assume that the indicators are standardized to have means of zero and unit variances. Moreover, each indicator is connected to one composite only. Hence the correlation matrix of the indicators can be calculated as $\boldsymbol{\Sigma} = \mathrm{E}(\boldsymbol{xx'})$ and the intra-block correlation matrix as $\boldsymbol{\Sigma}_{jj} = \mathrm{E}(\boldsymbol{x}_j \boldsymbol{x}_j')$. Moreover, the correlation matrix of the composites, $c_j = \boldsymbol{x}_j' \boldsymbol{w}_j$ is calculated as follows: $\boldsymbol{\Sigma}_c = \mathrm{E}(\boldsymbol{cc'})$. In general, GCCA chooses the weights to maximize the correlation between the composites. In doing so, GCCA offers the several following options: *sumcor*, *maxvar*, *ssqcor*, *minvar*, and *genvar*.[9]

In the following part, we use *maxvar* under the constraint that each composite has a unit variance, $\boldsymbol{w}_j' \boldsymbol{\Sigma}_{jj} \boldsymbol{w}_j = 1$, to estimate the weights, the composites, and the resulting composite correlations.[10] In doing so, the weights are chosen to maximize the largest eigenvalue of the composite correlation matrix. Thus, the total variation of the composites is explained as well as possible by one underlying 'principal component' and the weights to form the composite c_j are calculated as follows (Kettenring, 1971):

$$\boldsymbol{w}_j = \boldsymbol{\Sigma}_{jj}^{-\frac{1}{2}} \tilde{\boldsymbol{a}}_j / \sqrt{\tilde{\boldsymbol{a}}_j' \tilde{\boldsymbol{a}}_j}. \tag{2.6}$$

The subvector $\tilde{\boldsymbol{a}}_j$, of length K_j, corresponds to the largest eigenvalue of the matrix $\boldsymbol{\Sigma}_D^{-\frac{1}{2}} \boldsymbol{\Sigma} \boldsymbol{\Sigma}_D^{-\frac{1}{2}}$, where the matrix $\boldsymbol{\Sigma}_D$, of dimension $K \times K$, is a block-diagonal matrix containing the the intra-block correlation matrices $\boldsymbol{\Sigma}_{jj}$, $j = 1, ..., J$ on its diagonal. For empirical work, the population matrix $\boldsymbol{\Sigma}$ is replaced by its empirical counterpart $\boldsymbol{S}$ to obtain the estimates of the weights, the composites, and their correlations.

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[8]GCCA builds composites in a way that they are maximally correlated.

[9]For an overview we refer to Kettenring (1971)

[10]In general, GCCA offers several composites (canonical variates); but in our study, we have focused only on the canonical variates of the first stage.

2.5 Assessing composites models

2.5.1 Tests of overall model fit

In CFA and factor-based SEM a goodness-of-fit test has been naturally supplied by the maximum-likelihood estimation in form of the chi-square test (Jöreskog, 1967), while CCA inherently lacks in terms of such a test. However, we contribute a combination of a bootstrap procedure with several distance measures to statistically test how well the assumed composites model fits to the collected data.

The existing literature provides several measures with which to assess the discrepancy between the perfect fit and the model fit. In fact, every distance measure known from CFA can be used to assess the goodness-of-fit of a composites model. They all capture the discrepancy between the sample covariance matrix $\boldsymbol{S}$ and the model implied covariance matrix $\hat{\boldsymbol{\Sigma}}$ of the indicators. In our study, we consider the following three distance measures: squared Euclidean distance (d_L), geodesic distance (d_G), and standardized root mean square residual (SRMR).

The squared Euclidean distance between the sample and the model implied covariance matrix is calculated as follows:

$$d_{\mathrm{L}} = \frac{1}{2} \sum_{i=1}^{K} \sum_{j=1}^{K} (s_{ij} - \hat{\sigma}_{ij})^2, \tag{2.7}$$

where K is the total number of indicators, and s_{ij} and $\hat{\sigma}_{ij}$ are the elements of the sample and the model-implied covariance matrix respectively. It is obvious that the squared Euclidean distance is zero for a perfectly fitting model, $\hat{\boldsymbol{\Sigma}} = \boldsymbol{S}$.

Moreover, the geodesic distance stemming from a class of distance functions proposed by Swain (1975) can be used to measure the discrepancy between the sample and model-implied covariance matrix. It is given by the following:

$$d_{\mathrm{G}} = \frac{1}{2} \sum_{i=1}^{K} (\log(\varphi_i))^2, \tag{2.8}$$

where φ_i is the i-th eigenvalue of the matrix $\boldsymbol{S}^{-1}\hat{\boldsymbol{\Sigma}}$ and K is the number of indicators. The geodesic distance is zero when and only when all eigenvalues equal one, i.e., when and only when the fit is perfect.

Finally, the standardized root mean square residual (SRMR) (Hu and Bentler, 1999)

can be used to test the goodness-of-fit. The SRMR is calculated as follows:

$$\text{SRMR} = \sqrt{\left[2 \sum_{i=1}^{K} \sum_{j=1}^{i} ((s_{ij} - \hat{\sigma}_{ij})/(s_{ii}s_{jj}))^2 \right] / (K(K+1))}, \qquad (2.9)$$

where K is the number of indicators. It reflects the average discrepancy between the empirical and the model implied correlation matrix. Thus, for a perfectly fitting model, the SRMR is zero, as $\hat{\sigma}_{ij}$ equals s_{ij}.

Since all distance measures considered are functions of the sample covariance matrix, a procedure proposed by Beran and Srivastava (1985) can be used to test the overall model fit: $H_0 : \boldsymbol{\Sigma} = \hat{\boldsymbol{\Sigma}}$.[11] The reference distribution of the distance measures as well as the critical values are obtained from the transformed sample data as follows:

$$\boldsymbol{X} \boldsymbol{S}^{-\frac{1}{2}} \hat{\boldsymbol{\Sigma}}^{\frac{1}{2}}, \qquad (2.10)$$

where the data matrix $\boldsymbol{X}$ of dimension $(N \times K)$ contains the N observations of all K indicators. This transformation ensures that the new dataset satisfies the null hypothesis, i.e., the sample covariance matrix of the transformed dataset equals the model implied covariance matrix. The reference distribution of the distance measures is obtained by bootstrapping from the transformed dataset. In doing so, the estimated distance based on the original dataset can be compared to the critical value from the reference distribution (typically the empirical 95% or 99% quantile) to decide if the null hypothesis, $H_0 : \boldsymbol{\Sigma} = \hat{\boldsymbol{\Sigma}}$ is rejected or not (Bollen and Stine, 1992).

2.5.2 Fit indices for composites models

Additional to the test of overall model fit, we provide some fit indices as measures of the overall model fit. In general, fit indices can indicate whether or not a model is misspecified by providing an absolute value of the misfit; however, we advise to use them with caution as they are based on heuristic rules-of-thumb rather than statistical theory. Moreover, it is recommended to calculate the fit indices based on the indicator correlation matrix instead of the covariance matrix.

The standardized root mean square residual (SRMR) was already introduced as a measure of overall model fit (Henseler et al., 2014). As described above, it represents the average discrepancy between the indicator sample and model-implied correlation

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[11]This procedure is known as Bollen-Stine bootstrap (Bollen and Stine, 1992) in the factor-based SEM literature. The model must be over-identified for this test.

matrix. Values below 0.10 and, following a more conservative view, below 0.08 indicate a good model fit (Hu and Bentler, 1998).

Furthermore, the normed fit index (NFI) is suggested as a measure of goodness of fit (Bentler and Bonett, 1980). It measures the relative discrepancy between the fit of baseline model and the fit of the estimated model. In this context, a model where all indicators are assumed to be uncorrelated (the model-implied correlation matrix equals the unit matrix) can serve as a baseline model (Lohmöller, 2013, Chap. 2.4.4). To assess the fit of the baseline model and the estimated model several measures can be used, e.g., the log likelihood function used in CFA or the geodesic distance. Values of the NFI close to one imply a good model fit. However, cut-off values still need to be determined.

Finally, we suggest to consider the root mean square residual covariance of the outer residuals ($\text{RMS}_{\text{theta}}$) as a further fit index (Lohmöller, 2013). It is defined as the square root of the average residual correlations. Since the indicators of one block are allowed to be freely correlated, the residual correlations within a block should be excluded and only the residual correlations across the blocks should be taken into account during its calculation. Small values close to zero for the $\text{RMS}_{\text{theta}}$ indicate a good model fit. However, threshold values still need to be determined.

2.6   A Monte Carlo simulation

In order to assess our proposed procedure of statistically testing the overall model fit of composites models and to examine the behavior of the earlier presented discrepancy measures, we conduct a Monte Carlo simulation. In particular, we investigate the type I error rate (false positive rate) and the power which are the most important characteristics of a statistical test. In designing the simulation, we choose a number of constructs used several times in the literature to examine the performance of fit indices and tests of overall model fit in CFA: a model containing two composites and a model containing three composites (Heene et al., 2012; Hu and Bentler, 1999). To investigate the power of the test procedure, we consider various misspecifications of these models. Tables 2.2 and 2.3 summarize the designs investigated in our simulation study.

Table 2.2: Simulation design for the model containing two composites

Table 2.3: Simulation design for the model containing three composites

Experimental condition	Population model	Correlation matrix	Estimated model

4) No misspecification

	x_{11}	x_{12}	x_{13}	x_{21}	x_{22}	x_{23}	x_{31}	x_{32}	x_{33}
x_{11}	1.000								
x_{12}	0.500	1.000							
x_{13}	0.500	0.500	1.000						
x_{21}	0.108	0.096	0.084	1.000					
x_{22}	0.216	0.192	0.168	0.200	1.000				
x_{23}	0.216	0.192	0.168	0.000	0.400	1.000			
x_{31}	0.326	0.290	0.254	0.116	0.232	0.232	1.000		
x_{32}	0.306	0.272	0.238	0.109	0.218	0.218	0.250	1.000	
x_{33}	0.333	0.296	0.259	0.118	0.237	0.237	0.400	0.160	1.000

5) Unexplained correlation

	x_{11}	x_{12}	x_{13}	x_{21}	x_{22}	x_{23}	x_{31}	x_{32}	x_{33}
x_{11}	1.000								
x_{12}	0.500	1.000							
x_{13}	0.500	0.500	1.000						
x_{21}	0.108	0.096	0.250	1.000					
x_{22}	0.216	0.192	0.168	0.200	1.000				
x_{23}	0.216	0.192	0.168	0.000	0.400	1.000			
x_{31}	0.326	0.290	0.254	0.116	0.232	0.232	1.000		
x_{32}	0.306	0.272	0.238	0.109	0.218	0.218	0.250	1.000	
x_{33}	0.333	0.296	0.259	0.118	0.237	0.237	0.400	0.160	1.000

Values in the population correlation matrices are rounded to three decimal places.

2.6.1 Two composites model

All models containing two composites are estimated using the specification illustrated in the last column of Table 2.2. The indicators x_{11} to x_{13} are specified to build composite c_1, while the remaining three indicators build composite c_2. Moreover, the composites are allowed to freely correlate. The parameters of interest are the correlation between the two composites, and the weights, w_{11} to w_{23}. As column 'Population model' of Table 2.2 shows, we consider three types of population models with two composites.

Design 1: no misspecification

First, in order to examine whether the rejection rates of the test procedure are close to the predefined significance level in cases in which the null hypothesis is true, a population model is considered that has the same structure as the specified model. The correlation between the two composites is set to $\rho = 0.3$ and the composites are formed by its connected standardized indicators as follows: $c_i = \boldsymbol{x}_i' \boldsymbol{w}_i$ with $i = 1, 2$, where $\boldsymbol{w}_1' = \begin{pmatrix} 0.6 & 0.2 & 0.4 \end{pmatrix}$ and $\boldsymbol{w}_2' = \begin{pmatrix} 0.4 & 0.2 & 0.6 \end{pmatrix}$. All correlations between the indicators of one block are set to 0.5, which leads to the population correlation matrix given in Table 2.2 (see row *No misspecification*).

Design 2: false assignment

The second design is used to investigate whether the test procedure is capable of detecting misspecified models. It presents a situation where the researcher falsely assigns two indicators to wrong constructs. The correlation between the two composites and the weights are the same as in population model 1: $\rho = 0.3$, $\boldsymbol{w}_1' = \begin{pmatrix} 0.6 & 0.2 & 0.4 \end{pmatrix}$, and $\boldsymbol{w}_2' = \begin{pmatrix} 0.4 & 0.2 & 0.6 \end{pmatrix}$. However, in contrast to population model 1, the indicators x_{13} and x_{21} are interchanged. Moreover, the correlations among all indicators of one block are 0.5. The population correlation matrix of the second model is presented in Table 2.2 (see row *Confounded indicators*).

Design 3: unexplained correlation

The third design is chosen to further investigate the capabilities of the test procedure to detect misspecified models. It shows a situation where the correlation between the

two indicators x_{13} and x_{21} is not fully explained by the two composites.[12] As in the two previously presented population models, the two composites have a correlation of $\rho = 0.3$. The correlations among the indicators of one block are set to 0.5, and the weights for the construction of the composites are set to $\boldsymbol{w}_1' = \begin{pmatrix} 0.6 & 0.2 & 0.4 \end{pmatrix}$, and $\boldsymbol{w}_2' = \begin{pmatrix} 0.4 & 0.2 & 0.6 \end{pmatrix}$. The population correlation matrix of the indicators is presented in Table 2.2 (see row *Unexplained correlation*).

2.6.2 Three composites model

Furthermore, we investigate a more complex model consisting of three composites. Again, each composite is formed by three indicators and the composites are allowed to freely correlate. The column 'Estimated model' of Table 2.3 illustrates the specification to be estimated in case of three composites. We assume that the composites are built as follows: $c_1 = \boldsymbol{x}_1' \boldsymbol{w}_1$, $c_2 = \boldsymbol{x}_2' \boldsymbol{w}_2$, and $c_3 = \boldsymbol{x}_3' \boldsymbol{w}_3$. Moreover, the composites are allowed to freely correlate. Again, we examine two different population models.

Design 4: no misspecification

The fourth design is used to further investigate whether the rejection rates of the test procedure are close to the predefined significance level in cases in which the null hypothesis is true. Hence, the structure of the fourth population model matches the specified model. All composites are assumed to be freely correlated. In the population the composite correlations are set to $\rho_{12} = 0.3$, $\rho_{13} = 0.5$, and $\rho_{23} = 0.4$. Each composite is built by three indicators using the following population weights: $\boldsymbol{w}_1' = \begin{pmatrix} 0.6 & 0.4 & 0.2 \end{pmatrix}$, $\boldsymbol{w}_2' = \begin{pmatrix} 0.3 & 0.5 & 0.6 \end{pmatrix}$, and $\boldsymbol{w}_3' = \begin{pmatrix} 0.4 & 0.5 & 0.5 \end{pmatrix}$. The indicators correlations of each block can be read from Table 2.3. The population correlation matrix of model 4 is given in Table 2.3 (see row *No misspecification*).

Design 5: unexplained correlation

In the last design, number 5, we investigate a situation where the correlation between two indicators is not fully explained by the underlying composites, similar to what is observed in design 3. Consequently, population model 5 does not match the model to be estimated and is used to investigate the power of the overall model test. It equals

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[12]The model implied correlation between the two indicators is calculated as follows, $0.8 \cdot 0.3 \cdot 0.8 \neq 0.5$.

population model 4 with the exception that the correlation between the indicators x_{13} and x_{21} is only partly explained by the composites. Since the original correlation between these indicators is 0.084, a correlation of 0.25 presents only a weak violation. The remaining model stays untouched. The population correlation matrix is illustrated in Table 2.3 (see row *Unexplained correlation*).

2.6.3 Further simulation conditions and expectations

To assess the quality of the proposed test of the overall model fit, we generate 10,000 standardized samples from the multivariate normal distribution having zero means and a covariance matrix, according to the respective population model. Moreover, we vary the sample size from 50 to 1,450 observations and the significance level α from 10% to 1%. To obtain the reference distribution of the discrepancy measures considered, 200 bootstrap samples are drawn from the transformed and standardized dataset. Each dataset is used in the maxvar procedure to estimate the model parameters.

All simulations are conducted in the statistical programming environment R (R Core Team, 2016). The samples are drawn from the multivariate normal distribution, using the *mvrnorm* function of the *MASS* packages (Venables and Ripley, 2002). The results for the test of overall model fit are obtained by user-written functions[13] and the *matrixpls* package (Rönkkö, 2016).

Since population model 1 and 4 fit the respective specification, we expect rejection rates close to the predefined level of significance α. Additionally, we expect that for an increasing sample size the predefined significance level is kept with more precision. For population model 2, 3, and 5, much larger rejection rates are expected as these population models do not match the respective specification. Moreover, we expect that the power of the test to detect misspecifications would increase with an increasing sample size. Regarding the different discrepancy measures, we have no expectations only that the squared Euclidean distance and the SRMR should lead to identical results. For standardized datasets, the only difference is a constant factor that does not affect the order of the observations in the reference distribution and, therefore, does not affect the decision about the null hypothesis.

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[13]These functions are provided by the authors upon request.

2.6.4 Results

Figure 2.3 illustrates the rejection rates for population model 1 matching the specification estimated. Besides the rejection rates, the figure also depicts the 95% confidence intervals (shaded area) constructed around the rejection rates to clarify whether or not a rejection rate is significantly different from the predefined significance level.[14]
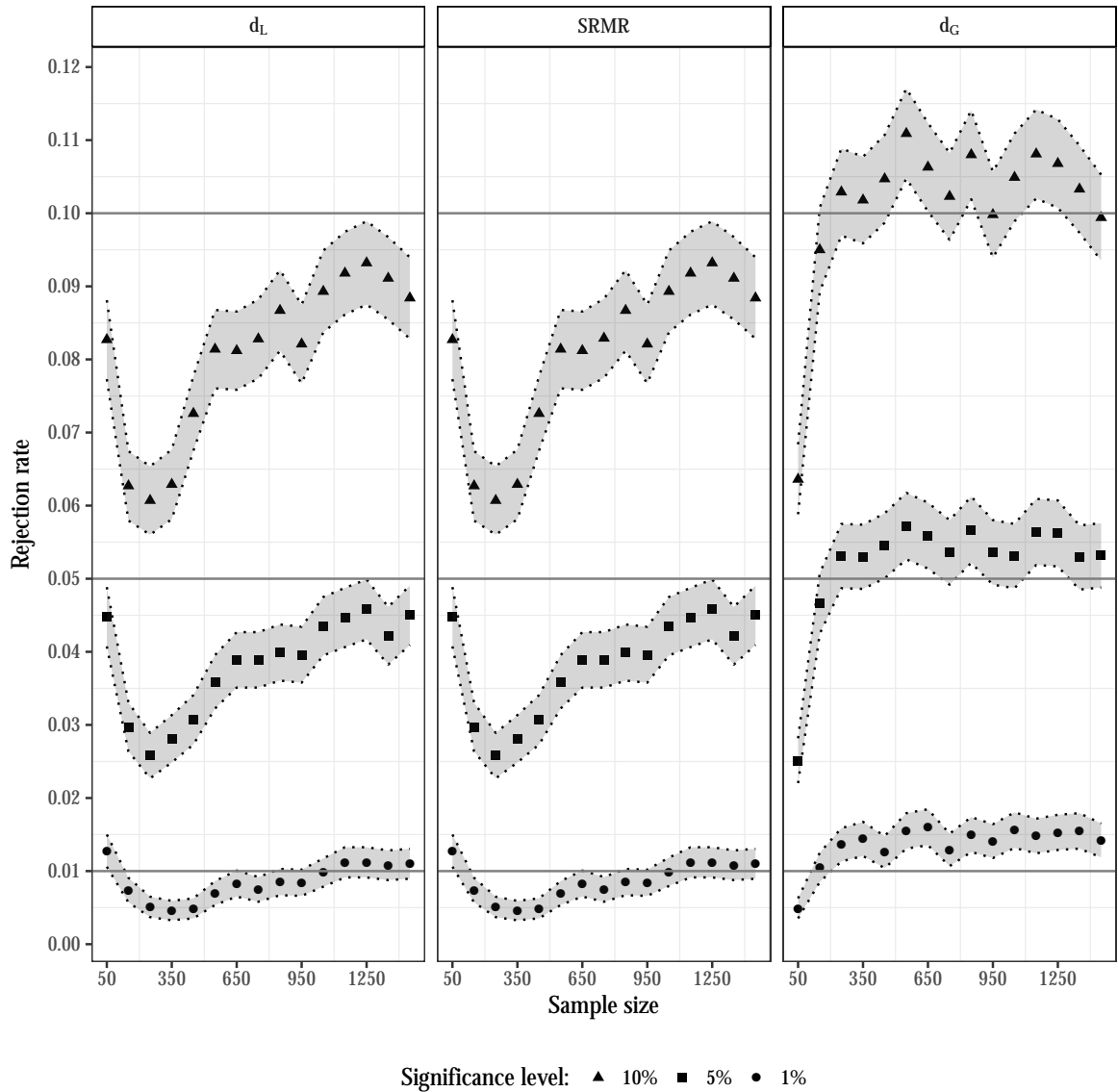
Figure 2.3: Rejection rates for population model 1

First, as expected, the squared Euclidean distance (d_L) as well as the SRMR lead to identical results. The test using the squared Euclidean distance and the SRMR rejects the model too rarely in case of $\alpha = 10\%$ and $\alpha = 5\%$ respectively; however, for

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[14]The limits of the 95% confidence interval are calculated as, $\hat{p} \pm \Phi^{-1}(0.975)\sqrt{\hat{p}(1-\hat{p})/10000}$, where $\hat{p}$ represents the rejection rate and $\Phi^{-1}()$ is the quantile function of the standard normal distribution.

an increasing sample size, the rejection rates converge to the predefined significance level without reaching it. For the 1% significance level, a similar picture is observed; however, for larger sample sizes the significance level is retained more often compared to the larger significance levels. In contrast, the test using the geodesic distance mostly rejects the model too often for the 5% and 10% significance level. However, the obtained rejection rates are less often significantly different from the predefined significance level compared to the same situation where the SRMR or the Euclidean distance is used. In case of $\alpha = 1\%$ and sample sizes larger than $n = 100$, the test using the geodesic distance rejects the model significantly too often.

Figure 2.4 displays the rejection rates for population model 2 and 3. The horizontal line at 80% depicts the commonly recommended power for a statistical test (Cohen, 1988).
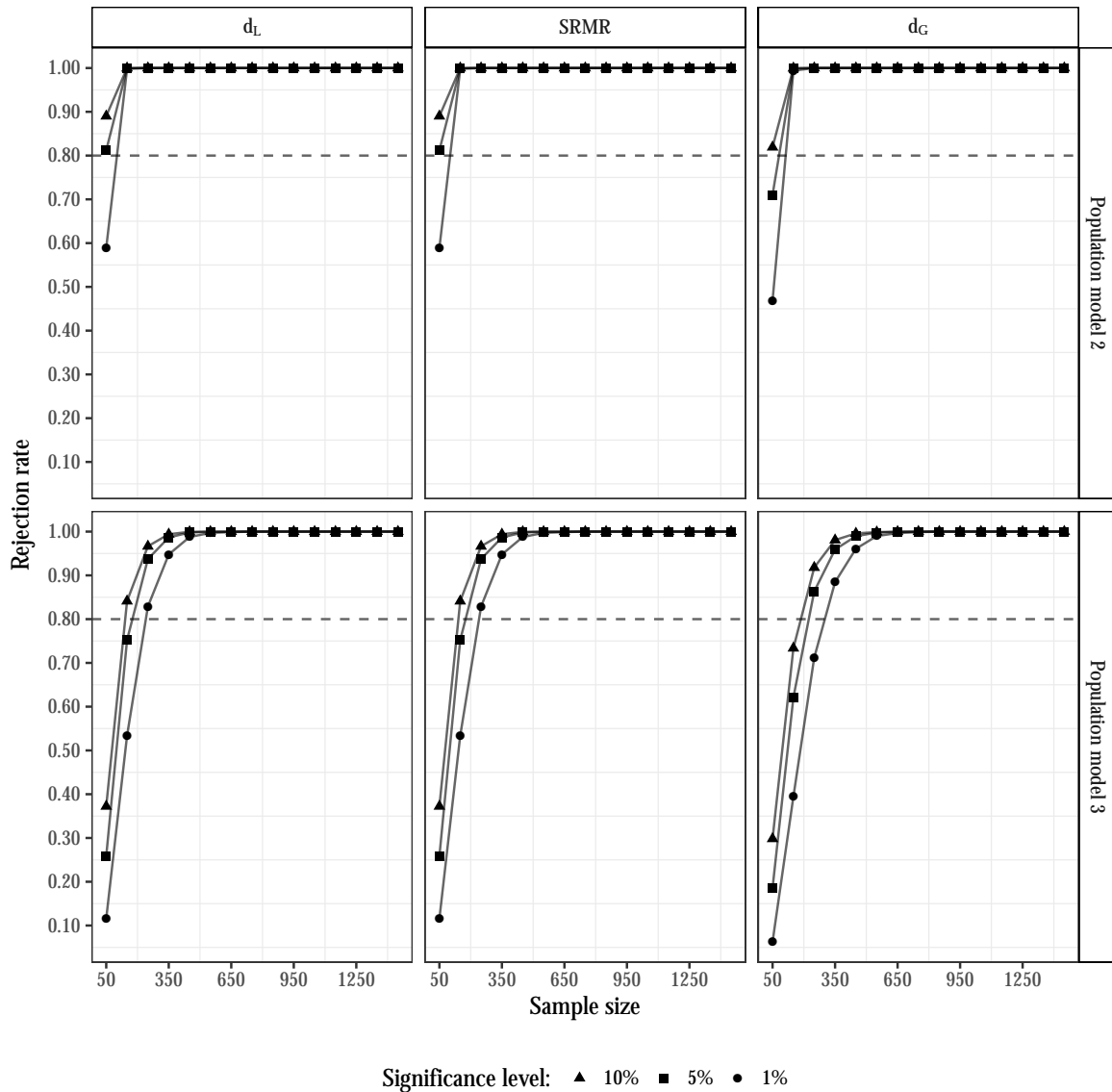
Figure 2.4: Rejection rates for population model 2 and 3

For the two cases where the specification does not match the underlying data generating process, the test using the squared Euclidean distance as well as the SRMR has more power than the test using the geodesic distance, i.e., the test using former discrepancy measures rejects the wrong model more often. For model 2 (confounded indicators) the test produces higher or equal rejection rates compared to model 3 (unexplained correlation). Furthermore, as expected, the power decreases for an increasing level of significance and increases with increasing sample sizes.

Figure 2.5 depicts the rejection rates for population model 4 and 5. Again, the 95% confidence intervals are illustrated for population model 4 (shaded area) matching the specification estimated.
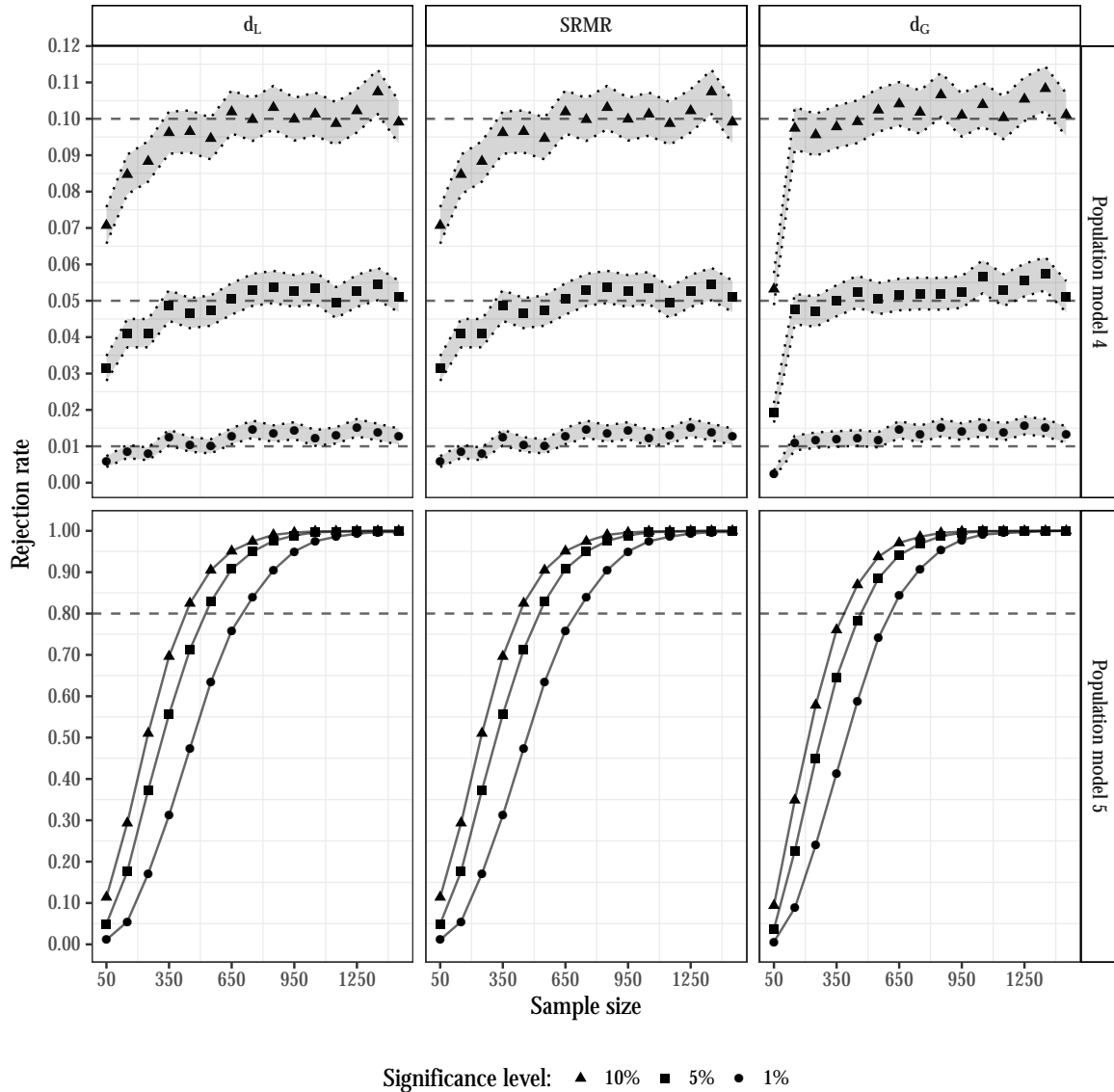
Figure 2.5: Rejection rates for population model 4 and 5

Considering population model 4 which matches the estimated model, the test leads to similar results for all three discrepancy measures. However, the rejection rate of the test using the geodesic distance converges faster to the predefined significance level, i.e., for smaller sample sizes $n \geq 100$. Again, among the three discrepancy measures considered, the geodesic distance performs best in terms of keeping the significance level.

As the misspecification in population model 5 is only of minor extent, the test

struggles to detect the model misspecification up to sample sizes $n = 350$, regardless of the discrepancy measure used. However, for sample sizes larger than 350 observations, the test detects the model misspecification satisfactorily. For sample sizes larger than 1050 observations, the misspecification was identified in almost all cases regardless of the significance level and the discrepancy measure used. Again, this confirms the anticipated relationship between sample size and statistical power.

2.7 Discussion

We introduced the confirmatory composite analysis (CCA) as a full-fledged technique for confirmatory purposes that employs composites to model theoretical constructs. In doing so, it carries the spirit of CFA and SEM to research domains where composites models prevail. Thus, CCA is appropriate in situations where the research goal is to explore whether or not an artifact is useful rather than to establish whether or not a certain entity exists. It follows the same steps usually applied in SEM and enables researchers to analyze a variety of situations, in particular, abroad the realm of social and behavioral sciences. Hence, CCA allows for dealing with research questions that could not be appropriately dealt with yet in the framework of CFA or in more generally SEM.

The results of the Monte Carlo simulation confirmed that CCA can be used for confirmatory purposes. They revealed that the bootstrap-based approach, in combination with different discrepancy measures, can be used to statistically assess the overall model fit of the composites model. For specifications matching the population model, the rejection rates were in the acceptable range, i.e., close to the predefined significance level. Moreover, the results of the power analysis showed that the boostrap-based test can reliably detect misspecified models. However, caution is needed in case of small sample sizes where the rejection rates were low which means that misspecified models were not reliably detected.

In future research, the usefulness of the composites model in empirical studies needs to be examined, accompanied and enhanced by simulation studies. In particular, the extensions outlined by Dijkstra (2018), to wit interdependent systems of equations for the composites estimated by classical econometric methods (like 2SLS and 3SLS) warrant further analysis and scrutiny. Robustness with respect to non-normality and

misspecification also appear to be relevant research topics. Additionally, devising ways to efficiently predict indicators and composites might be of particular interest (see for example the work by Shmueli et al. (2016)).

Moreover, to contribute to the confirmatory character of CCA, we recommend to further study the performance and limitations of the proposed test procedure: consider more misspecifications and the ability of the test to reliably detect them, find further discrepancy measures and examine their performance, and investigate the behavior of the test under the violation of the normality assumption, similar as Nevitt and Hancock (2001) did for CFA. Finally, cut-off values for the fit indices need to be determined for CCA.

2.8 Appendix to Chapter 2

Rejection rates of the test for overall model fit

Table 2.4: Results: 2 composites model

(a) Population model 1

Obs.	α	d_{LS}	d_G	SRMR
	10%	8.3%	6.4%	8.3%
50	5%	4.5%	2.5%	4.5%
	1%	1.3%	0.5%	1.3%
	10%	6.3%	9.5%	6.3%
150	5%	3.0%	4.7%	3.0%
	1%	0.7%	1.1%	0.7%
	10%	6.1%	10.2%	6.1%
250	5%	2.6%	5.3%	2.6%
	1%	0.5%	1.4%	0.5%
	10%	6.3%	10.2%	6.3%
350	5%	2.8%	5.3%	2.8%
	1%	0.5%	1.4%	0.5%
	10%	7.3%	10.1%	7.3%
450	5%	3.1%	5.5%	3.1%
	1%	0.5%	1.3%	0.5%
	10%	8.1%	11.1%	8.1%
550	5%	3.6%	5.7%	3.6%
	1%	0.7%	1.6%	0.7%
	10%	8.1%	10.6%	8.1%
650	5%	3.9%	5.6%	3.9%
	1%	0.8%	1.6%	0.8%
	10%	8.3%	10.2%	8.3%
750	5%	3.9%	5.4%	3.9%
	1%	0.8%	1.3%	0.8%
	10%	8.7%	10.8%	8.7%
850	5%	4.0%	5.7%	4.0%
	1%	0.9%	1.5%	0.9%
	10%	8.2%	10.0%	8.2%
950	5%	4.0%	5.4%	4.0%
	1%	0.8%	1.4%	0.8%
	10%	8.9%	10.5%	8.9%
1050	5%	4.4%	5.3%	4.4%
	1%	1.0%	1.6%	1.0%
	10%	9.2%	10.8%	9.2%
1150	5%	4.5%	5.6%	4.5%
	1%	1.1%	1.5%	1.1%
	10%	9.3%	10.7%	9.3%
1250	5%	4.6%	5.6%	4.6%
	1%	1.1%	1.5%	1.1%
	10%	9.1%	10.3%	9.1%
1350	5%	4.2%	5.3%	4.2%
	1%	1.1%	1.6%	1.1%
	10%	8.8%	9.9%	8.8%
1450	5%	4.5%	5.3%	4.5%
	1%	1.1%	1.4%	1.1%

(b) Population model 2

Obs.	α	d_{LS}	d_G	SRMR
	10%	89.0%	81.9%	89.0%
50	5%	81.2%	71.0%	81.2%
	1%	58.9%	46.9%	58.9%
	10%	100%	100%	100%
150	5%	100%	99.9%	100%
	1%	99.8%	99.4%	99.8%
	10%	100%	100%	100%
250	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
350	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
450	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
550	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
650	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
750	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
850	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
950	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
1050	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
1150	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
1250	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
1350	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
1450	5%	100%	100%	100%
	1%	100%	100%	100%

(c) Population model 3

Obs.	α	d_{LS}	d_G	SRMR
	10%	37.2%	29.8%	37.2%
50	5%	25.8%	18.6%	25.8%
	1%	11.6%	6.2%	11.6%
	10%	84.1%	73.4%	84.1%
150	5%	75.2%	62.1%	75.2%
	1%	53.4%	39.4%	53.4%
	10%	96.7%	91.8%	96.7%
250	5%	93.7%	86.3%	93.7%
	1%	82.9%	71.2%	82.9%
	10%	99.4%	98.1%	99.4%
350	5%	98.7%	95.9%	98.7%
	1%	94.8%	88.5%	94.8%
	10%	100%	99.6%	100%
450	5%	99.8%	99.0%	99.8%
	1%	98.8%	96.1%	98.8%
	10%	100%	99.9%	100%
550	5%	100%	99.8%	100%
	1%	99.7%	99.0%	99.7%
	10%	100%	100%	100%
650	5%	100%	99.9%	100%
	1%	99.9%	99.7%	99.9%
	10%	100%	100%	100%
750	5%	100%	100%	100%
	1%	100%	99.9%	100%
	10%	100%	100%	100%
850	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
950	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
1050	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
1150	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
1250	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
1350	5%	100%	100%	100%
	1%	100%	100%	100%
	10%	100%	100%	100%
1450	5%	100%	100%	100%
	1%	100%	100%	100%

Table 2.5: Results: 3 composites model

(a) Population model 4

| Obs. | Rejection rates | | | |
	α	d_{LS}	d_G	SRMR
	10%	7.1%	5.3%	7.1%
50	5%	3.1%	1.9%	3.1%
	1%	0.6%	0.2%	0.6%
	10%	8.5%	9.7%	8.5%
150	5%	4.1%	4.8%	4.1%
	1%	0.9%	1.1%	0.9%
	10%	8.8%	9.6%	8.8%
250	5%	4.1%	4.7%	4.1%
	1%	0.8%	1.2%	0.8%
	10%	9.6%	9.8%	9.6%
350	5%	4.9%	5.0%	4.9%
	1%	1.2%	1.2%	1.2%
	10%	9.7%	9.9%	9.7%
450	5%	4.7%	5.3%	4.7%
	1%	1.1%	1.2%	1.1%
	10%	9.5%	10.2%	9.5%
550	5%	4.7%	5.1%	4.7%
	1%	1.0%	1.2%	1.0%
	10%	10.2%	10.4%	10.2%
650	5%	5.1%	5.2%	5.1%
	1%	1.3%	1.5%	1.3%
	10%	10.0%	10.2%	10.0%
750	5%	5.3%	5.2%	5.3%
	1%	1.5%	1.3%	1.5%
	10%	10.3%	10.7%	10.3%
850	5%	5.4%	5.2%	5.4%
	1%	1.4%	1.5%	1.4%
	10%	10.0%	10.1%	10.0%
950	5%	5.3%	5.2%	5.3%
	1%	1.4%	1.4%	1.4%
	10%	10.1%	10.4%	10.1%
1050	5%	5.4%	5.7%	5.4%
	1%	1.2%	1.5%	1.2%
	10%	9.9%	10.0%	9.9%
1150	5%	5.0%	5.3%	5.0%
	1%	1.3%	1.4%	1.3%
	10%	10.2%	10.5%	10.2%
1250	5%	5.3%	5.6%	5.3%
	1%	1.5%	1.6%	1.5%
	10%	10.7%	10.8%	10.7%
1350	5%	5.5%	5.7%	5.5%
	1%	1.4%	1.5%	1.4%
	10%	9.9%	10.1%	9.9%
1450	5%	5.1%	5.1%	5.1%
	1%	1.3%	1.3%	1.3%

(b) Population model 5

| Obs. | Rejection rates | | | |
	α	d_{LS}	d_G	SRMR
	10%	11.4%	9.4%	11.4%
50	5%	5.0%	3.7%	5.0%
	1%	1.1%	0.6%	1.1%
	10%	29.3%	34.9%	29.3%
150	5%	17.6%	22.6%	17.6%
	1%	5.5%	8.8%	5.5%
	10%	51.0%	57.8%	51.0%
250	5%	37.3%	44.9%	37.3%
	1%	17.1%	24.0%	17.1%
	10%	69.6.1%	76.1%	69.6%
350	5%	55.6%	64.6%	55.6%
	1%	31.2%	41.4%	31.2%
	10%	82.5%	87.0%	82.5%
450	5%	71.3%	78.3%	71.3%
	1%	47.4%	58.8%	47.4%
	10%	90.5%	93.7%	90.5%
550	5%	82.9%	88.5%	82.9%
	1%	63.4%	74.1%	63.4%
	10%	95.1%	97.1%	95.1%
650	5%	90.8%	94.1%	90.8%
	1%	75.9%	84.3%	75.9%
	10%	97.4%	98.6%	97.4%
750	5%	95.0%	96.9%	95.0%
	1%	83.9%	90.8%	83.9%
	10%	99.0%	99.5%	99.0%
850	5%	97.6%	98.7%	97.6%
	1%	90.5%	95.3%	90.5%
	10%	99.6%	99.8%	99.6%
950	5%	98.9%	99.5%	98.9%
	1%	95.0%	97.8%	95.0%
	10%	99.9%	100%	99.9%
1050	5%	99.7%	99.9%	99.7%
	1%	97.5%	99.1%	97.5%
	10%	99.9%	100%	99.9%
1150	5%	99.8%	99.9%	99.8%
	1%	98.6%	99.5%	98.6%
	10%	100%	100%	100%
1250	5%	99.9%	100%	99.9%
	1%	99.3%	99.7%	99.3%
	10%	100%	100%	100%
1350	5%	100%	100%	100%
	1%	99.7%	99.9%	99.7%
	10%	100%	100%	100%
1450	5%	100%	100%	100%
	1%	99.7%	100%	99.7%

Further insights to the composites model

As demanded in the discussion (Section 2.7), I further compare different estimators for the measurement model (PLS and maxvar) and the structural model (two-stage least squares and three-stage least squares) in a scenario where composites are embedded in a structural equation model. For this purpose, I adopt a simulation study from Dijkstra and Henseler (2015a) and Dijkstra (2018) based on a model from Summers (1965).

Setup of the Monte Carlo simulation

Figure 2.6 depicts the structural model used in the Monte Carlo simulation. It contains four exogenous $(c_{exo,j}, j = 1, ..., 4)$[15] and two endogenous composites $(c_{endo,j}, j = 1, 2)$, illustrated by hexagons.
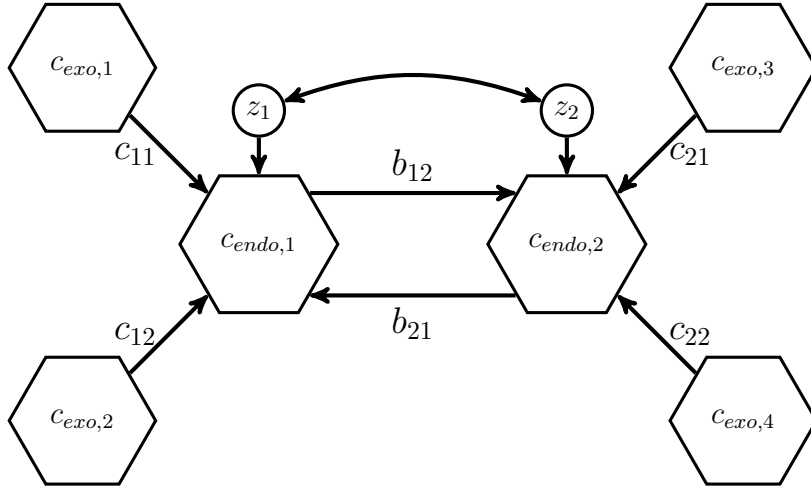
Figure 2.6: Structural model of Summers' model

The structural model can be summarized by the following equation:

$$(\boldsymbol{I} - \boldsymbol{B})\boldsymbol{c}_{endo} = \boldsymbol{C}\boldsymbol{c}_{exo} + \boldsymbol{z}. \tag{2.11}$$

For the simulation study, I use the following population path coefficients:

$$\boldsymbol{B} = \begin{pmatrix} 0 & 0.25 \\ 0.5 & 0 \end{pmatrix} \quad \text{and} \quad \boldsymbol{C} = \begin{pmatrix} -0.3 & 0.5 & 0 & 0 \\ 0 & 0 & 0.5 & 0.25 \end{pmatrix}. \tag{2.12}$$

Furthermore, each composite is built as a linear combination of three indicators. For the composites $c_{exo,1}$ and $c_{exo,4}$, I choose unit weights, for $c_{exo,2}$ and $c_{endo,1}$, the weights

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[15] Since composites are built by the indicators, exogeneity of the composites refers to the structural model.

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are proportional to $(1, 2, 3)$, and for $c_{exo,3}$ and $c_{endo,2}$, the unscaled weights are $(1, 4, 9)$. Before the analysis, the weights are scaled to obtain composites with unit variance. In addition, I vary the correlation between the endogenous composites $c_{endo,1}$ and $c_{endo,2}$ from 0 to $\sqrt{0.6}$, leading to correlated structural error terms in order to investigate the efficiency gains of 3SLS over 2SLS. While 3SLS is known to be asymptotically more efficient than 2SLS for structural equation models with observable variables only (Zellner and Theil, 1962), for structural equation models containing composites, an additional source of uncertainty is introduced by the estimation of the weights.[16] Table 2.6 contains the resultant variances and covariances between the error terms of the structural model ζ_1 and ζ_2, depending on the correlation between the endogenous composites.

Table 2.6: Variances and covariance of the structural error terms z_1 and z_2 depending on the correlation between $c_{endo,1}$ and $c_{endo,2}$

$\mathrm{cor}(c_{endo,1}, c_{endo,2})$	$\mathrm{var}(z_1)$	$\mathrm{var}(z_2)$	$\mathrm{cov}(z_1, z_2)$
$\sqrt{0.0}$	0.8725	0.8125	-0.8250
$\sqrt{0.1}$	0.7144	0.4963	-0.4692
$\sqrt{0.2}$	0.6489	0.3653	-0.3219
$\sqrt{0.3}$	0.5986	0.2648	-0.2088
$\sqrt{0.4}$	0.5563	0.1800	-0.1135
$\sqrt{0.5}$	0.5189	0.1054	-0.0295
$\sqrt{0.6}$	0.4852	0.0379	0.0464

As was observed in the original simulation of Dijkstra (2018), my simulation comprises 10,000 runs, using samples of size $n = 300$. Apart from replicating the Monte Carlo simulation using maxvar (Kettenring, 1971), I rerun the simulation using PLS (Wold, 1982b). For PLS, the all-adjacent centroid scheme and Mode B are used.[17] The whole simulation is conducted in R (R Core Team, 2016), using the matrixpls package (Rönkkö, 2016) in combination with several user-written functions. The user-written functions are provided by the author upon request.

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[16]This might entail an adjustment of the weighting matrix in 3SLS, which is object of future research.

[17]The use of the usual centroid scheme leads to average weight estimates substantially far away from the population weights and, therefore, the average path coefficient estimates deviate from their population value.

Results

The results confirm that 3SLS outperforms 2SLS if structural error terms are substantially correlated, i.e., 3SLS produces smaller standard errors (SEs) (blue line is below the red line). The SEs presented in Figure 2.7 are obtained as standard deviation of the parameter estimates obtained in each of the 10,000 runs.
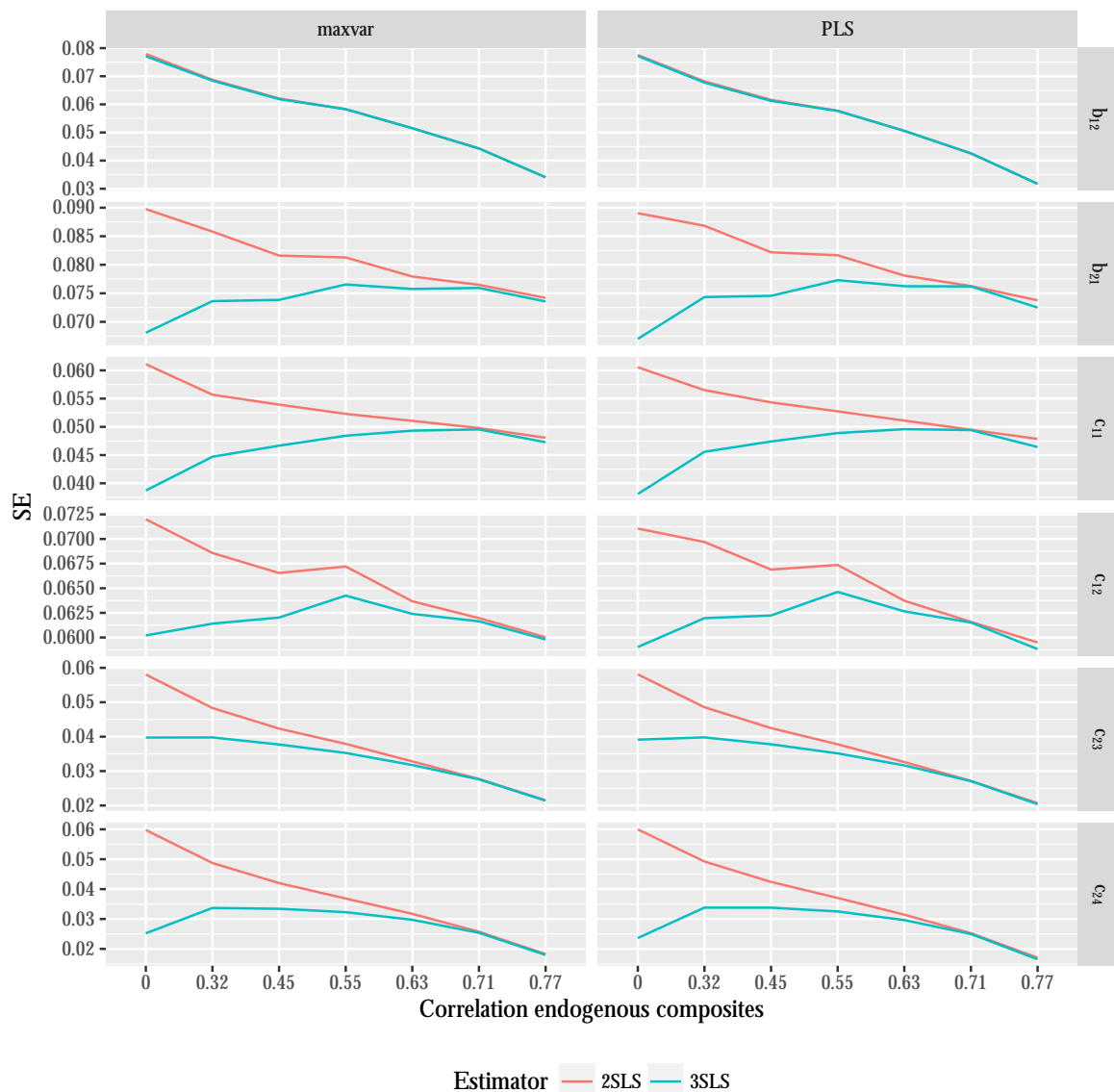
Figure 2.7: SEs for 2SLS and 3SLS, using the Summers' model with composites

While the standard deviations are for most path coefficient estimates as expected, they are smaller for 3SLS than for 2SLS. It is surprising that the standard deviations of $\hat{b}_{12}$ are very similar for 2SLS and 3SLS.

Furthermore, I present the deviation of the average path coefficient estimates from their population value for 2SLS and 3SLS. The deviations using PLS and maxvar

are illustrated in Figure 2.8 and 2.9 respectively. Across the columns, the correlation between the endogenous composites $c_{endo,1}$ and $c_{endo,2}$ is varied. The results of maxvar are in line with those obtained by Dijkstra (2018). To view this, compare column 6 of Figure 2.9 with the results presented in Dijkstra (2018, Table p. 19). Furthermore, the results confirm that PLS leads to similar results as is obtained with maxvar.
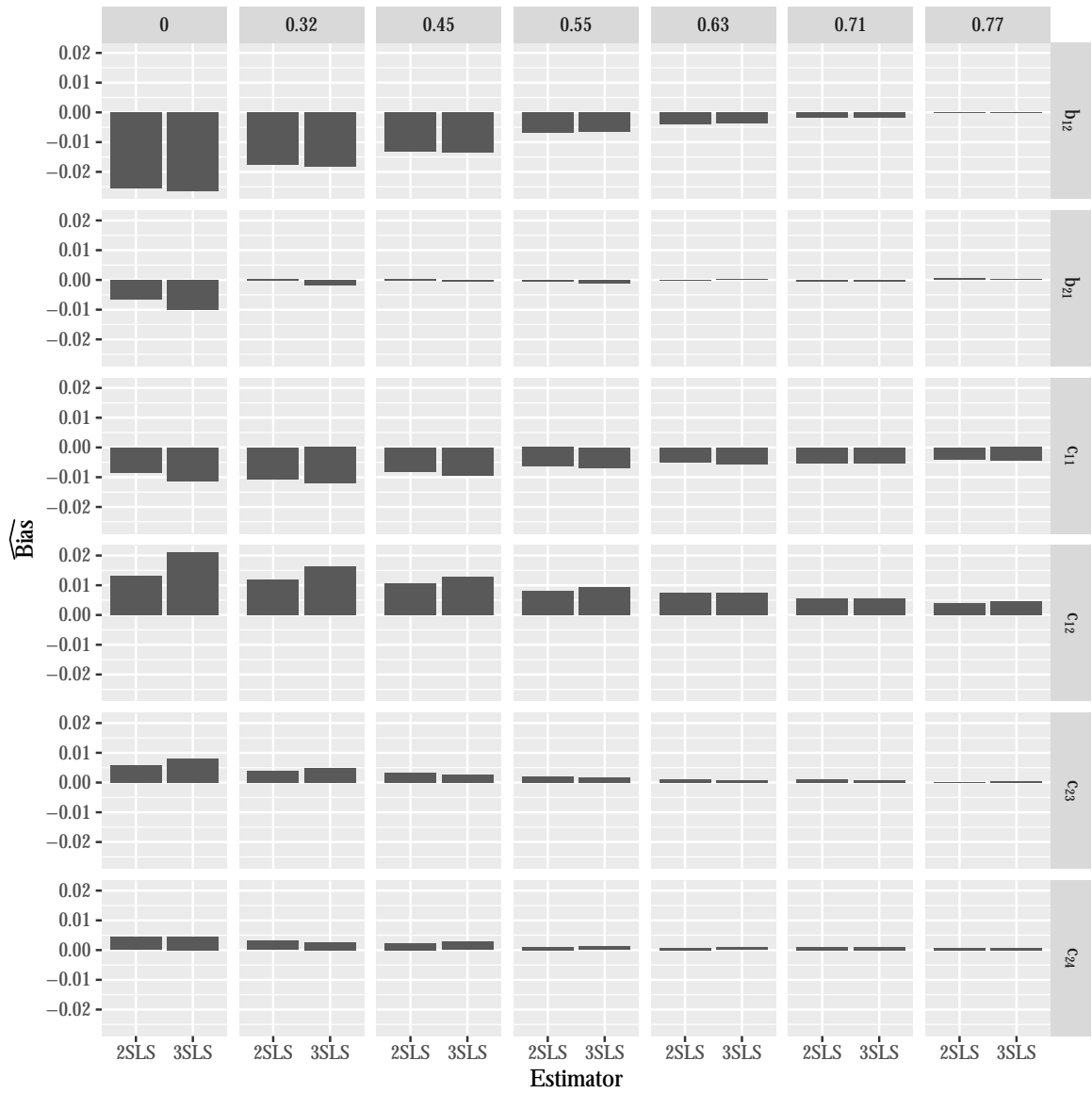
Figure 2.8: Average deviations from the population path coefficients for 2SLS and 3SLS using PLS weights
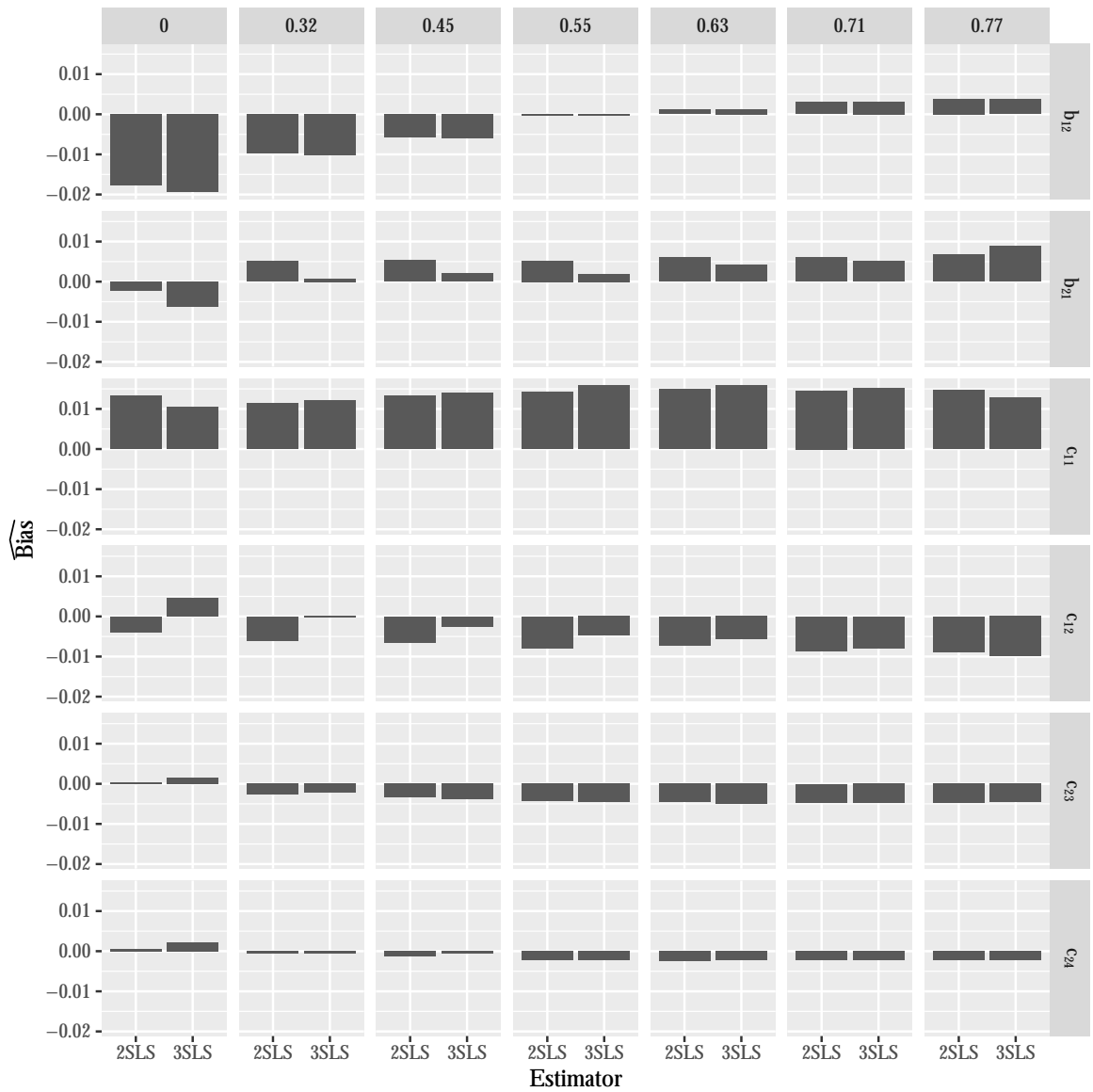
Figure 2.9: Average deviations from the population path coefficients for 2SLS and 3SLS using maxvar weights

Chapter 3

Assessing statistical differences between parameter estimates in Partial Least Squares path modeling

3.1 Introduction[1]

Structural equation modeling with latent variables (SEM) have become a mainstream modeling approach in various disciplines, such as marketing, information systems, and innovation management (Hair et al., 2013; Henseler et al., 2014). Its ability to model complex relationships between constructs, to configure associations between indicators and constructs, and to account for various forms of measurement errors makes SEM a powerful statistical method for dealing with a variety of research questions. Among the various approaches to SEM, including variance- and covariance-based estimators, the partial least squares path modeling (PLS) approach (Wold, 1982b) has particularly gained increasing attention over the last decades (Hair et al., 2014). Representing a

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[1]This chapter is based on a published article with Macario Rodríguez-Entrena and Carsten Gelhard (Rodríguez-Entrena et al., 2016).

two-step approach, PLS first creates proxies for the latent constructs and, subsequently, it estimates model parameters. Since PLS is based on separate OLS regressions, no distributional assumptions are imposed on the data ('soft modeling approach'), and complex models can be estimated using a relatively small number of observations compared to the number of indicators and constructs (Henseler, 2010).

Since any research method can only play to its strengths if properly applied, in this specific research context, scholars incessantly study the limits of PLS (Sarstedt et al., 2014; Hair et al., 2013). In so doing, scholars steadily advance PLS to broaden its applicability as well as reinforce its methodological foundations. The latest advancements to PLS refer to the following: (i) a bootstrap-based test for evaluating the overall model fit (Dijkstra and Henseler, 2015b), (ii) the heterotrait-monotrait ratio of common factor correlations as a new criterion for discriminant validity (Henseler et al., 2015), and (iii) consistent partial least squares (PLSc) as an extension of PLS, which allows for the consistent estimation of common factor and composite models (Dijkstra and Henseler, 2015a). The ability to model latent constructs as both composites and common factors makes PLSc an outstanding and appealing estimator for SEM. Thus, in its most modern appearance, PLS can be understood as full-fledged SEM method,[2] which enables the hybridization of two complementary paradigms of analysis – behavioral and design research. However, PLS is still continuously enhanced. Particularly, PLS-users very often struggle with issues that are of greater practical relevance and have not been sufficiently addressed yet. One of those issues is the lack of appropriate guidance and techniques that are necessary for exploring and interpreting statistical differences between various parameter estimates (e.g., Doreen (2009) in the SmartPLS[3] internet forum). By exploring the existence of significant differences between various parameter estimates, scholars become enabled to deepen the knowledge of both the structural model (e.g., ranking different management instruments) as well as the measurement model (e.g., identifying outstanding indicators). Commonly used practices, such as ranking various indicators/constructs based on differences in the p-values of weight/loading/path coefficient estimates or deriving conclusions solely based on effect size differences are prone to misleading findings and misinterpretations (e.g., Kline (2004); Hubbard and Lindsay (2008); Schochet (2008); Vandenberg (2009);

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[2]For more detailed information on the state of the art of PLS, please refer to Henseler et al. (2016a).

[3]SmartPLS is a commercial software where PLS is implemented.

Nieuwenhuis et al. (2011); Gross (2015)). Gelman and Stern (2006, p. 328), for instance, accentuate that 'large changes in significance levels can correspond to small, not significant changes in the underlying quantities'. Hence, drawing conclusion about parameter differences solely based on differing p-values must be regarded with caution, since the difference between 'significant' and 'non-significant' does not necessarily have to be significant (Gelman and Stern, 2006).

A comparison of two estimated effects requires rather a statistical test that is based on the difference between two parameter estimates as opposed to two separate tests for each parameter estimate. Since the mere presence of differences in p-values does not allow one to make any inferences about the nature of these differences, more sophisticated steps need to be taken to fully exploit the information inherent in the estimated model. Otherwise, important parameter differences might remain undetected (Gelman and Stern, 2006). Figure 3.1 provides an overview of common misconceptions by exemplary comparing three variables (η_1, η_2, and η_3) and their related estimated effects ($\hat{\beta}_1$, $\hat{\beta}_2$, and $\hat{\beta}_3$, where $\hat{\beta}_1 > \hat{\beta}_2$). The p-values used in the figure refer to the hypothesis assuming that the true coefficient is equal to zero.
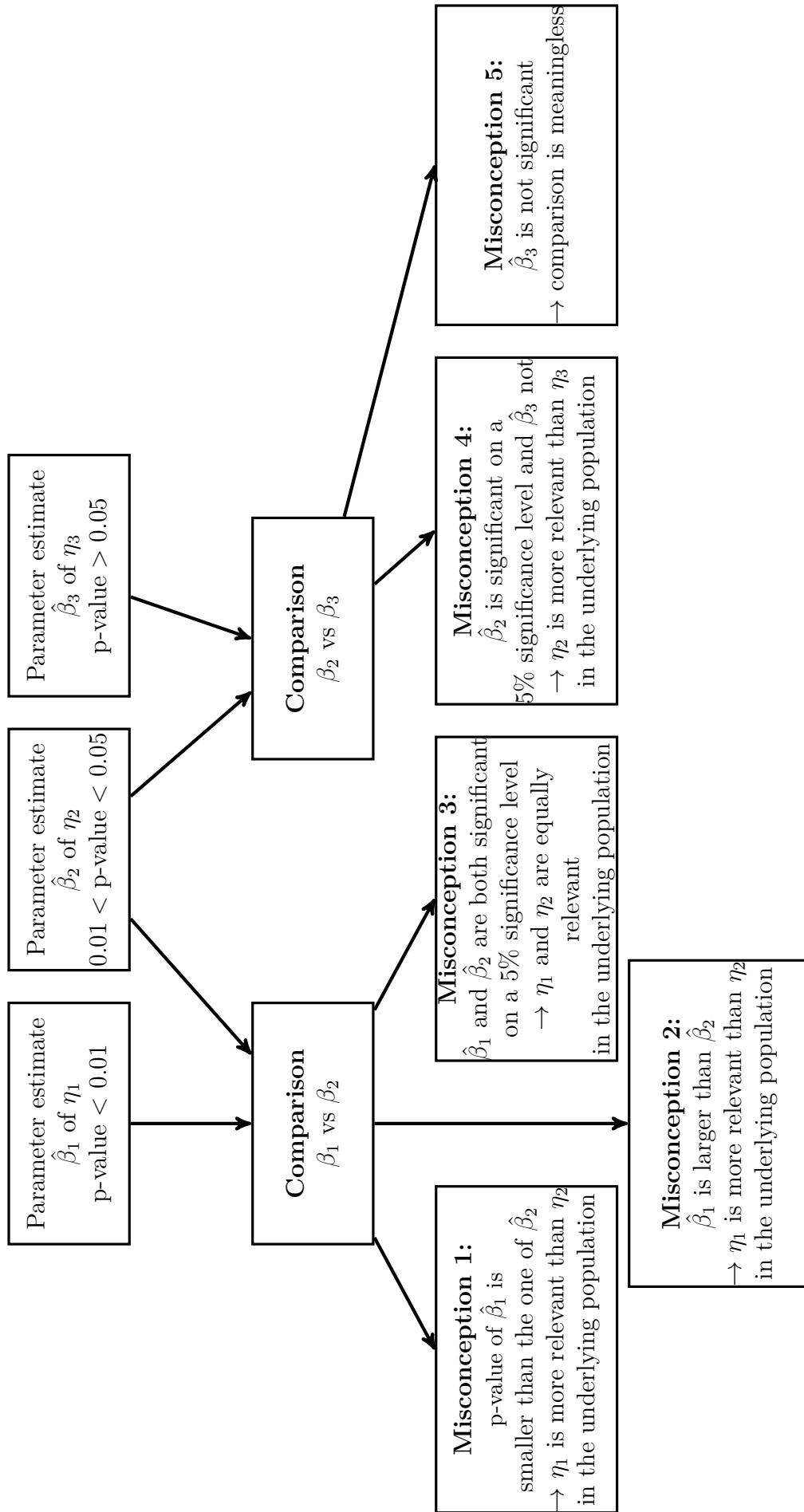
Figure 3.1: Common misconceptions in testing parameter differences

To eliminate these sources of misinterpretation and to support PLS users in fully leveraging information inherent in the underlying data set, the study at hand introduces a practical guideline on how to statistically assess a parameter difference in SEM using PLS. For assessing the statistical significance of a difference between two parameter estimates, we use several bootstrap techniques that are commonly applied to test single parameter estimates in PLS. To be more precise, we construct confidence intervals for the difference between two parameter estimates belonging to the same sample. The procedure is compiled in a user-friendly guideline for commonly used PLS software packages such as SmartPLS (Ringle et al., 2015) or ADANCO (Henseler and Dijkstra, 2015). By introducing this advancement, we not only fill an important gap in the existing literature on PLS (McIntosh et al., 2014), but we also draw attention to the commonly made mistake of relying on individual p-values when prioritizing effects (Gelman and Stern, 2006).

3.2 Field of application

While most studies solely consider the estimated net effect of various predicting variables on the outcome of interest, they usually do not test whether two parameter estimates are statistically different. This prevents researchers from fully exploiting the information captured in the estimated model. Evaluating the statistical difference between two parameter estimates might be particularly valuable when model estimates are proposed for guiding decision-makers while handling budget constraints (e.g., selection of marketing strategies, success factors or investment in alternative instruments of innovation, process, product, and the like.). In situations in which two management instruments coexist with both wielding impact on the outcome of interest, a ranking of priority based on their explanatory power supports managers in selecting the most relevant one. In the following, we present some empirical examples, illustrating the practical relevance of assessing whether the difference between two parameter estimates belonging to the same model (i.e., comparisons within a single sample) is statistically significant.[4]

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[4]For an overview of techniques for assessing statistical significance of differences between parameter estimates in a multi-group setting, i.e., comparing the estimated coefficients across different submodels, please refer to Sarstedt et al. (2011) or Henseler (2012a).

Figures 3.2a and 3.2b display two excerpts of the well-known corporate reputation model (CRM) by Eberl and Schwaiger (2005) and the technological acceptance model (TAM) by Davis (1989).

(a) Corporate reputation model   (b) Technology acceptance model
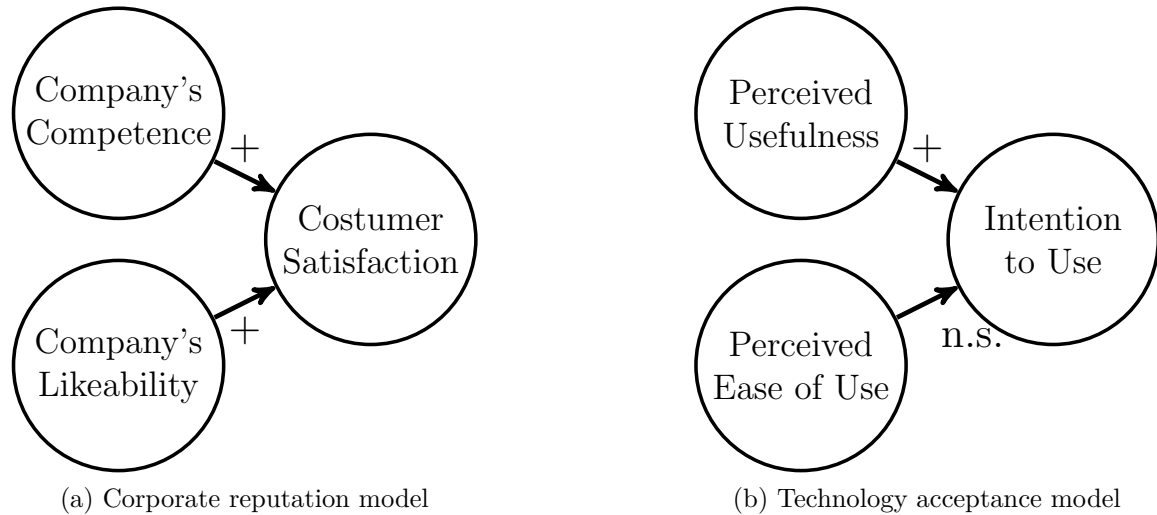
Figure 3.2: Practical examples for testing parameter differences

Testing parameter differences might be applied to examine which of the two predictors has a greater influence on the endogenous construct. To be more precise, researchers might be potentially interested in exploring whether 'Company's Competence' or 'Company's Likeability' has a higher impact on 'Customer Satisfaction' in the context of the CRM or, with regard to the TAM, they might be interested in statistically testing whether 'Perceived Usefulness' is more relevant than 'Perceived Ease of Use' for explaining 'Intention to Use'. In general, drawing conclusions solely based on the individual p-values of the estimated coefficients is not recommended (Gelman and Stern, 2006) as p-values provide no information about the substantiality of a variable or the magnitude of an effect. Hence, claims such as 'Perceived Usefulness' is more relevant than 'Perceived Ease of Use' might be misleading (see the TAM in Figure 3.2b).

In addition to the previously described examples, Figure 3.3 illustrates a less common though highly interesting and important scenario wherein the two estimated parameters of both antecedents are approximately equal in magnitude but differ with regard to their signs ($|\hat{\beta}_1| \approx |\hat{\beta}_2|$) (Eggert et al., 2012). To eventually assess the total impact of the two antecedents on the outcome of interest (here: 'Channel Switching'), researchers might need to test whether the difference of the absolute estimated effect

between both antecedents (here: 'Distributor Loyalty' and 'Brand Loyalty') differs significantly from zero (H_0: $|\beta_1| = |\beta_2|$).
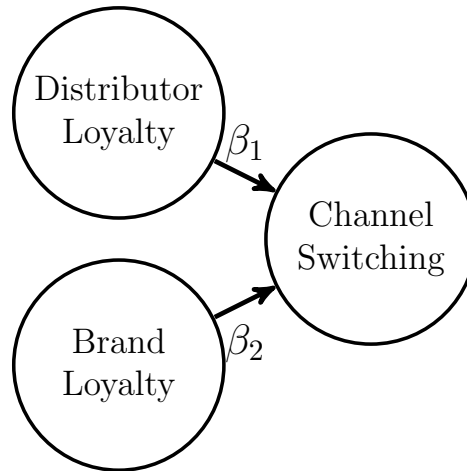
Figure 3.3: Example from Eggert et al. (2012)

3.3 Methodological framework for testing differences between parameters

Typically, in PLS, bootstrap-based confidence intervals (CIs) are constructed to draw conclusions about population parameters. In general, a CI is designed to cover the population parameter with a confidence level $1 - \alpha$. We suggest the same approach for testing parameter differences of the following form: $\theta_k - \theta_l = 0$, see Section 3.4.[5]

In the following, we summarize the commonly used bootstrap procedures to construct CIs (Davison and Hinkley, 1997) for a single parameter θ and show how these approaches can be used to statistically assess parameter differences.[6]

3.3.1 The standard/ Student's t confidence interval

For the standard/ Student's t CI, it is assumed that $(\hat{\theta} - \theta)/\widehat{\mathrm{Var}(\hat{\theta})}^{\frac{1}{2}}$ is approximately standard normally or t-distributed respectively. For this purpose, the central limit theorem is often used to justify the distribution of the standardized parameter estimates.

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[5]Using a slight modification, hypotheses of the form $\theta_k - \theta_l \geq a$ can also be tested, where $a = $ constant.

[6]We refer to Davison and Hinkley (1997) for further procedures that have overcome some limitations of the approaches presented here.

The standard/Student's t CI for a certain significance level α is constructed as follows:

$$\left[\hat{\theta} - F^{-1}\left(1 - \frac{\alpha}{2}\right)\sqrt{\widehat{\text{Var}(\hat{\theta}^*)}},\ \hat{\theta} - F^{-1}\left(\frac{\alpha}{2}\right)\sqrt{\widehat{\text{Var}(\hat{\theta}^*)}}\right], \tag{3.1}$$

where $\hat{\theta}$ is the parameter estimate based on the original sample, and F^{-1} is the quantile function of the standard normal or the t-distribution with $n - k$ degrees of freedom, where n denotes the number of observations and k the number of estimated parameters. Since PLS does not provide a closed-form expression of the variance, the bootstrap-based estimator $\widehat{\text{Var}(\hat{\theta}^*)}$ for the variance is used. This approach is problematic when the distribution of the parameter estimates is not normal. This is especially true for small sample sizes. Moreover, the standard/Student's t CI does not adjust when dealing with skewness in the underlying population (Efron and Tibshirani, 1994).

3.3.2 The basic percentile bootstrap confidence interval

In contrast to the previous CI, the basic percentile bootstrap CI is not based on distributional assumptions. The boundaries are directly calculated from the bootstrap sample distribution of the estimated parameter as follows:

$$\left[\hat{F}_{\theta^*}^{-1}\left(\frac{\alpha}{2}\right),\ \hat{F}_{\theta^*}^{-1}\left(1 - \frac{\alpha}{2}\right)\right], \tag{3.2}$$

where $\hat{F}_{\theta^*}^{-1}$ is the empirical quantile function of the bootstrap sample distribution of $\hat{\theta}$. This approach only works well if a transformation, even an unknown one, exists, which makes the bootstrap distribution symmetric around zero (Wehrens et al. 2000). In case of no such transformation, the percentile method must be be adjusted.[7] However, the percentile method is really appealing due to its simplicity (Sarstedt et al., 2011).

3.3.3 The basic bootstrap confidence interval

The basic bootstrap CI assumes that the distribution of $\hat{\theta} - \theta$ can be approximated by $\hat{\theta}^* - \hat{\theta}$ and, therefore, the quantiles of $\hat{\theta} - \theta$ are estimated by the empirical quantiles of $\hat{\theta}^* - \hat{\theta}$ (Wehrens et al., 2000). The basic bootstrap CI is constructed as follows:

$$\left[2\hat{\theta} - \hat{F}_{\theta^*}^{-1}\left(1 - \frac{\alpha}{2}\right);\ 2\hat{\theta} - \hat{F}_{\theta^*}^{-1}\left(\frac{\alpha}{2}\right)\right], \tag{3.3}$$

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[7]A well-known approach to achieve the adjustment is the bias corrected (BC) estimator (Efron and Tibshirani, 1994) that is not discussed in this chapter.

where $\hat{\theta}$ represents the parameter estimate from the original sample, and $\hat{F}_{\theta^*}^{-1}(1 - \frac{\alpha}{2})$ and $\hat{F}_{\theta^*}^{-1}(\frac{\alpha}{2})$ are the $1 - \frac{\alpha}{2}$ and $\frac{\alpha}{2}$ quantiles of the empirical bootstrap sample distribution of $\hat{\theta}$.

3.4 Guideline on testing parameter differences in partial least squares path modeling

Following Gelman and Stern (2006), when comparing two treatments, we recommend taking into consideration the statistical significance of the difference between two parameter estimates rather than the difference between their individual p-values. Thus, we provide a user guideline on testing a parameter difference in PLS as well as in PLSc (see Table 3.1).

Table 3.1: Guideline on testing parameter differences based on different CI

1. Use PLS or PLSc[a] to obtain the model parameter estimates: $(\hat{\theta}_k; \hat{\theta}_l)$.

2. Calculate the difference of the parameter estimates: $\Delta\hat{\theta} = \hat{\theta}_k - \hat{\theta}_l$.

3. Create B bootstrap samples of the original data set and calculate the parameter estimates $\hat{\theta}_{ki}^*$ and $\hat{\theta}_{li}^*$, and their difference $\Delta\hat{\theta}_i^* = \hat{\theta}_{ki}^* - \hat{\theta}_{li}^*$ for every bootstrap sample, with $i = 1, ..., B$.

4. Estimate the variance of the estimated parameter difference as

$$\widehat{\mathrm{Var}(\Delta\hat{\theta}^*)} = (B-1)^{-1} \sum_{i=1}^{B} (\Delta\hat{\theta}_i^* - \overline{\Delta\hat{\theta}^*})^2, \quad \text{with} \quad \overline{\Delta\hat{\theta}^*} = B^{-1} \sum_{i=1}^{B} \Delta\hat{\theta}_i^*. \quad (3.4)$$

5. Estimate the $\frac{\alpha}{2}$ and $1 - \frac{\alpha}{2}$ sample quantile of $\Delta\hat{\theta}^*$ given by $\hat{F}_{\Delta\theta^*}^{-1}(\frac{\alpha}{2})$ and $\hat{F}_{\Delta\theta^*}^{-1}(1 - \frac{\alpha}{2})$.

[a] PLSc should be used if constructs are modeled as common factors in the model.

First, the parameters of interest need to be obtained by PLS or PLSc (Step 1). For this purpose, every common PLS software such as SmartPLS or ADANCO can be used. Second, the difference between the parameter estimates of interest is calculated (Step 2). Third, the bootstrap estimates of the parameters need to be obtained (Step 3) and inserted into a spreadsheet in order to manually calculate the parameter difference for every bootstrap sample. Depending on the CI used (see Table 3.2), Step 4 comprises

the estimation of the variance of the estimated parameter difference. The command VAR.S() in MS Excel can be used for this purpose. If the basic percentile bootstrap CI or the basic bootstrap CI is used, Step 5 needs to be conducted, comprising the determination of the empirical quantiles of the bootstrapped parameter difference, e.g., the command PERCENTILE.INC() in MS Excel can be applied.

Table 3.2: Necessary steps for the construction of the different CIs

- Steps 1 and 2 are needed for all approaches except for the basic percentile bootstrap CI.

- To apply the standard/Student's t CI (Equation (3.1)), additionally Step 3 and 4 are necessary.

- In contrast, the construction of the basic percentile bootstrap CI (Equation (3.2)) and the basic bootstrap CI (Equation (3.3)) of the parameter difference requires the Steps 3 and 5.

Based on the CI, the null hypothesis is rejected or not rejected. If the zero is covered by the CI, it cannot be assumed that a difference between the two considered parameters exists in the population regarding the type I error. For an illustration of the described procedure, see Figure 3.4.
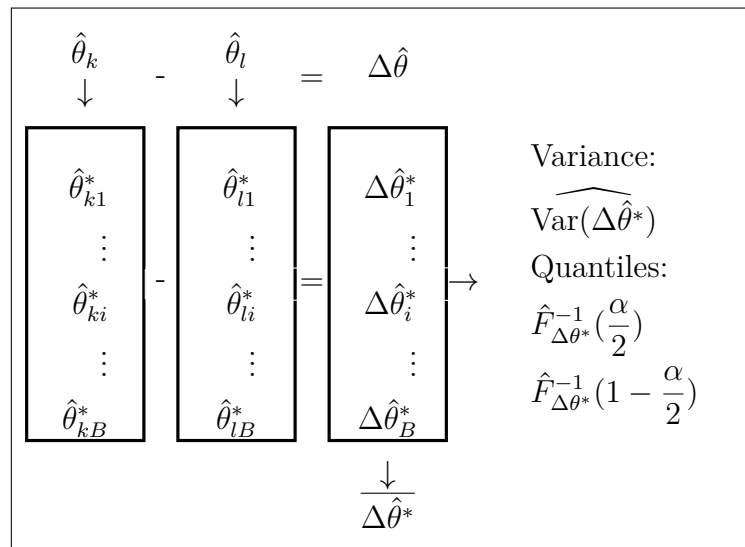
Figure 3.4: Construction of the CIs

3.5 Empirical example

To illustrate our proposed procedure, we refer to the TAM developed originally by (Davis, 1989; Davis et al., 1992), suggesting 'Perceived Usefulness' and 'Perceived Ease of Use' as potential predictors of IT adoption intention. More precisely, we demonstrate our procedure by referring to Chin et al. (2003), who followed Davis' (1989) theoretical framework when investigating the intention to regularly use electronic mail within an organization. The data set consists of 12 indicators and 250 respondents from a single organization that had recently installed an electronic mail system.[8] The respondents worked at different organization levels, including managers, engineers, technicians, and clerical workers. The dependent construct 'Intention to regularly use electronic mail' (INT) is explained by both 'Perceived Usefulness' (USE) and 'Enjoyment' (ENJ). The structural model is depicted by the following equation (see also Figure 3.5):

$$INT = \beta_1 \cdot USE + \beta_2 \cdot ENJ + \zeta. \tag{3.5}$$

Following Chin et al. (2003), all constructs are modeled as common factors. While USE is connected to six indicators, both ENJ and INT are connected to three items each. All indicators are measured on a seven-point Likert scale.
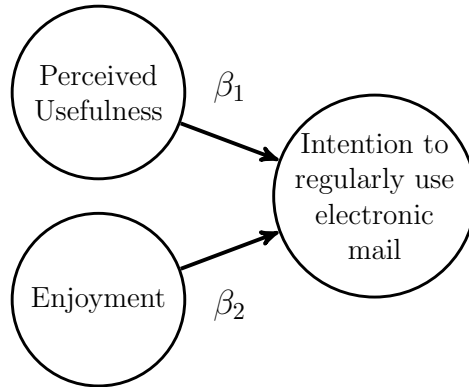
Figure 3.5: Structural model of the reduced TAM

Using our proposed procedure for statistically testing the difference between two parameter estimates, we seek to answer whether USE (extrinsic motivation) has a statistically different impact on INT than ENJ (intrinsic motivation) (H_0: $\beta_1 = \beta_2$). Since this model was originally estimated by traditional PLS but represents a common factor model, we use both approaches PLS and PLSc (Dijkstra and Henseler, 2015a)

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[8]For a detailed description of the indicators, please refer to Chin et al. (2003).

for model estimation.[9] The analysis eventually leads to the following estimated path coefficients: $\hat{\beta}_1 = 0.517$ and $\hat{\beta}_2 = 0.269$ for the model estimation with PLS and $\hat{\beta}_1 = 0.507$ and $\hat{\beta}_2 = 0.313$ for the model estimation with PLSc.

Table 3.3: Results of PLS

Type of CI	95% CI	
Standard	0.046	0.450
Percentile	0.044	0.496
Basic	0.001	0.452

Table 3.4: Results of PLSc

Type of CI	95% CI	
Standard	-0.099	0.488
Percentile	-0.048	0.508
Basic	-0.120	0.437

The limits of the CIs derived from the bootstrap procedure with 5000 draws (see Section 3.3) are displayed in Tables 3.3 and 3.4. Since the CIs do not contain the zero with regard to the estimation using PLS, we infer that both path coefficient estimates ($\hat{\beta}_1$ and $\hat{\beta}_2$) are significantly different. With regard to the estimation with PLSc, all CIs cover the zero. We, therefore, conclude that the difference between the two path coefficient estimates ($\hat{\beta}_1$ and $\hat{\beta}_2$) is not statistically significant.[10] Hence, if the underlying measurement models are conceptualized as composites (i.e., model estimation using PLS), the null hypothesis of no parameter difference (H_0: $\beta_1 = \beta_2$) must be rejected. If the measurement models, on the other hand, are conceptualized as common factors (i.e., model estimation with PLSc), there is not enough evidence against the null hypothesis.

3.6 Discussion

The purpose of this chapter is to provide a practical guideline as well as the technical background for statistically assessing the difference between two parameter estimates in SEM using PLS. This guideline is intended for testing a parameter difference based on the parameter estimates and the bootstrap distribution. The input required for the proposed methodological procedure directly builds on the output of the most popular variance-based SEM statistical software packages such as ADANCO or SmartPLS. The methodological procedure serves as a functional toolbox that can be considered as a

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[9]As outer weighting scheme, we use *mode A* and the *factorial* scheme is used as inner weighting scheme.

[10]As PLSc path coefficient estimates are known to have a larger standard deviation compared to PLS estimates (Dijkstra and Henseler, 2015a), it is not surprising that PLSc produced larger CIs than PLS.

natural extension of PLS. As it is common practice in PLS to use bootstrap approaches to draw conclusions about single parameters, we use these approaches and the resulting CIs to draw conclusions about a parameter difference. As the study at hand shows, the same procedure can also be employed for PLSc to assess a parameter difference in models where constructs are modeled as common factors instead of as composites.

Using the well-established TAM, we eventually demonstrated the application of our proposed assessment technique. In accordance with Chin et al. (2003), we made use of PLS to test for a statistical difference between the estimated influence of 'Perceived Usefulness' (extrinsic motivation) and 'Enjoyment' (intrinsic motivation) on 'Intention to regularly use electronic mail'. Since no CI covered the zero, we conclude that a difference between the parameters exists. We also performed our proposed procedure using PLSc because existing literature has shown that traditional PLS tends to overestimate factor loadings and underestimate path coefficients when referring to common factor models (Schneeweiss, 1993). Contrasting the estimation with PLS, we cannot infer that the estimated influence of 'Perceived Usefulness' and 'Enjoyment' on 'Intention to regularly use electronic mail' is statistically different. Considering the concrete example used in this study, our proposed technique is proven to be useful, i.e., when estimating the SEM using traditional PLS, we could show that the estimated effects of the two antecedents explaining the outcome of interest are significantly different.

Contrasting established methods for assessing whether various parameter estimates are statistically different (e.g., parametric and non-parametric approaches in PLS multi-group analysis (PLS-MGA) (Sarstedt et al., 2011)), the procedure introduced in this study enables PLS users to test whether two parameter estimates from one sample ($\hat{\beta}_k^1$ and $\hat{\beta}_l^1$) are statistically different. Approaches used in PLS-MGA, for instance, are not suitable for this framework, since the underlying assessment approach is based on the hypothesis that a parameter β_k differs for two subpopulations (H_0: β_k^1 = β_k^2), which can be tested, for instance, by using an unpaired t-test in the PLS-MGA framework (e.g., (Keil et al., 2000)). In the PLS-MGA framework, the proposed research model is estimated for different subsamples, followed by a comparison of the coefficient estimates across the various models. Taken together, while techniques used in PLS-MGA represent proper approaches for statistically assessing the difference between the same parameter estimate for different subsamples (H_0: $\beta_k^i = \beta_k^j$, where i and j refer to the different subpopulations and k to the parameter tested), the procedure

proposed in the study at hand represents the first choice when assessing the difference between two parameter estimates derived from the same sample (H_0: $\beta_k^i = \beta_l^i$, where i refers to the population, and k and l to the parameters tested).

Although the present study only considered path coefficient estimates while testing for differences, the proposed approach might also be performed with regard to other parameter estimates, such as weights, factor-loadings, or cross-loadings. Thus, for instance, testing for statistically significant differences between factor-loading and cross-loading estimates, might prove to be a promising approach for evaluating discriminant validity (e.g., (Hair et al., 2011; Henseler et al., 2009)). Analyzing whether estimated weights are significantly different might further be useful for identifying key indicators of composites.

3.7 Limitations and future research

Though we are able to introduce a diagnostic procedure for statistically assessing the differences between two parameter estimates, the study at hand is not without limitations. First, we only consider the difference between one pair of parameter estimates. We, thus, recommend future research to develop procedures for testing more than two parameter estimates, employing the following two potential approaches: (i) performing several single tests and adjusting the assumed level of significance (e.g., Bonferroni correction) (Rice, 1989) or (ii) performing a joint test, similar to an F-test in regression analysis.

Second, the procedure proposed in this study solely makes use of basic bootstrap approaches when calculating the required CIs. Therefore, scholars might also want to consider more sophisticated techniques, such as studentized, bias-corrected, tilted, balanced, ABC, antithetic, or m-out-of-n bootstrap techniques.

Third, in general, scholars could, in more detail, investigate the performance and limitations of the various bootstrap procedures when using PLS and PLSc, in particular, for small sample sizes, which can be done through a simulation study.

Chapter 4

Partial least squares path modeling using ordinal categorical indicators

4.1 Introduction[1]

Structural equation modeling (SEM) has become an established method in the fields of business and social sciences, and its application goes even beyond. Its capacity to model constructs, to take into account various forms of measurement error, and to test entire theories makes it a prime candidate for dealing with a variety of research issues.

For SEM, two types of estimators need to be differentiated, which are covariance- and variance-based estimators. Covariance-based parameter estimates are obtained by minimizing the distance between the empirical variance-covariance matrix of the indicators and its model-implied counterpart. Variance-based estimators, on the contrary, create proxies for constructs first and, subsequently, estimate model parameters based on these proxies. While covariance-based methods are preferred if the model contains constructs modeled as common factors, variance-based estimators are favored if the underlying model consists of constructs modeled as composites, in particular, when

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the composites are endogenous in the structural model.

Among variance-based estimators, partial least squares path modeling (PLS) is regarded as the "most fully developed and general system" (McDonald, 1996, p. 240), and it was even called a "silver bullet" (Hair et al., 2011). The use of PLS is prevalent in many fields, e.g., information systems research (Marcoulides and Saunders, 2006) or marketing (Hair et al., 2012b). Because of its capability to model both factors and composites[2], the latest version of PLS, known as consistent PLS, is considered to be a vigorous method for estimation and is acknowledged by researchers across different disciplines. Common factors can be used to model constructs of behavioral research, such as attitudes or personality traits, whereas composites can be applied to model strong concepts (Höök and Löwgren, 2012), i.e., the abstraction of artefacts such as management instruments, innovations, or information systems. Consequently, PLS is a preferred statistical tool for success factor studies (Albers, 2010).

Recently, a lot of development has been done in the field of PLS. For example, a new criterion for discriminant validity based on heterotrait-monotrait ratio of common factor correlations (Henseler et al., 2015), the standardized root mean square residual (SRMR) as a measure of overall model fit (Henseler et al., 2014), and bootstrap-based tests for overall model fit (Dijkstra and Henseler, 2015a) have been introduced. Since PLS creates composites as proxies for all kinds of constructs, its estimates suffer from attenuation and are inconsistent in case of an underlying common factor model (Schneeweiss, 1993). Therefore, a consistent PLS (PLSc) version was developed in order to rectify for the attenuation bias to consistently estimate SEMs with common factors (Dijkstra and Henseler, 2015b). All these developments are based on the PLS algorithm and, therefore, on ordinary least squares (OLS) regression analysis, implicitly assuming that all indicators are continuous.

Since numerous studies are based on data collected by questionnaires, the indicators used are rarely measured on a metric scale. Hence, in many situations researchers are faced with data measured on ordinal categorical scales, e.g., in marketing research, in particular customer satisfaction surveys (Hair et al., 2012b; Coelho and Esteves, 2007).

It is well-known in the PLS literature as well as in literature pertaining to other fields that treating categorical variables as continuous can lead to biased estimates and, therefore, to invalid inferences and erroneous conclusions. Lohmöller recognizes that

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[2]For a comparison of constructs modeled as composites or common factors, see Rigdon (2012).

the "[...] standard procedures cannot be used for the categorical and ordinal-scaled variables [...]" (Lohmöller, 2013, Chap. 4). Additionally, Hair et al. (2012b) mention that PLS is often used with categorical indicators but that their use in a procedure like PLS, which uses OLS as estimator, can be problematic. Several approaches to address this issue in the context of PLS are provided by the literature, e.g., ordinal PLS (OrdPLS) an innovative approach to deal with ordinal categorical indicators in a psychometric way (Cantaluppi, 2012; Cantaluppi and Boari, 2016). As OrdPLS is based on the traditional PLS algorithm, its use is limited to models where all constructs are modeled as composites. However, researchers often deal with models containing constructs that are modeled as common factors instead of as composites (Ringle et al., 2012; Hair et al., 2012b). Hence, there is a real need for improving methods like OrdPLS to equip it to deal with common factors, composites, and ordinal categorical indicators.

In this chapter, we present ordinal consistent partial least squares (OrdPLSc) (Schuberth et al., 2016) which is a combination of PLSc and OrdPLS, thus providing the advantages of both. OrdPLSc is an estimator that is capable of consistently estimating structural equation models, including not only composites but common factors and ordinal categorical indicators as well. Figure 4.1 compares the properties of traditional PLS, PLSc, OrdPLS, and OrdPLSc with respect to dealing with common factors and taking into account the scale of ordinal categorical indicators.
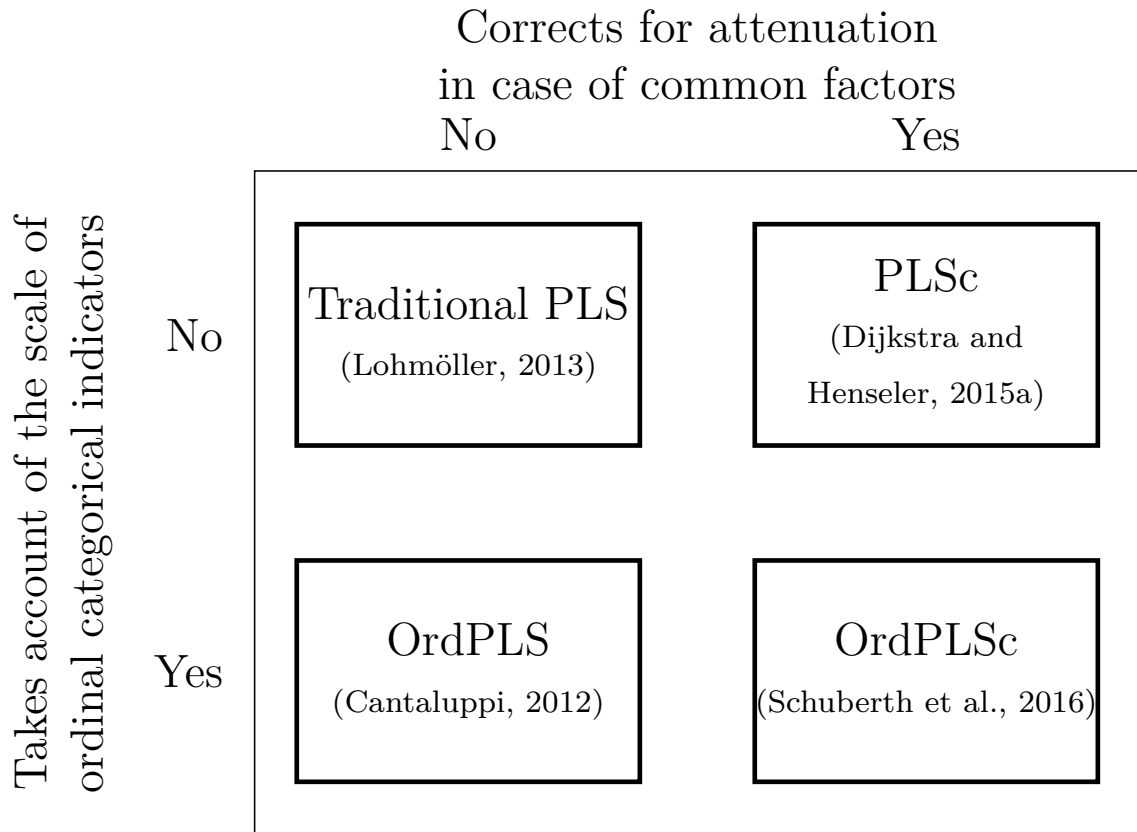
Figure 4.1: A typology of PLS methods

First, we run a Monte Carlo simulation to investigate the performance of Ord-PLSc in different conditions and compare it as benchmark to the means and variance adjusted weighted least squares (WLSMV) estimator. The latter approach is a consistent covariance-based estimator, which is typically used for structural equation models with common factors and ordinal categorical indicators. Moreover, we show how traditional PLS, PLSc, and OrdPLS behave for different kinds of models, and we also show how PLS and PLSc are affected when the scale of ordinal categorical indicators is ignored. Second, apart from running a Monte Carlo simulation, we also reestimate the well-known European customer satisfaction model for the mobile phone industry (Tenenhaus et al., 2005), using OrdPLSc, thereafter which, we compare the results with those obtained from PLS, PLSc, and OrdPLS. We also provide commonly used instruments in PLS to assess construct validity and composite reliability, taking into account the qualitative scale of ordinal categorical indicators. Additionally, we show how construct scores can be obtained from OrdPLSc.

The remainder of the chapter is organized as follows. The next section shows the development from PLS to PLSc and provides a reformulation of the two procedures

in terms of indicator correlation matrices. In Section 4.3, we present the development from PLS to OrdPLS utilizing a literature review of the existing approaches dealing with categorical indicators in the framework of PLS, and, in particular, we present the idea of the OrdPLS and how it treats ordinal categorical indicators. In Section 4.3, we propose our approach, ordinal consistent PLS (OrdPLSc), combining PLSc and OrdPLS. Section 4.5 provides first attempts of calculating construct scores for OrdPLSc as well as OrdPLS. In the following Section 4.6, we present the setup of our Monte Carlo simulation, which is conducted to examine the performance of OrdPLSc and different other estimators under several conditions. We present these findings in Section 4.7. In the following Section 4.8, we present ways to assess the results from OrdPLSc. In Section 4.9, we assess the results from OrdPLSc and compare them with those obtained from PLS, PLSc, and OrdPLS, using an empirical example. The chapter closes with the discussion of the results in Section 4.10. An Appendix covers the figure of the threshold parameter distribution used in the Monte Carlo simulation and several additional results from the empirical example.

4.2 The development from PLS path modeling to consistent PLS path modeling

PLS was developed by Wold (1975) for the analysis of high-dimensional data in a low-structure environment, and it has since then undergone various extensions and modifications. It is an approach similar to generalized canonical correlation analysis (GCCA), and, in addition, it can emulate several of Kettenring's (1971) techniques for the canonical analysis of several sets of variables (Tenenhaus et al., 2005).

In its most modern appearance known as consistent PLS (PLSc) (Dijkstra and Henseler, 2015a,b), it can be understood as a well-developed SEM method. It is capable of estimating recursive and non-recursive structural models with constructs modeled as composites and common factors. Both of these obtain the outer weights and the final stand-ins for the constructs by the classical PLS algorithm. While traditional PLS simply relies on OLS to estimate the model parameters, its extended version, PLSc, uses two-stage least squares (2SLS) to consistently estimate even non-recursive path models. Furthermore, PLSc can handle both constructs modeled as composites and as common factors by using a post-correction for attenuation of the correlations among

common factors as well as of the correlations between common factors and indicators.

The classical common factor model assumes that the variance of a block of indicators $(x_1, \ldots, x_K)$ is completely explained by the underlying common factor (ξ in the large circle) and by their random errors ($\epsilon_1, \ldots, \epsilon_K$), see Figure 4.2a. Hence, the indicators reflect the underlying common factor (reflective measurement model). This sort of indicator is also known as effect indicators (Bollen and Bauldry, 2011). Common factors are usually used in behavioral research.

(a) Common factor model   (b) Composite model
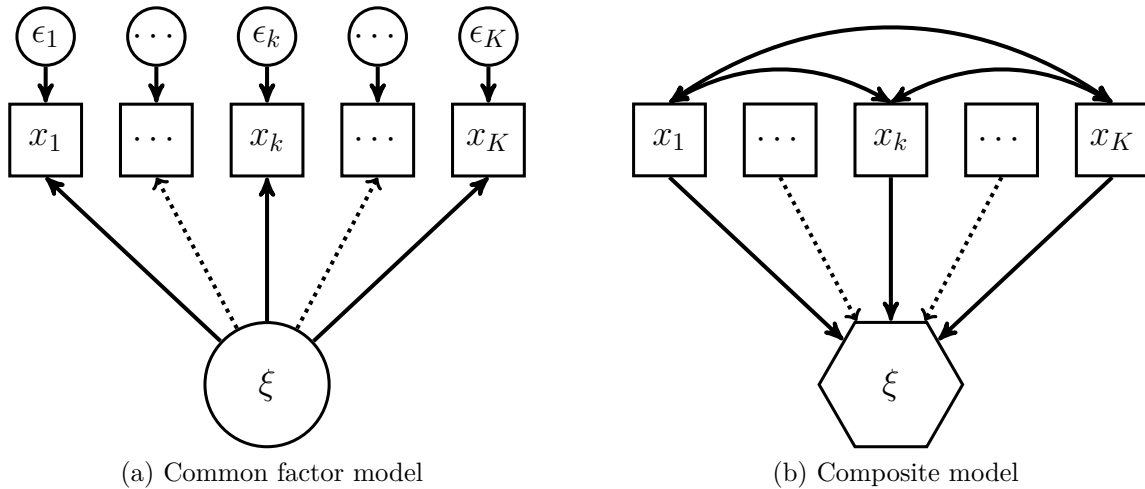
Figure 4.2: Common factor vs. composite

As Figure 4.2b depicts, composites (ξ in the hexagon) are formed as linear combinations of their belonging indicators $(x_1, \ldots, x_K)$. Since the indicators form the composite, they are related to composite-formative measurement models.[3] Furthermore, the composite model does not put any restrictions on the covariances of the indicators belonging to one block, and hence, it relaxes the assumption that all covariation between the indicators has to be explained by the common factor. Composites are often used as proxies for scientific concepts of interest (Ketterlinus et al., 1989; Maraun and Halpin, 2008; Rigdon, 2012; Tenenhaus, 2008).

For the derivation of OrdPLS(c), it is crucial to describe the well-known PLS algorithm (Wold, 1975) and its extension to PLSc in terms of indicator covariances or correlations respectively. Since in PLS no distinction between exogenous and endogenous constructs is made, we use the following notation: $\boldsymbol{\eta}$ is a $(J \times 1)$ vector containing all

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[3]In general, the existing literature provides the two following definitions of a formative measurement model: (i) the (composite) indicators that completely determine composite (Fornell and Bookstein, 1982) and (ii) the (causal) indicators that do not completely explain the underlying latent variable. See Bollen and Bauldry (2011) for a more detailed description.

modeled constructs that are connected by the structural model, regardless of whether they are modeled as common factors or as composites. The $(K \times 1)$ vector $\boldsymbol{x}$ contains all indicators that are connected to the common factors or build the composites.

4.2.1 Partial least squares path modeling

For a sample of size n, all observations of the K indicators are stacked in a data matrix $\boldsymbol{X}$ of dimension $(n \times K)$. For simplicity, the K_j indicators belonging to one common factor or one composite η_j are grouped to form block j with $j = 1, \ldots, J$. Observations of block j are stacked in the data matrix $\boldsymbol{X}_j$ of dimension $(n \times K_j)$ with $\sum_{j=1}^{J} K_j = K$. Furthermore, we assume that each indicator is standardized, as is customary in PLS, to have mean zero and unit variance, such that the sample covariance matrix $\boldsymbol{S}$ equals the sample correlation matrix.

The PLS estimation procedure consists of three parts. In the first part, for each block j initial arbitrary outer weights $\hat{\boldsymbol{w}}_j^{(0)}$ $(K_j \times 1)$ are chosen, which satisfy the following condition: $\hat{\boldsymbol{w}}_j^{(0)\prime} \boldsymbol{S}_{jj} \hat{\boldsymbol{w}}_j^{(0)} = 1$, where the $(K_j \times K_j)$ matrix $\boldsymbol{S}_{jj}$ contains the sample correlations of the indicators of block j. This condition holds true for all outer weights in each iteration (i) and can be achieved by using the scaling factor $(\hat{\boldsymbol{w}}_j^{(i)\prime} \boldsymbol{S}_{jj} \hat{\boldsymbol{w}}_j^{(i)})^{-\frac{1}{2}}$ for the outer weights $\hat{\boldsymbol{w}}_j^{(i)}$ in each iteration.

In the second part, the iterative PLS algorithm starts with step one, the outer approximation of η_j as follows:

$$\hat{\boldsymbol{\eta}}_j^{(i)} = \boldsymbol{X}_j \hat{\boldsymbol{w}}_j^{(i)} \quad \text{with} \quad \hat{\boldsymbol{w}}_j^{(i)\prime} \boldsymbol{S}_{jj} \hat{\boldsymbol{w}}_j^{(i)} = 1, \tag{4.1}$$

where $\hat{\boldsymbol{\eta}}_j^{(i)}$ is a column vector of length n. Since outer weights are scaled, all outer proxies also have mean zero and unit variance.

In the second step, the inner proxy of η_j is calculated as a linear combination of inner weights and outer proxies of η_l:

$$\tilde{\boldsymbol{\eta}}_j^{(i)} = \sum_{l=1}^{J} e_{jl}^{(i)} \hat{\boldsymbol{\eta}}_l^{(i)}, \tag{4.2}$$

where $\tilde{\boldsymbol{\eta}}_j^{(i)}$ is again a column vector of length n. The inner weight e_{jl} defines how the inner proxy $\tilde{\boldsymbol{\eta}}_j$ is built. The following three different schemes for the calculation of e_{jl} are commonly used: *centroid* (Wold, 1982b), *factorial* (Lohmöller, 2013), and *path weighting*. However, all schemes yield essentially the same results (Noonan and Wold,

1982), and hence, we only consider the *centroid* scheme.[4] The inner weight is chosen according to the sign of the correlation between the outer proxies:

$$e_{jl}^{(i)} = \begin{cases} \text{sign}(\hat{\boldsymbol{w}}_j^{(i)\prime} \boldsymbol{S}_{jl} \hat{\boldsymbol{w}}_l^{(i)}), \text{ for } j \neq l & \text{if construct } j \text{ and } l \text{ are adjacent} \\ 0, & \text{otherwise,} \end{cases} \quad (4.3)$$

where adjacent refers to the constructs j and l directly connected by the structural model. All inner proxies $\tilde{\boldsymbol{\eta}}_j^{(i)}$ are again scaled to have unit variance.

In the third and last step of the iterative part, new outer weights are calculated. This can be done in the following three ways: *mode A*, *mode B*, and *mode C*. For *mode A*, estimated outer weights of block j equal the estimated coefficients of a multivariate regression from the indicators of block j on its related inner proxy. Due to standardization, the new estimated outer weights $\hat{\boldsymbol{w}}_j^{(i+1)}$ equal the correlations between inner proxy and its related indicators:

$$\hat{\boldsymbol{w}}_j^{(i+1)} \propto \sum_{l=1}^{J} \boldsymbol{S}_{jl} \hat{\boldsymbol{w}}_l^{(i)} e_{jl}^{(i)} \quad \text{with} \quad \hat{\boldsymbol{w}}_j^{(i+1)\prime} \boldsymbol{S}_{jj} \hat{\boldsymbol{w}}_j^{(i+1)} = 1. \quad (4.4)$$

In contrast, for *mode B*, the new outer weights equal the estimated coefficients of a regression from the inner proxy on its connected indicators:

$$\hat{\boldsymbol{w}}_j^{(i+1)} \propto \boldsymbol{S}_{jj}^{-1} \sum_{l=1}^{J} \boldsymbol{S}_{jl} \hat{\boldsymbol{w}}_l^{(i)} e_{jl}^{(i)} \quad \text{with} \quad \hat{\boldsymbol{w}}_j^{(i+1)\prime} \boldsymbol{S}_{jj} \hat{\boldsymbol{w}}_j^{(i+1)} = 1. \quad (4.5)$$

Mode C, also known as *MIMIC mode*, is a mixture of *mode A* and *mode B* and is not considered here.[5]

As the traditional PLS algorithm has no single optimization criteria to be minimized, the new outer weights $\hat{\boldsymbol{w}}_j^{(i+1)}$ are checked for significant changes compared to the outer weights from the iteration step before $\hat{\boldsymbol{w}}_j^{(i)}$. If there is a significant change in the weights, the algorithm starts again at step one by building new outer proxies with the new outer weights; otherwise, it stops.

In the last part, the obtained stable outer weights $\hat{\boldsymbol{w}}_j$ are used to build final composites as stand-ins for the theoretical constructs, regardless of being modeled as common factors or composites as follows:

$$\hat{\boldsymbol{\eta}}_j = \boldsymbol{X}_j \hat{\boldsymbol{w}}_j. \quad (4.6)$$

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[4]For more details on the other schemes, see Tenenhaus et al. (2005).

[5]A consistent version of *mode C*, for any of its $2^J - 2$ implementations, can be obtained by using the properties of *mode A* and *mode B*, see Dijkstra (1985, Chap.2 Par. 5.2), but since *mode C* is intermediate between the other modes, adding *mode C* does not really contribute to achieving further understanding.

For constructs that are modeled as common factors, the factor loadings are estimated by OLS in accordance with the measurement model. In contrast, for constructs that are modeled as composites, the final weights equal the stable weights from the last iteration. Finally, path coefficients are estimated by OLS with respect to the structural model.

4.2.2 Consistent PLS

PLS is based on composites, which implies that estimates are inconsistent if constructs are modeled as common factors.[6] However, a transformation of the model-implied correlation matrix of a composite model into the model-implied correlation matrix of a common factor model can be achieved by a correction for attenuation (Cohen et al., 2003, Chap. 2.10). Consistent PLS (PLSc) uses this correction to obtain consistent estimates for models containing common factors (Dijkstra and Henseler, 2015a,b). The correction requires that each common factor is connected to at least two indicators and uses the proportionality between the population factor loadings and the population outer weights, $\boldsymbol{\lambda}_j = c_j \boldsymbol{w}_j$. The estimated correction factor for block j satisfies the following condition:

$$\text{plim}(\hat{c}_j) = \sqrt{\boldsymbol{\lambda}_j' \boldsymbol{\Sigma}_{jj} \boldsymbol{\lambda}_j}, \tag{4.7}$$

where $\boldsymbol{\lambda}_j$ is a column vector of length K_j, containing the population loadings of common factor η_j, and $\boldsymbol{\Sigma}_{jj}$ is the $K_j \times K_j$ population correlation matrix of the indicators of block j.[7] The squared correction factor $\hat{c}_j^2$ can be obtained as follows:

$$\hat{c}_j^2 = \frac{\hat{\boldsymbol{w}}_j'(\boldsymbol{S}_{jj} - \text{diag}(\boldsymbol{S}_{jj}))\hat{\boldsymbol{w}}_j}{\hat{\boldsymbol{w}}_j'(\hat{\boldsymbol{w}}_j\hat{\boldsymbol{w}}_j' - \text{diag}(\hat{\boldsymbol{w}}_j\hat{\boldsymbol{w}}_j'))\hat{\boldsymbol{w}}_j}. \tag{4.8}$$

It is chosen such that the Euclidean distance between

$$\boldsymbol{S}_{jj} - \text{diag}(\boldsymbol{S}_{jj}) \quad \text{and} \quad (c_j\hat{\boldsymbol{w}}_j)(c_j\hat{\boldsymbol{w}}_j)' - \text{diag}((c_j\hat{\boldsymbol{w}}_j)(c_j\hat{\boldsymbol{w}}_j')) \tag{4.9}$$

is minimized (Dijkstra and Henseler, 2015a). Factor loadings of block j are consistently estimated as follows:

$$\hat{\boldsymbol{\lambda}}_j = \hat{c}_j \hat{\boldsymbol{w}}_j. \tag{4.10}$$

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[6] Both, common factors as well as composites are legit ways of construct modeling, see Rigdon (2012).

[7] The use of *mode B* for common factors is not considered here. For a consistent version of PLS using *mode B*, see Dijkstra (2011).

Moreover, PLSc can consistently estimate the path coefficients of recursive and non-recursive models,[8] using OLS or 2SLS, according to the structural model. Since all variables are standardized, the estimated path coefficients are based on the correlations between the columns of $\hat{\boldsymbol{\eta}}$ ($n \times J$). The correlation between the common factors j and l is consistently estimated by the following:

$$\widehat{\text{cor}}(\eta_j, \eta_l) = \frac{\hat{\boldsymbol{w}}_j' \boldsymbol{S}_{jl} \hat{\boldsymbol{w}}_l}{\sqrt{\hat{c}_j^2 \hat{\boldsymbol{w}}_j' \hat{\boldsymbol{w}}_j \hat{c}_l^2 \hat{\boldsymbol{w}}_l' \hat{\boldsymbol{w}}_l}}. \tag{4.11}$$

Using the corrected correlation of Equation (4.11) for the estimation of the structural model, one obtains consistently estimated path coefficients between the common factors.[9] For constructs that are modeled as composites, no correction of the correlation is required, because, by assumption, they are not affected by attenuation. For example, if construct j is modeled as a common factor and construct l as a composite, the consistently estimated correlation is obtained as follows:

$$\widehat{\text{cor}}(\eta_j, \eta_l) = \frac{\hat{\boldsymbol{w}}_j' \boldsymbol{S}_{jl} \hat{\boldsymbol{w}}_l}{\sqrt{\hat{c}_j^2 \hat{\boldsymbol{w}}_j' \hat{\boldsymbol{w}}_j}}. \tag{4.12}$$

4.3   The development from PLS to ordinal PLS

Since incorrectly handling ordinal categorical variables as continuous can lead to biased inferences and, therefore, to erroneous conclusions, the PLS literature provides several approaches to deal with discrete indicators: dichotomize the ordinal categorical indicator, a mixture of PLS and correspondence analysis (CA), Partial Maximum Likelihood PLS (PML-PLS), and non-metric PLS (NM-PLS).

Common practice in PLS is to replace a categorical indicator by a dummy matrix which is known as dichotomizing. Since each categorical indicator is replaced by $M-1$ dummy variables, where M is the number of observed categories, $M-1$ outer weights are obtained for the original variable. This contradicts the idea of treating an indicator as a whole.

Betzin and Henseler (2005) use correspondence analysis to quantify ex-ante categorical indicators. As the quantified indicators are obtained, PLS is used to estimate

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[8]PLSc relaxes the assumptions of the *basic design* (Wold, 1982b) where non-recursive structural models are not allowed.

[9]For more details, e.g., the consistent estimation of non-recursive models and the correction for nonlinear structural equation models, see Dijkstra (1983, 1985, 2010, 2011); Dijkstra and Schermelleh-Engel (2014).

the model parameters. As a result, individual weights are obtained for each category of the categorical indicator. Again, this has the drawback that no single outer weight for a categorical indicator is calculated.

Partial Maximum Likelihood Partial Least Squares (PML-PLS) is a modified version of the original PLS algorithm (Jakobowicz and Derquenne, 2007). It is a combination of PLS and generalized linear models designed to deal with indicators of any scale. For categorical indicators, individual outer weights are computed for each category by ANOVA. Based on those, one 'global' weight per categorical indicator is calculated. However, statistical properties like the proportionality of outer weights to factor loadings are unknown for the global weights, thus necessitating further investigation. Moreover, the authors note that PML-PLS "is especially advantageous in the case of nominal or binary variables" (Jakobowicz and Derquenne, 2007); however, we focus on ordinal categorical indicators.

The last approach, non-metric partial least squares (NM-PLS) combines the PLS algorithm with optimal scaling to quantify qualitative indicators (Trinchera and Russolillo, 2010; Russolillo, 2012). Optimal scaling is a procedure that quantifies qualitative variables by preserving properties of the original measurement scales. In case of NM-PLS, the categorical indicator is quantified in a way that the correlation between the inner LV estimate and the quantified categorical indicator is maximized. As a result, for each variable one outer weight is obtained as is the case in traditional PLS for continuous indicators.

However, the evaluation of the presented approaches is based on empirical studies, and, to our knowledge, no simulation studies have been conducted to investigate their statistical properties. For an extension to PLSc, in order to deal with common factors, it is necessary that the outer weights are proportional to the factor loadings. Moreover, the modified PLS procedures are often applied to common factor models that represent a misspecified model in the context of PLS. Hence, an assessment of their statistical properties is hardly possible, and hence, we decide not to pursue any of the previously mentioned methods.

4.3.1 Ordinal PLS

A promising approach to deal with ordinal categorical indicators is ordinal PLS (Ord-PLS[10]) (Cantaluppi, 2012). It is a modified procedure for handling ordinal categorical variables in a classical econometric way. In Section 4.2, we showed that all parameters can be obtained using the correlation matrix $\boldsymbol{S}$. Traditional PLS uses the Bravais-Pearson (BP) correlation matrix which requires all indicators to be continuous for consistency. The observation of an ordinal categorical variable is a qualitative measure, yet it is often coded numerically and, therefore, mistakenly treated as a quantitative measure by researchers. This routinely happens in applications with binary and ordinal categorical indicators, which, in turn, results in biased BP correlation estimates (Carroll, 1961; O'Brien and Homer, 1987; Quiroga, 1992; Wylie, 1976). To fix this, OrdPLS uses a consistent correlation matrix as input for the traditional PLS algorithm. An advantage of OrdPLS over the approaches previously introduced is that it offers a transparent way of dealing with ordinal categorical variables. Moreover, the original PLS algorithm remains untouched, and it is just provided by a consistent correlation matrix as input for the algorithm.

Since OrdPLS does not correct for attenuation, it shows the same drawbacks as PLS if common factors are included in the model. Nevertheless, we consider OrdPLS as a powerful extension of PLS when applied under appropriate circumstances, i.e., for models with only composites. Furthermore, it is straightforward to extend by PLSc for overcoming its drawback for common factor models (see Section 4.4). In the following subsection we present Pearson's considerations of ordinal categorical variables to provide a better understanding of the polychoric and polyserial correlation.

4.3.2 Ordinal categorical variables according to Pearson

Pearson (1900, 1913) considers an ordinal categorical variable as a crude measure of an underlying continuous random variable, while Yule (1900) assumes categorical variables as being inherently discrete. In this chapter, we follow Pearson's idea which states that an observed ordinal categorical indicator x is the result of a polytomized standard

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[10]OrdPLS was originally called OPLS (Cantaluppi, 2012). An anonymous reviewer suggested to use a different name in order to avoid confounding with O-PLS (Trygg and Wold, 2002). We came to an agreement with Gabriele Cantaluppi to speak of OrdPLS in the future. We thank the anonymous reviewer for suggesting such a disambiguation.

normally distributed random variable x^* seen as follows:

$$x = x_m, \quad \text{if} \quad \tau_{m-1} \leq x^* < \tau_m \quad m = 1, \ldots, M, \qquad (4.13)$$

where the threshold parameters $\tau_0, \ldots, \tau_M$ determine the observed categories. The first and last threshold are fixed as follows: $\tau_0 = -\infty$ and $\tau_M = \infty$. Moreover, thresholds are assumed to be strictly increasing as follows: $\tau_0 < \tau_1 < \ldots < \tau_M$.
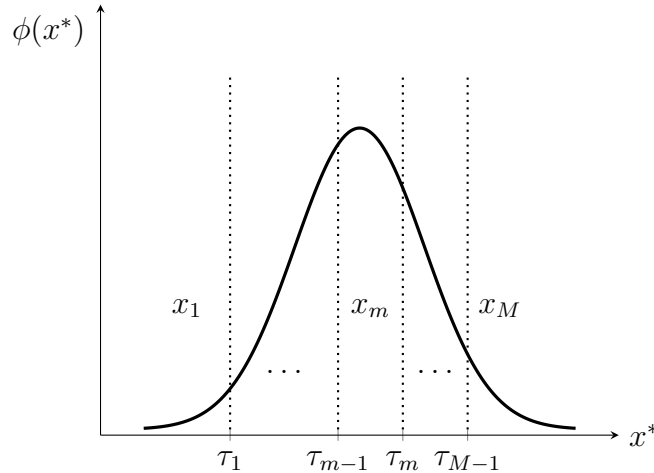
Figure 4.3: Pearson's idea of an ordinal categorical variable

Figure 4.3 depicts the idea of an underlying continuous variable: For indicator x category x_m is observed if the realization of the underlying continuous variable x^* is in between the thresholds τ_{m-1} and τ_m.

4.3.3 Polychoric and polyserial correlation

Since an ordinal categorical variable is determined by an underlying continuous variable, it is more appropriate to consider the correlation between these underlying quantitative continuous variables for evaluating the linear relationship of interest. This is achieved by using the polychoric or polyserial correlation (Drasgow, 1988). To illustrate the principles of the polychoric correlation, we consider two ordinal categorical variables, x_1 and x_2, with consecutive categories denoted by m_1 and m_2 for x_1 and x_2 respectively, with $m_1 = 1, \ldots, M_1$ and $m_2 = 1, \ldots, M_2$, see Equation (4.13). The two underlying continuous variables are assumed to be jointly bivariate standard normally distributed with correlation ρ. The correlation between x_1^* and x_2^* can be consistently

estimated by maximum likelihood, using the following log-likelihood function:

$$\ln L = \ln(c) + \sum_{m_1=1}^{M_1} \sum_{m_2=1}^{M_2} n_{m_1 m_2} \ln(\pi_{m_1 m_2}), \qquad (4.14)$$

where $\ln(c)$ is a constant term, $n_{m_1 m_2}$ denotes the observed joint absolute frequency of $x_1 = m_1$ and $x_2 = m_2$, and $\pi_{m_1 m_2}$ is the probability that category m_1 and m_2 are observed jointly. Due to the bivariate normality assumption, $\pi_{m_1 m_2}$ is obtained as follows:

$$\pi_{m_1 m_2} = \qquad (4.15)$$

$$\Phi_2(\tau_{m_1}, \tau_{m_2}, \rho) - \Phi_2(\tau_{m_1}, \tau_{m_2-1}, \rho) - \Phi_2(\tau_{m_1-1}, \tau_{m_2}, \rho_1) + \Phi_2(\tau_{m_1-1}, \tau_{m_2-1}, \rho),$$

where Φ_2 is the cumulative distribution function of the bivariate standard normal distribution. The parameters τ_{m_1}, τ_{m_2}, and ρ are chosen to maximize the function $\ln L$. In order to reduce computational burden, a two-step procedure can be used (Olsson, 1979). In the first step, estimated threshold parameters are separately calculated for both ordinal categorical indicators x_k, with $k = 1, 2$ as quantiles of cumulative marginal frequencies, $\hat{\tau}_{m_k} = \Phi^{-1}(F_{m_k})$, where F_{m_k} equals the cumulative marginal relative frequency up to category m_k. The function Φ^{-1} represents the quantile function of the univariate standard normal distribution. Second, given the estimated threshold parameters, Equation (4.14) is maximized with respect to ρ. In case of a continuous and an ordinal categorical variable, the correlation between the two continuous variables is obtained by the polyserial correlation (Olsson et al., 1982). For more than two variables, a multivariate version is used to estimate the correlations (Poon and Lee, 1987). Moreover, a less computational intensive two-step approach can be used for the multivariate version (Lee and Poon, 1987). OrdPLS as well as OrdPLSc make use of the polychoric and polyserial correlation when ordinal categorical indicators are part of the model.

4.4 Ordinal consistent partial least squares

We introduce a new approach that deals with common factors, composites, and ordinal categorical indicators. It is called ordinal consistent partial least squares (OrdPLSc) and is a combination of OrdPLS and PLSc. It uses the polychoric correlation, a consistent correlation matrix in case of ordinal categorical indicators, as input for the

PLS algorithm and corrects for attenuation if common factors are included in the model. Since the use of the polychoric correlation matrix does not affect the original PLS algorithm, the proportionality property of the outer weights is maintained, and the correction of attenuation can be applied to the inter-composite correlation matrix in the same manner as is done in PLSc. Figure 4.4 illustrates commonalities and differences of the three previously presented PLS approaches and OrdPLSc.
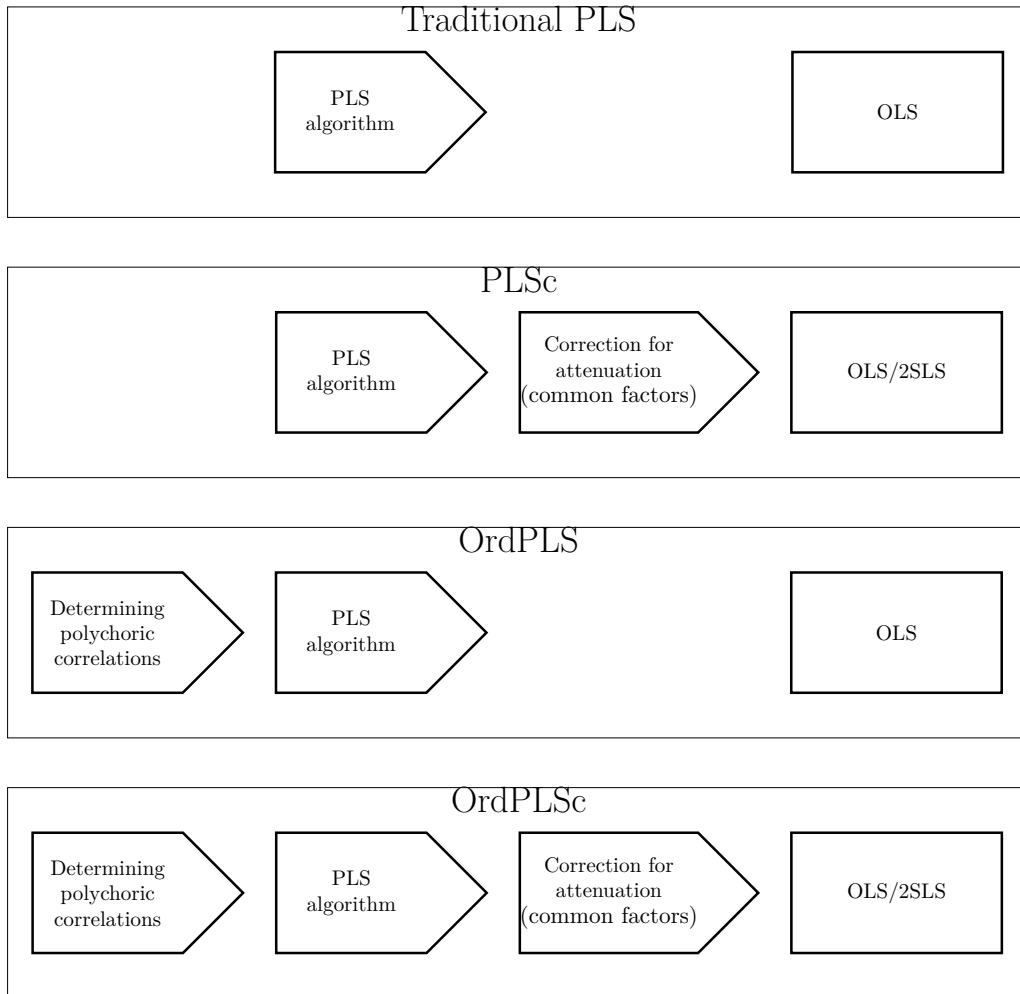
Figure 4.4: Conceptual differences between the four PLS approaches

The role of an ordinal categorical indicator x, more precisely its underlying continuous variable x^*, is influenced by its position in the model. As Figure 4.5a displays, when the ordinal categorical indicator belongs to a common factor, its outcome is indirectly influenced by the underlying common factor and a measurement error ϵ through the underlying continuous variable x^*. An ordinal categorical indicator that is part of a composite, see Figure 4.5b, is simply a crude measure of an underlying continuous variable (represented by a double headed arrow) that actually builds the composite

along with the other indicators belonging to this block.

(a) Exogenous common factor: ordinal categorical indicators

(b) Exogenous composite model: ordinal categorical indicators
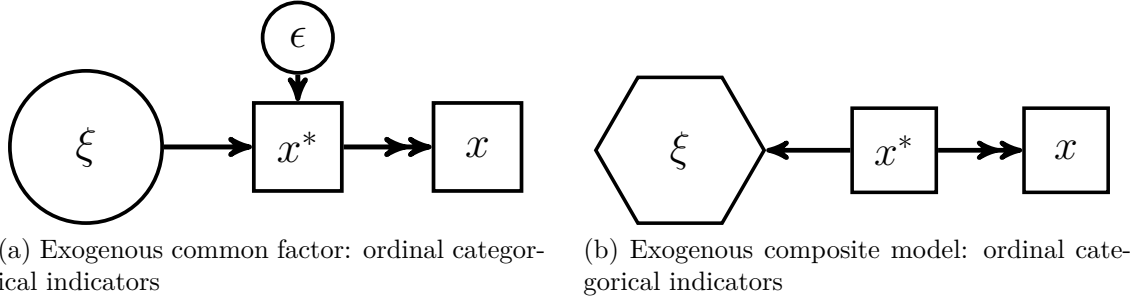
Figure 4.5: Ordinal categorical indicators in common factor and composite models

Ignoring the nature of the ordinal categorical indicators may cause serious problems. First, in common factor models, the correlation between the indicator and its underlying common factor is underestimated (O'Brien and Homer, 1987; Quiroga, 1992), which leads to biased estimates. Second, in the case of a composite, disregarding the scale of the ordinal categorical indicator leads to biased estimates as well. This is commonly known as the *error-in-variables* problem (Wooldridge, 2012, Chap. 15).

4.5 Evaluation of construct scores in OrdPLS and OrdPLSc

A useful feature of PLS is that construct scores can be calculated directly enabling, e.g., importance-performance matrix analysis (IPMA) (Ringle and Sarstedt, 2016).[11] In this section, we present three ways of calculating construct scores in the framework of OrdPLS and OrdPLSc[12] to obtain a category indication, which is expressed on the same common ordinal scale that characterizes the indicators[13] of the latent variable.[14] As the continuous variables $\boldsymbol{x}_j^*$ underlying each ordinal categorical indicator are not observable (see Figure 4.5), unique construct scores $\hat{\eta}_j$ cannot be calculated directly.

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[11]IPMA is a technique aimed at finding which construct is better to act on, in order to improve the average level of a target construct. It is based on a scatter plot diagram for each endogenous construct, representing summary location measures (performances) of its antecedent latent variables and their impacts (regression coefficients) on the analyzed endogenous construct.

[12]As the weights are unaffected by the correction for attenuation, the construct scores are the same for PLS and PLSc as well as for OrdPLS and OrdPLSc.

[13]We assume that all indicators have the same number of categories. Calculating construct scores in presence of ordinal categorical indicators with different numbers of categories will be considered in future research.

[14]In PLS, a linear transformation of standardized scores is sufficient to assign location and scale to construct scores as shown, e.g., in Bayol et al. (2000).

We are only able to determine the probability function of each composite $\hat{\eta}_j$ and an interval of possible values conditional on the threshold values pertaining to the latent variables x^*_{jk} that underlie each ordinal categorical indicator connected to η_j. This information can be used for approximating construct scores.

Each underlying latent variable x^*_{jk} with $k = 1, \ldots, K_j$ is assumed to be standard normally distributed. Therefore, the composite $\hat{\eta}_j$, defined by the following linear combination (analogous to Equation 4.6):

$$\hat{\eta}_j = \sum_{k=1}^{K_j} \hat{w}_{jk} x^*_{jk}, \tag{4.16}$$

is also normally distributed and, thus, classified on a continuous scale. In order to assign a location value to the composites $\hat{\eta}_j$, a set of threshold parameters for the composite $\tau_m^{\hat{\eta}_j}$, $m = 1, \ldots, M-1$, can be derived from the individual indicators threshold parameters $\tau_m^{x_{jk}}$ belonging to the underlying variable x^*_{jk}, $k = 1, \ldots, K_j$, where M denotes the number of categories for indicator x_{jk}, as follows:

$$\tau_m^{\hat{\eta}_j} = \sum_{k=1}^{K_j} \hat{w}_{jk} \tau_m^{x_{jk}}. \tag{4.17}$$

For practical reasons, threshold parameters equal to $\pm\infty$ are replaced by ± 4.

In the following, we first define an interval of $\hat{\eta}_{ji}$, with $i = 1, \ldots, n$, which is the image of x_{jki}, $k = 1, \ldots, K_j$, where x_{jki} is the observation of subject i for indicator x_{jk} linked to the corresponding composite $\hat{\eta}_j$. Using the interval, we propose three ways to obtain construct scores on the common ordinal scale characterizing the indicators.

In case subject i chooses the same category m for all the indicators connected to $\hat{\eta}_j$, $x_{j1i} = \cdots = x_{jK_j i} = m$ with $m \in \{1, \ldots, M\}$, the image is of the following type:

$$A_m \equiv (\tau_{m-1}^{\hat{\eta}_j}, \tau_m^{\hat{\eta}_j}] \tag{4.18}$$

which we call *homogeneous thresholds*. Otherwise, as illustrated in Figure 4.6, the set which is the image of all possible responses x_{jki}, will not correspond exactly to one subset A_m. Let us denote this set for subject i with

$$C_{ji} \equiv (\alpha_i^{\hat{\eta}_j}, \beta_i^{\hat{\eta}_j}], \tag{4.19}$$

where

$$\alpha_i^{\hat{\eta}_j} = \sum_{k=1}^{K_j} \hat{w}_{jk} \tau_{m-1}^{x_{jki}} \qquad \text{and} \qquad \beta_i^{\hat{\eta}_j} = \sum_{k=1}^{K_j} \hat{w}_{jk} \tau_m^{x_{jki}}. \tag{4.20}$$

The parameters $\tau_{m-1}^{x_{jki}}$ and $\tau_m^{x_{jki}}$ are the threshold parameters that determine the observed category for subject i of indicator x_{jk} and those that can be used to define the values for the interval of x_{jk}^*. To assign a category to the i-th observation of the composite $\hat{\eta}_j$, we propose one of the following options:

1. **Mode estimation:** Compute, see Figure 4.6, the probabilities for C_{ji} overlapping each set A_m defined by the 'homogeneous thresholds' as follows:

$$P\left(C_{ji} \cap A_m\right) \quad m = 1, \dots, M \tag{4.21}$$

and select for observation i the set A_m with the maximum probability. To the set A_m corresponds the assignment of category m as a score estimate for the construct η_j. In Figure 4.6, category 3 (interval from τ_2 to τ_3) is assigned.

2. **Median estimation:** Compute the median for each observation i of the variable $\hat{\eta}_j$ on the interval C_{ji} as follows:

$$\text{median}(\hat{\eta}_{ji} | \hat{\eta}_{ji} \in C_{ji}) = \Phi^{-1}\left(\frac{1}{2}(\Phi(\alpha_i^{\hat{\eta}_j}) + \Phi(\beta_i^{\hat{\eta}_j}))\right). \tag{4.22}$$

The category m pertaining the set A_m to which $\text{median}(\hat{\eta}_{ji} | \hat{\eta}_{ji} \in C_{ji})$ belongs, is assigned to subject i.

3. **Mean estimation:** Compute the mean of the variable $\hat{\eta}_{ji}$ on the interval C_{ji} as follows:

$$E(\hat{\eta}_{ji} | \hat{\eta}_{ji} \in C_{ji}) = \frac{\phi(\alpha_i^{\hat{\eta}_j}) - \phi(\beta_i^{\hat{\eta}_j})}{\Phi(\beta_i^{\hat{\eta}_j}) - \Phi(\alpha_i^{\hat{\eta}_j})}. \tag{4.23}$$

The category m pertaining the set A_m to which $E(\hat{\eta}_{ji} | \hat{\eta}_{ji} \in C_{ji})$ belongs, is assigned to subject i.
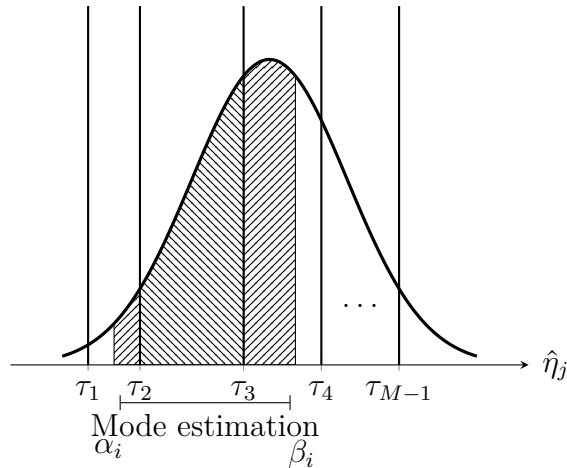
Figure 4.6: Categorical construct scores

4.6 Monte Carlo simulation

In order to investigate the performance of OrdPLSc under various conditions and to compare it to the performance of PLSc, OrdPLS, and PLS for structural equation models containing ordinal categorical indicators, we run a Monte Carlo simulation. In particular, we examine their unbiasedness and their efficiency – the most important properties of an estimator. Furthermore, we study the bias of PLS and OrdPLS for common factor models with ordinal categorical indicators. Also for PLSc, which is known to be a consistent estimator in the framework of continuous indicators (Dijkstra and Henseler, 2015a), we examine the behavior when ordinal categorical variables are used instead of continuous ones.

We conduct a Monte Carlo simulation with 1000 multivariate standard normally distributed samples with 500 observations each. The continuous indicators are categorized in the way presented in Section 4.3.2. We only consider consecutive categories, i.e., $1, 2, \ldots, M$. To compare all estimators in a fair way, inadmissible solutions[15] are removed and replaced by proper estimations before analysis.

We consider the following experimental conditions: two population models (a model with three common factors and a model with one common factor and two composites), four different number of categories (2, 3, 5, and, 7 categories), and five different distributions of the ordinal categorical indicators (symmetric, moderately asymmetric, extremely asymmetric, alternating moderately asymmetric, and alternating extremely asymmetric). Each condition is estimated by OrdPLSc, PLSc, OrdPLS, and PLS. As a benchmark comparison for the pure common factor model, we also estimate the model by WLSMV, a consistent covariance-based three stage least squares estimator (Muthén, 1984; Lee et al., 1990b), which is considered to be the golden standard for common factor models with ordinal categorical indicators.[16]

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[15]Inadmissible solutions are estimations with absolute factor loadings larger than 1, non positive-definite construct correlation matrix, or estimations that have not converged.

[16]The mixed model with an endogenous composite cannot be estimated by WLSMV because of identification problems. Moreover, as is the case in OrdPLS and OrdPLSc, covariance-based estimators for categorical indicators are typically based on polychoric correlation, see Lee et al. (1990a, 1992); De Leon (2005); Liu (2007); Katsikatsou et al. (2012).

4.6.1 Two population models

Starting point are the following two kinds of models: one model with only common factors and one model with one common factor and two composites. The pure common factor model is chosen to compare OrdPLSc to its covariance-based counterpart WLSMV. In designing the path structure of the models, we choose a structure that has been used several times in the literature (Hwang et al., 2010; Henseler, 2012b; Henseler and Sarstedt, 2013).

Population model with only common factors

First, we consider a pure common factor model with the following population structural equations:

$$\eta_1 = \gamma_1 \xi_1 + \zeta_1 \tag{4.24}$$

$$\eta_2 = \gamma_2 \xi_1 + \beta \eta_1 + \zeta_2, \tag{4.25}$$

where $\gamma_1 = 0.6, \gamma_2 = 0.0, \beta = 0.6, \mathrm{var}(\zeta_1) = 0.64, \mathrm{var}(\zeta_2) = 0.64$, and $\mathrm{cov}(\zeta_1, \zeta_2) = 0$. As Figure 4.7 depicts, each common factor is connected to three indicators with factor loadings $\boldsymbol{\lambda}'_x = \begin{pmatrix} 0.8 & 0.7 & 0.6 \end{pmatrix}$ for ξ, $\boldsymbol{\lambda}'_{y_1} = \begin{pmatrix} 0.7 & 0.7 & 0.7 \end{pmatrix}$ for η_1, and $\boldsymbol{\lambda}'_{y_2} = \begin{pmatrix} 0.5 & 0.7 & 0.9 \end{pmatrix}$ for η_2.
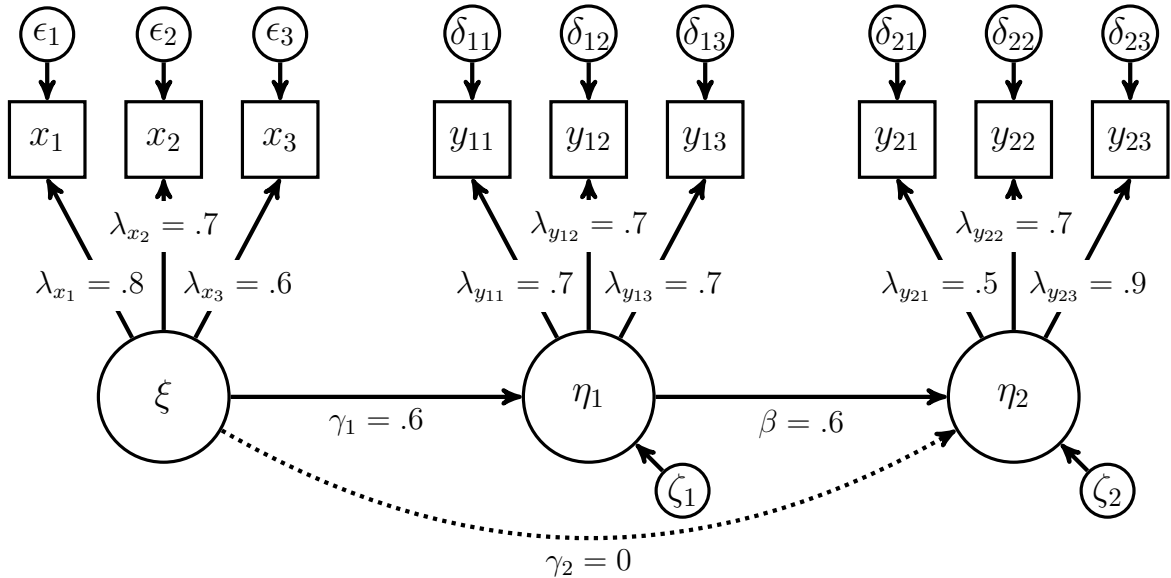
Figure 4.7: Population model with three common factors

All measurement errors and structural residuals are mutually independent and all common factors are assumed to be independent of the measurement errors. Therefore, the

indicators population correlation matrix is given by the following:

$$\mathbf{\Sigma} = \begin{array}{ccccccccc} \underline{x_1} & \underline{x_2} & \underline{x_3} & \underline{y_{11}} & \underline{y_{12}} & \underline{y_{13}} & \underline{y_{21}} & \underline{y_{22}} & \underline{y_{23}} \end{array}$$

$$\mathbf{\Sigma} = \begin{pmatrix} 1.0000 & & & & & & & & \\ 0.5600 & 1.0000 & & & & & & & \\ 0.4800 & 0.4200 & 1.0000 & & & & & & \\ 0.3360 & 0.2940 & 0.2520 & 1.0000 & & & & & \\ 0.3360 & 0.2940 & 0.2520 & 0.4900 & 1.0000 & & & & \\ 0.3360 & 0.2940 & 0.2520 & 0.4900 & 0.4900 & 1.0000 & & & \\ 0.1440 & 0.1260 & 0.1080 & 0.2100 & 0.2100 & 0.2100 & 1.0000 & & \\ 0.2016 & 0.1764 & 0.1512 & 0.2940 & 0.2940 & 0.2940 & 0.3500 & 1.0000 & \\ 0.2592 & 0.2268 & 0.1944 & 0.3780 & 0.3780 & 0.3780 & 0.4500 & 0.6300 & 1.0000 \end{pmatrix} .$$

(4.26)

Population model with two composites and one common factor

Second, we consider a model with the identical structural model as used for the model with three common factors, but two of the constructs are modeled as composites instead of as common factors. Figure 4.8 depicts the population model in terms of common and composite factors. We deliberately choose this representation of the composites and not the one used in Figure 4.2b to be able to clarify the construction of the population correlation matrix of the indicators.
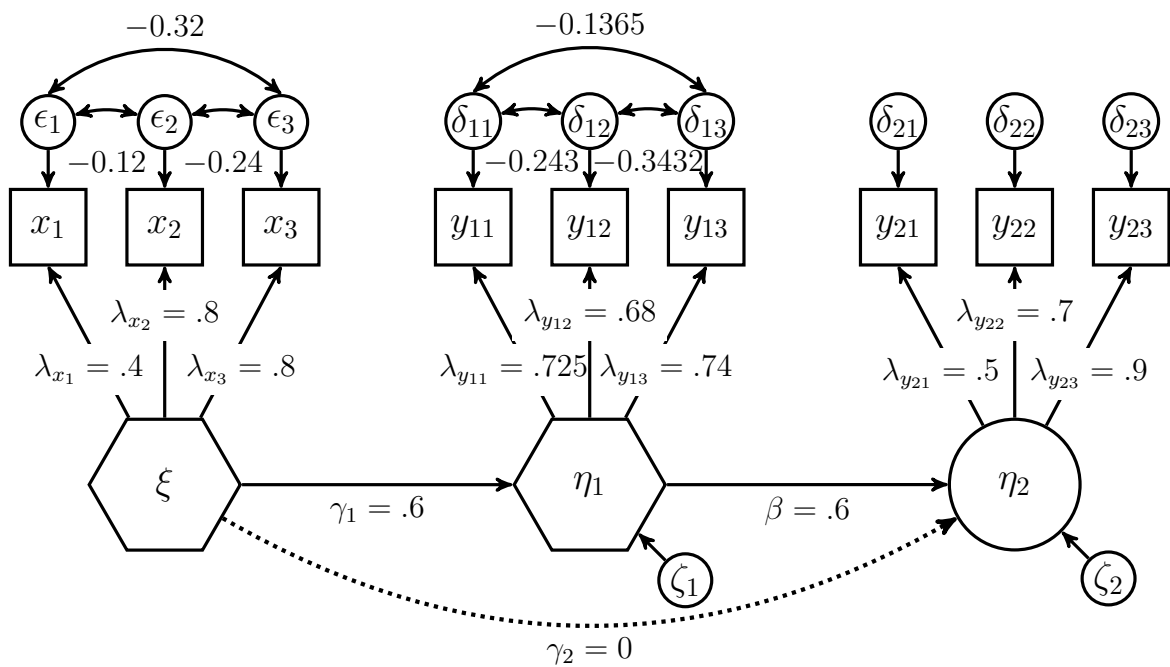
Figure 4.8: Population model with two composites and one common factor

Here ξ and η_1 are constructs modeled as composites. Since the relationship between a composite and its indicators can be expressed by composite loadings (Figure 4.8) or weights, we also report the weights: the composites are formed by their connected indicators as follows: $\xi = \boldsymbol{x}'\boldsymbol{w_x}$ where $\boldsymbol{w_x'} = (0.3, 0.5, 0.6)$ and $\eta_1 = \boldsymbol{y_1'}\boldsymbol{w_{y_1}}$ where $\boldsymbol{w_{y_1}'} = (0.4, 0.5, 0.5)$. The common factor η_2 is again connected to three indicators with the following loadings: 0.5, 0.7, and 0.9. The population correlation matrix of the

indicators has the following form:

$$\boldsymbol{\Sigma} = \begin{pmatrix}
\underline{x_1} & \underline{x_2} & \underline{x_3} & \underline{y_{11}} & \underline{y_{12}} & \underline{y_{13}} & \underline{y_{21}} & \underline{y_{22}} & \underline{y_{23}} \\
1.0000 \\
0.2000 & 1.0000 \\
0.0000 & 0.4000 & 1.0000 \\
0.1740 & 0.3480 & 0.3480 & 1.0000 \\
0.1632 & 0.3264 & 0.3264 & 0.2500 & 1.0000 \\
0.1776 & 0.3552 & 0.3552 & 0.4000 & 0.1600 & 1.0000 \\
0.0720 & 0.1440 & 0.1440 & 0.2175 & 0.2040 & 0.2220 & 1.0000 \\
0.1008 & 0.2016 & 0.2016 & 0.3045 & 0.2856 & 0.3108 & 0.3500 & 1.0000 \\
0.1296 & 0.2592 & 0.2592 & 0.3915 & 0.3672 & 0.3996 & 0.4500 & 0.6300 & 1.0000
\end{pmatrix}.$$

(4.27)

4.6.2 Number of categories

We consider four different numbers of indicator categories: 2, 3, 5, and 7. An increasing number of categories diminishes the bias of the BP correlation (O'Brien and Homer, 1987). Hence, we expect a decreasing difference between PLS and OrdPLS as well as PLSc and OrdPLSc as the number of categories increases.

4.6.3 Threshold parameter distribution

We investigate differently skewed ordinal categorical indicators by varying threshold parameter distributions for each number of categories. We consider the following threshold parameter distributions that has already been used in the literature before (Rhemtulla et al., 2012): symmetrically, moderately asymmetrically, extremely asymmetrically, alternating moderately asymmetrically, and alternating extremely asymmetrically distributed threshold parameters. In the alternating asymmetric threshold distribution scenario, the same thresholds are used; however, the direction of asymmetry is reversed for the indicators, x_2, y_{11}, y_{13}, and y_{22}.[17] Since BP correlations are more downward biased for more asymmetrical threshold distributions (Bollen and Barb, 1981; Faber, 1988; Holgado-Tello et al., 2010), and even more for alternating skewed indicators (Olsson, 1980), we expect an increasing difference between OrdPLSc and

[17]For an exact description of the threshold parameter distribution, see the Appendix.

PLSc estimates as well as between OrdPLS and PLS estimates from the symmetrical to the alternating extreme threshold distribution.

4.6.4 Data generation and analysis

All simulations are conducted within the R (version 3.2.2) statistical programming environment (R Core Team, 2015). Multivariate standard normally distributed data sets are drawn using the *mvrnorm* function of the *MASS* package (Venables and Ripley, 2002). To obtain PLS and PLSc estimates, we primarily use functions provided by the *matrixpls* package (Rönkkö, 2015), which allows for the use of the empirical correlation matrix as input for PLS and PLSc. A slightly modified version of those functions is also used for OrdPLS and OrdPLSc. The modified version is provided by the authors upon request. Since *matrixpls* is still under development, we also partly verify our results obtained with ADANCO (Henseler and Dijkstra, 2015). The polychoric correlation is calculated by the *polychoric* function from the *psych* package (Revelle, 2015), using the two-step approach.[18] WLSMV estimation is carried out using the *lavaan* package (Rosseel, 2012).

4.7 Results

This section shows the results of our study.[19] In the following, we summarize our findings in terms of bias with respect to the quality of the parameter estimates for the model containing only common factors and the mixed model. The bias is evaluated as follows by the deviation of the estimated parameter mean from its population counterpart across all Monte Carlo simulation runs:

$$\widehat{\mathrm{Bias}} = \frac{1}{1000} \sum_{i=1}^{1000} \hat{\theta}_i - \theta, \tag{4.28}$$

where θ represents the population parameter and $\hat{\theta}_i$ is the estimated parameter from the i-th Monte Carlo run. The estimated bias provides information about the estimators' unbiasedness and is used as performance measure to compare OrdPLSc estimates with the estimates obtained from the other approaches. Moreover, we assess the estimators'

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[18]If the polychoric correlation matrix is not positive definite, an eigenvector smoothing is done to assure its positive definiteness. Moreover, we follow the recommendation of Savalei (2011) and use the 'ADD' approach (0.5) for empty cells in the case of two categories and the 'NONE' approach for the other cases. The same is done for WLSMV.

[19]The complete results are provided in the supplementary material.

efficiency in terms of standard deviation across all Monte Carlo simulation runs. We finish the section by summarizing inadmissible results.

In general, for the moderate asymmetric and the alternating moderate asymmetric threshold parameter distribution, the estimators lead to similar results. The same is observed for extremely and alternating extremely asymmetrically distributed threshold parameters. For latter conditions, all estimators show a poorer performance, which confirms our expectations.

4.7.1   Bias of the parameter estimates

Figures 4.9 and 4.10 display the average deviation of the path coefficient estimates for $\beta(= 0.6)$ and $\gamma_2(= 0.0)$, and factor loading estimates for $\lambda_{x_1}(= 0.5)$ and $\lambda_{y_{21}}(= 0.8)$ of the pure common factor model from their population value for the different number of categories and the different threshold parameter distributions. An asterisk above a bar indicates that the deviation is statistically significant on a 5% level. Due to space constraints, we omit the results for the estimated path coefficient $\hat{\gamma}_1$ and the other factor loading estimates. They behave very similarly to the ones presented.
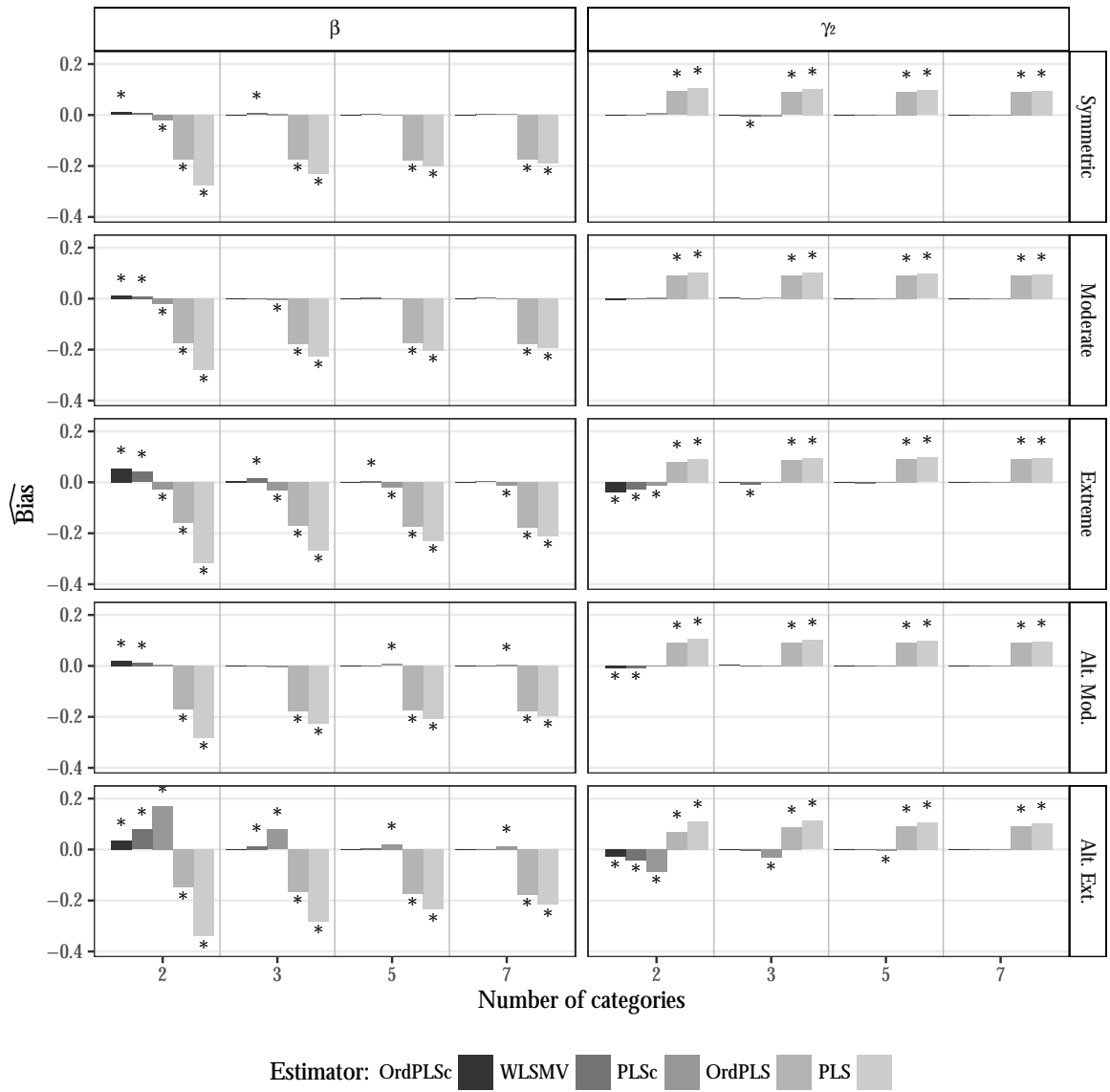
*: significant on a 5% level

Figure 4.9: Model with only common factors: average deviations from β and γ_2
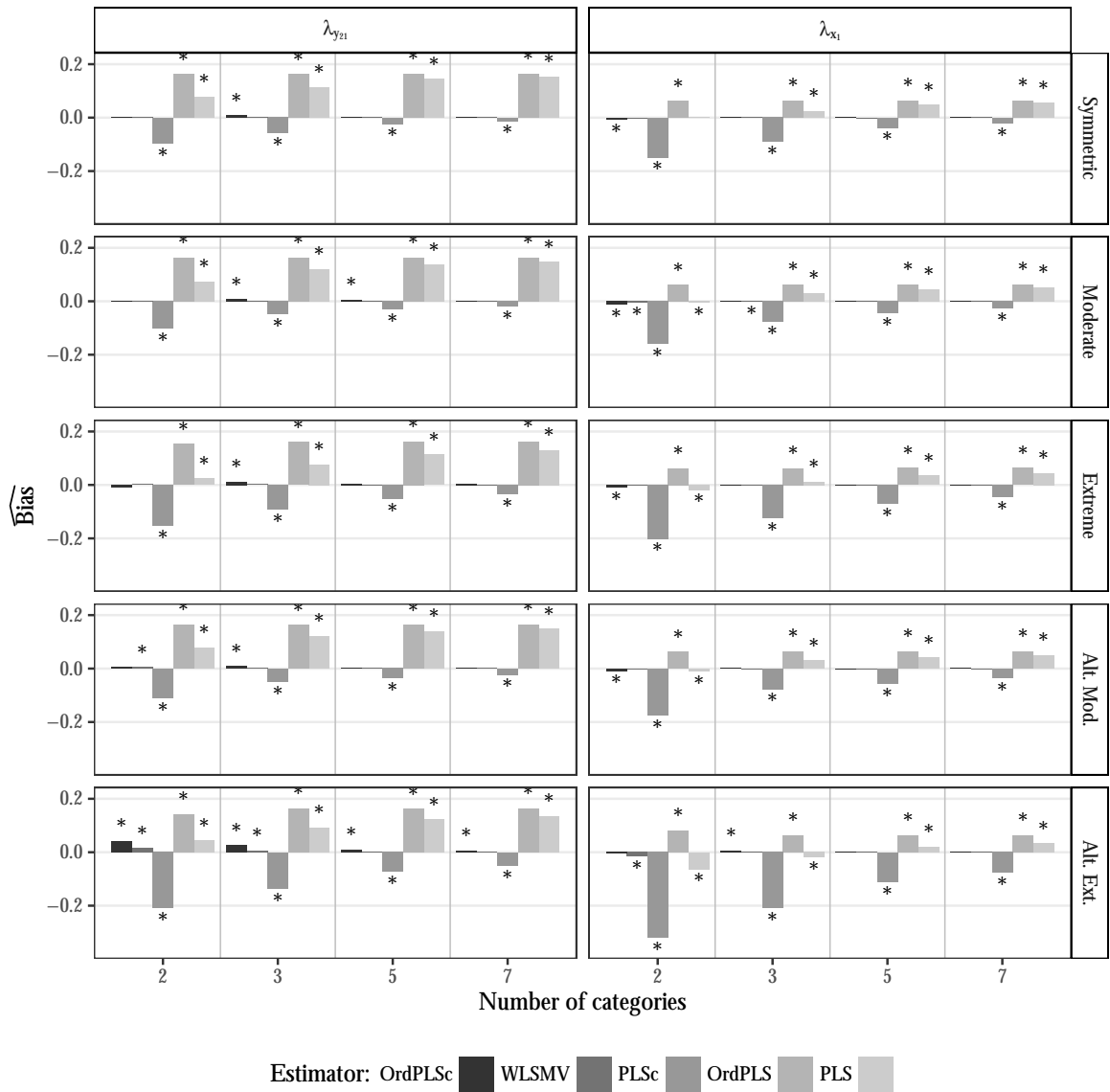
*: significant on a 5% level

Figure 4.10: Model with only common factors: average deviations from $\lambda_{y_{21}}$ and λ_{x_1}

These figures offer evidence that OrdPLSc and WLSMV lead to almost the same results for the estimated path coefficients and factor loadings under all conditions. Most parameter means are not significantly different from their population values, indicating that both estimators are hardly biased. In case of extremely and alternating extremely skewed indicators, the means of the path coefficient estimates significantly differ from the population values. This deviation diminishes and becomes insignificant with an increasing number of categories.

In contrast, PLSc path coefficient estimates behave surprisingly well in most of the conditions. For non-extremely distributed threshold parameters, the path coefficient estimates are, upon averaging, close to their population values. However, in case of the

extreme and, in particular, the alternating extreme threshold parameter distribution, the path coefficient means are significantly different from the true values. This deviation declines with an increase in the number of categories and becomes insignificant. In contrast, factor loadings are significantly under-estimated on average in all conditions but the deviation dramatically declines as the number of categories increases. However, the deviation is still significant for seven categories.

We obtain different results for OrdPLS that lead to fairly constant and statistically significant deviations of the means from their true parameters in all conditions, unaffected by the number of categories. In particular, the path coefficients β and γ_1 are significantly underestimated on average while the zero-path coefficient γ_2 is significantly overestimated on average. Factor loadings are all overestimated on average, except the largest factor loading $\lambda_{y_{23}} = 0.9$. All deviations are largely unaffected by the number of categories.

PLS produces average path coefficient estimates for γ_1 and β_1 that differ most from their population value. While the deviation of the average OrdPLS estimates from the true parameter is fairly constant in all conditions, the difference between the average PLS estimates and their population values converges to the average deviation of OrdPLS estimates with an increasing number of categories. A similar pattern is observed for PLS factor loading estimates. Mean factor loading estimates slightly deviate from the population value in case of two categories, but the deviation becomes more pronounced and converges to the deviation of the average OrdPLS factor loading estimates as the number of categories increases. In all conditions, these deviations are significant.

Next, we examine the estimates obtained for the mixed population model. Again, for the sake of simplicity, Figures 4.11 and 4.12 only depict the deviations for the path coefficients, $\beta(= 0.6)$ and $\gamma_2(= 0)$, for the factor loading $\lambda_{y_{22}}(= 0.7)$ and for the weight $w_{y_{12}}(= 0.5)$ of the model with two composites and one common factor. An asterisk above a bar signalizes a significant difference between the average parameter estimate and its population value on a 5% level.
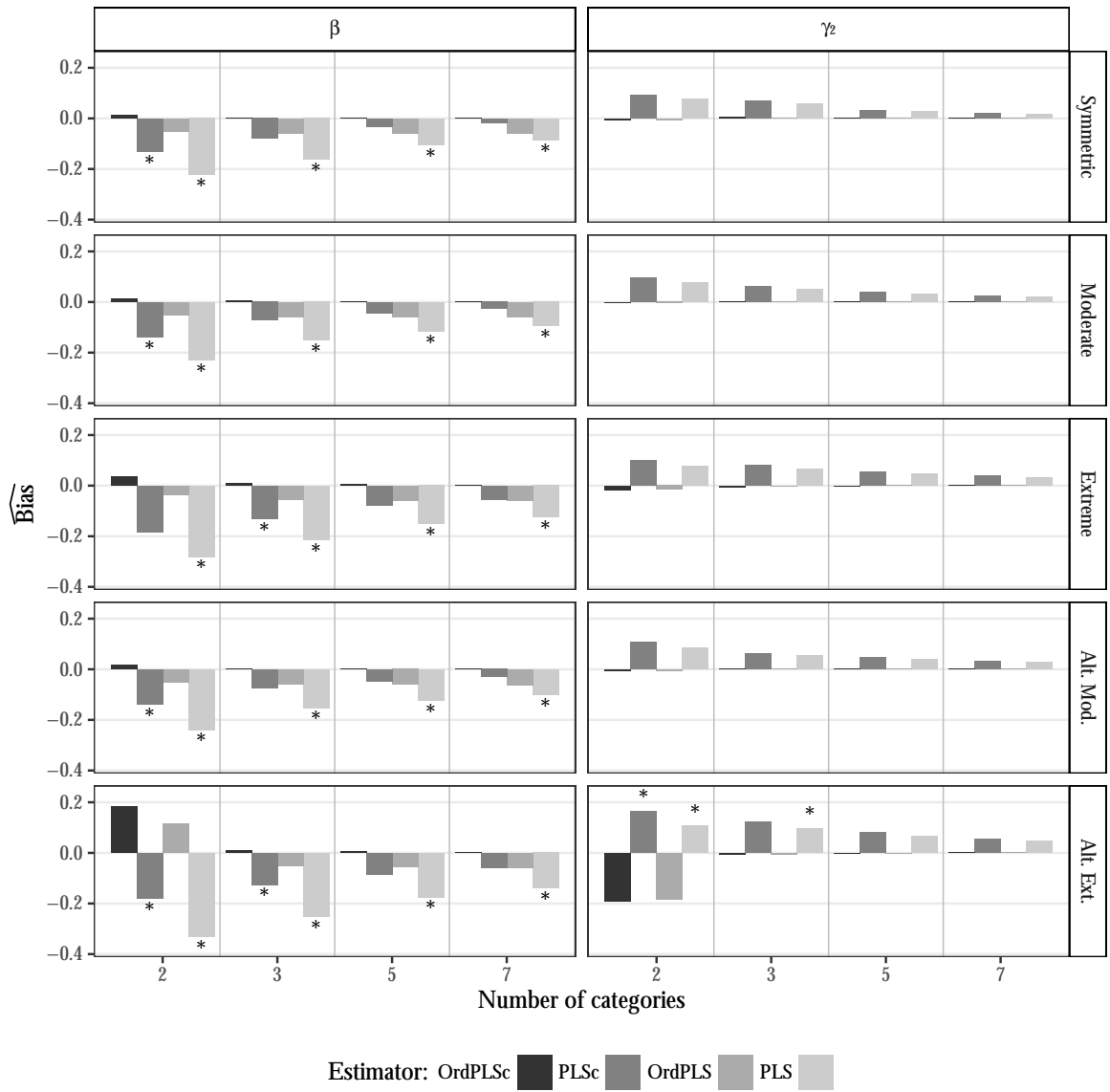
*: significant on a 5% level

Figure 4.11: Mixed model: average deviations from β and γ_2
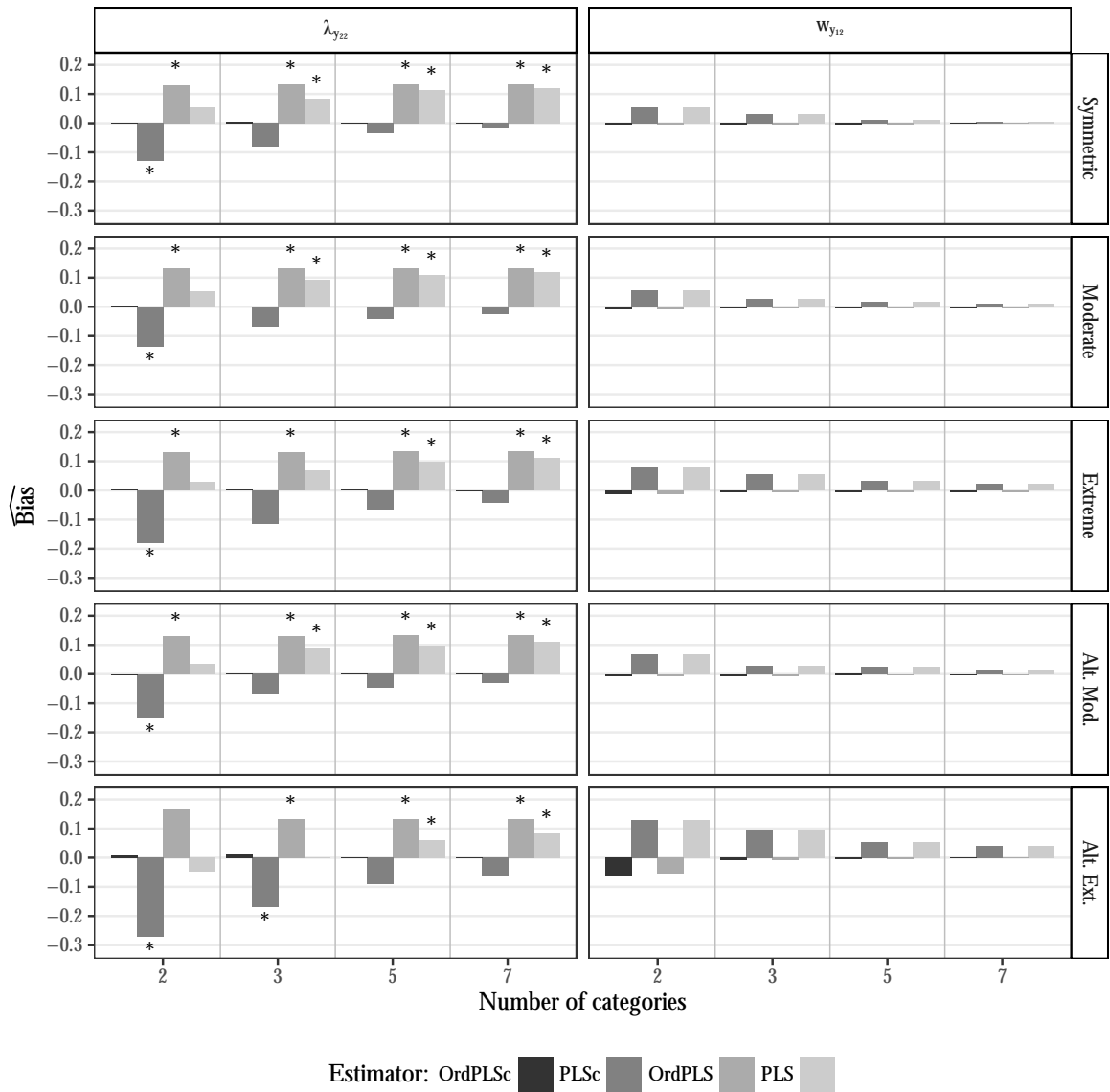
*: significant on a 5% level

Figure 4.12: Mixed model: average deviations from $\lambda_{y_{22}}$ and $w_{y_{12}}$

The OrdPLSc parameter means, again, show virtually no deviation from the population values. However, in case of an alternating extreme asymmetric threshold parameter distribution with two categories, a significant deviation of the average estimated path coefficient from its true value is observed.

OrdPLS leads to very similar results compared to OrdPLSc for estimates affected only by composites ($\hat{\gamma}_1$ and estimated weights). The estimated zero-path $\hat{\gamma}_2$ is after averaging very close to zero, while the mean of the path coefficient estimate for β, which is only affected by one common factor, constantly deviates from its population value. However, the difference is not significant. Factor loadings are again significantly overestimated on average under almost every threshold parameter distributions. The

deviation is neither affected by the number of categories nor by the threshold parameter distribution.

In contrast, for path coefficient β, average PLSc estimates differ significantly from the population value. However, the deviations become insignificant in case of more than two categories. For γ_2, the average PLSc estimates deviate from the population value, but this difference is only significant in case of two categories and alternating extremely asymmetrically distributed threshold parameters. In general, deviations of the factor loading estimates from the true parameters show a very similar behavior as those seen in the model with only common factors: factor loadings are underestimated on average. However, the difference is almost only significant in case of two categories. The weight means are not statistically different from their population values. All deviations decrease and average PLSc estimates converge to the average OrdPLSc estimates as the number of categories increases.

PLS produces almost the same parameter means for path coefficient γ_1 and weights as PLSc. The means of the other path coefficients differ significantly from their population counterparts under all conditions. While this difference decreases with an increasing number of categories, the deviations of factor loading means become even larger for an increasing number of categories. Again, average PLS factor loading estimates tend to converge to OrdPLS average factor loading estimates.

4.7.2 Efficiency

Apart from parameter recovery, an estimator's efficiency is of interest to assess its quality. Therefore, we evaluate the standard deviations of the standardized path coefficient, loading, and weight estimates. In general, all standard deviations decrease with an increasing number of categories but increase for more asymmetric threshold parameter distributions.

Considering the pure common factor model, WLSMV is always more efficient than OrdPLSc. Since comparing estimators' efficiency is only meaningful for unbiased or consistent estimators, the other results for the pure common factor model are not evaluated.

Also, the estimates for the composite model become more efficient with an increasing number of categories. For estimated parameters between composites only, PLS and PLSc as well as OrdPLS and OrdPLSc produce almost the same standard er-

rors. Estimated parameters connected with at least one common factor show larger standard deviations for OrdPLSc than for OrdPLS. In most cases, path coefficient and weight estimates are less efficient for OrdPLS than PLS, while factor loadings are more efficiently estimated by OrdPLS.

4.7.3 Inadmissible solutions

We finish the results part by comparing the inadmissible solutions. Inadmissible solutions are results with absolute factor loadings greater than one, construct correlation matrix that are not positive semi-definite, or results where the estimation algorithm does not converge. Figure 4.13 depicts the relative frequencies of inadmissible results.
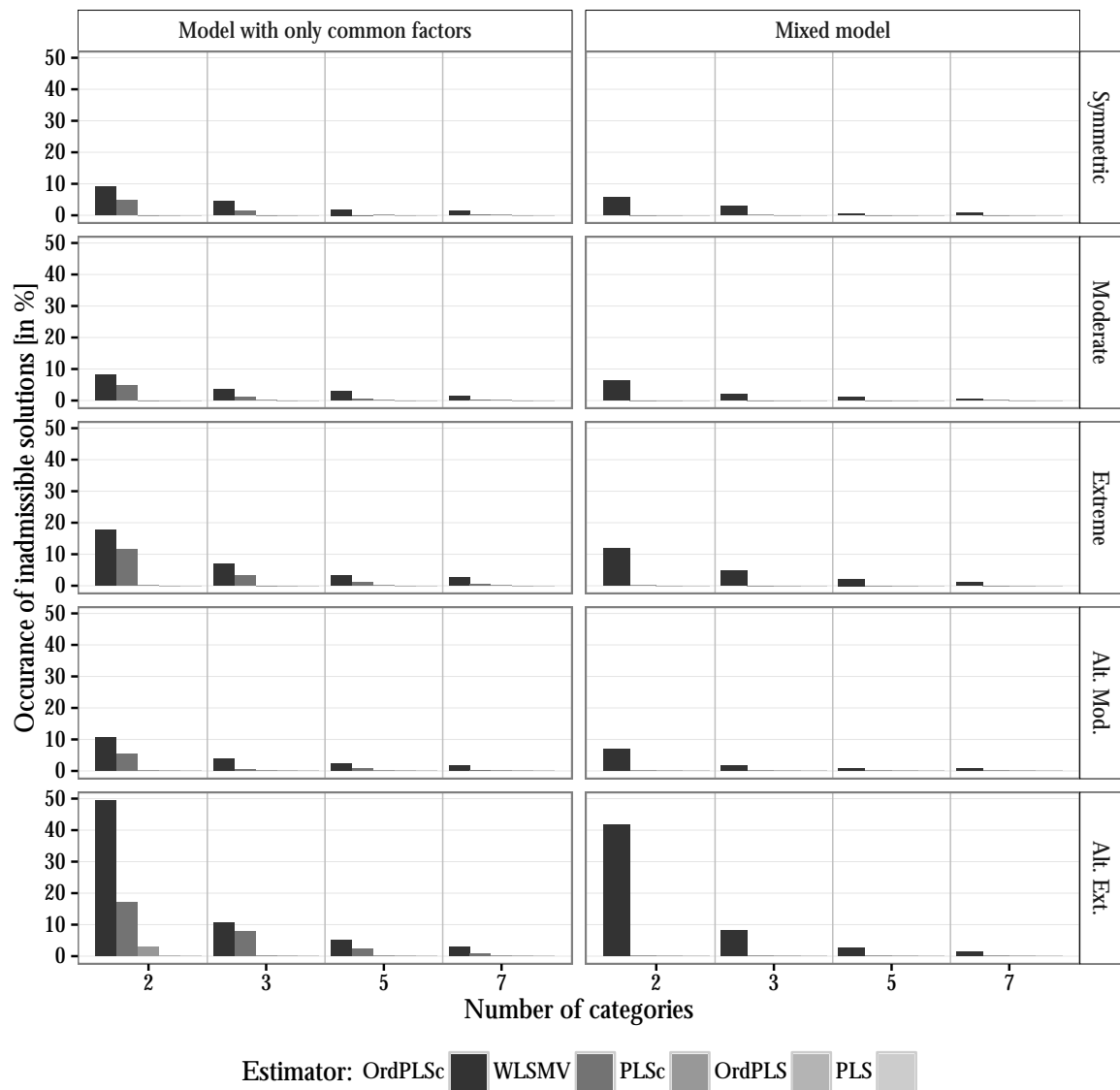
Figure 4.13: Inadmissible solutions

PLS, OrdPLS, and PLSc produce almost no inadmissible solutions for both kind of models. In contrast, OrdPLSc and WLSMV produce a few inadmissible solutions under every condition. The total number of inadmissible results increases for more skewed distributed indicators. The most inadmissible results are produced for alternating extremely asymmetrically distributed threshold parameters.

A similar pattern is observed for inadmissible results during the bootstrap procedure. PLS and OrdPLS, again, produce no improper solutions. In general, the number of inadmissible results during the bootstrap procedure increases for PLSc with an increasing number of categories, while it decreases for OrdPLSc and WLSMV.

4.8   Assessing the results of OrdPLSc

The main focus of this section is the assessment of the OrdPLSc results. In the following, we give a brief overview of approaches commonly followed in PLS and PLSc, which can be also used to assess the results obtained from OrdPLSc. Furthermore, we present approaches for the model evaluation in the case of ordinal categorical indicators.

4.8.1   Overall model evaluation

Statistical tests for the evaluation of the overall-model fit were not available for a long time in case of PLS. Most recently, a bootstrap-based test was developed for PLSc (Dijkstra and Henseler, 2015a). It is a combination of a bootstrap-based test about the model implied covariance matrix (Beran and Srivastava, 1985; Bollen and Stine, 1992) and PLSc. In the context of OrdPLSc, this approach is under development and the object of future research.[20] Nevertheless, the standardized root mean square residual (SRMR) (Hu and Bentler, 1999) can be used as a measure of model fit. It captures the sum of the squared differences between the empirical and the model-implied correlation matrix. Hence, the smaller the SRMR, the better the model fit. Furthermore, as PLS was developed as prediction method (Wold, 1982a), models estimated by PLS should be compared with regard to their predictive power (Shmueli et al., 2016).[21]

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[20]Applying simply the transformation proposed by Beran and Srivastava (1985) is not recommended since the transformation of the qualitative categorical indicators is not clear.

[21]We will investigate the predictive power of OrdPLSc and compare it to other approaches that can deal with ordinal categorical indicators in a future study.

4.8.2 Measurement model

In the following, we focus on criteria to assess convergent validity, discriminant validity, and internal consistency in the case of OrdPLSc.

Convergent validity

Convergent validity refers to the extent to which the reflective indicators connected to one construct are in fact related. A typically used measure for convergent validity is the average variance extracted (AVE) (Fornell and Larcker, 1981; Fornell and Cha, 1994; Farrell, 2010), which can be appropriately used in the context of OrdPLSc.

Discriminant validity

Discriminant validity refers to the extent to which a given construct differs in fact from the other constructs in the nomological network. It can be examined for OrdPLSc in the same manner as for PLSc, and it is usually assessed by the Fornell-Larcker criterion (Fornell and Larcker, 1981). In addition, in PLSc, the heterotrait-monotrait ratio of common factor correlations (HTMT) (Henseler et al., 2015) and the cross-loadings are used to investigate whether different common factors are also statistically different. Since all approaches mentioned are based on the factor loading estimates or the indicator correlation matrix, it is straightforward to use them in the context of OrdPLSc.

Internal consistency

Internal consistency relates to the correlations among the indicators of one block and reflects the reliability of the measurement model. To evaluate internal consistency for a block of indicators belonging to one construct modeled as common factor,[22] the use of the reliability measure ρ_A is recommended (Dijkstra and Henseler, 2015b; Henseler et al., 2016a). Furthermore, measures of composite reliability like Dillon-Goldstein's ρ (also known as Jöreskog ρ_c) (Chin, 1998) or Cronbach's α are usually considered. Since all these measures are based on the estimated factor loadings or the indicator

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[22]For constructs modeled as composites the assessment of internal consistency is meaningless since composites are by assumption fully reliable.

correlations, they can also be used in the context of OrdPLSc.[23]

In general, it is noted that measures used in the context of OrdPLSc refers to the underlying continuous latent variables $\boldsymbol{x}_j^*$ instead of referring to the ordinal categorical indicators $\boldsymbol{x}_j$ themselves.

4.8.3 Structural model

Since OrdPLSc is also based on OLS, the coefficient of determination R^2 of the endogenous constructs can be used to assess the structural model. It measures how well the explanatory constructs explain an endogenous construct.

4.9 An empirical example: customer satisfaction

Traditional PLS has been successfully applied to models aiming at measuring customer satisfaction: first at a national level (Fornell et al., 1996; Fornell, 1992), and later, also in a business context (Johnson et al., 2001). We replicate the study conducted by Bayol et al. (2000) and Tenenhaus et al. (2005) on customer satisfaction in the mobile phone industry to empirically investigate the performance of OrdPLSc in the presence of ordinal data collected through questionnaires with a large number of categories.[24]. Furthermore, we compare the results of OrdPLSc to those of PLS, PLSc, and OrdPLS.

The assumed underlying customer satisfaction model refers to a version of the European Customer Satisfaction Index (ECSI) with one exogenous and six endogenous constructs all modeled as common factors, see Figure 4.14 for a depiction of the structural model. The data set consists of 250 observations on 24 ordinal categorical indicators with 10 categories each: five measures of *Image* (IMG), three measures of *Customers Expectations* (EXP), seven measures of *Perceived Quality* (QUA), two measures of *Perceived Value* (VAL), three measures of *Customer Satisfaction* (SAT), one measure of *Complaints* (COM) and three measures of *Loyalty* (LOY). For more details on the questionnaire, see Tenenhaus et al. (2005).

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[23]The idea to calculate a Cronbach's α using the polychoric correlation is already known and denoted by the ordinal alpha (Zumbo et al., 2007). Ordinal alpha avoids the negative bias of Cronbach's α in the case of ordinal categorical indicators.

[24]The data set is public available, e.g., from the R package *plspm* (Sanchez et al., 2015).
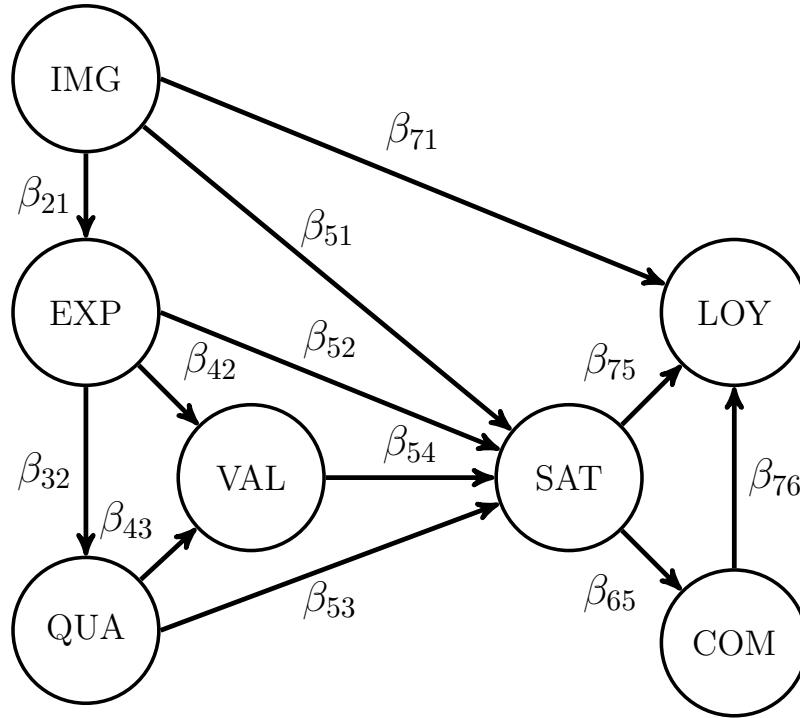
Figure 4.14: Path diagram of the mobile phone industry customer satisfaction model

The estimation of the model is conducted in R (R Core Team, 2016) using the package *matrixpls* (Rönkkö, 2016).[25] For the estimation, we use the *centroid scheme* for inner weighting, *mode A* for outer estimation, and the algorithm proposed by Wold (1982b) to obtain the final weights. To obtain the polychoric correlation for OrdPLS and OrdPLSc, we use a modified version[26] of the *polychoric* function of the *psych* package (Revelle, 2016). Moreover, we use the NONE approach in the case of non-occupied cells, which is recommended for indicators with more than two categories (Savalei, 2011). For the calculation of the construct scores, we use user-written functions, which are provided upon request. In the bootstrap procedures, improper solutions are discarded.

Since the SRMR is below the recommended cut-off value of 0.08 (Hu and Bentler, 1998) with regard to OrdPLSc, overall-model fit is established and we proceed with considering the parameter estimates.[27] In Table 4.1, we provide the path coefficient estimates of the mobile phone customer satisfaction model for PLS, PLSc, OrdPLS, and OrdPLSc.

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[25]As *matrixpls* is still under development, we cross-validate the results for PLS and PLSc with ADANCO (Henseler and Dijkstra, 2015).

[26]The original *polychoric* function does not allow for the calculation of the polychoric correlation between indicators with more than eight categories.

[27]It is mentioned that goodness of fit measures like the SRMR should be regarded with caution. A test for the overall model fit is not developed yet for OrdPLSc.

Table 4.1: Path coefficient estimates of the mobile phone customer satisfaction model

	PLS	CI^a		PLSc	CI^b		OrdPLS	CI^a		OrdPLSc	CI^c	
β_{21}	**0.493**	0.379	0.610	**0.887**	0.646	0.940	**0.584**	0.474	0.669	**0.902**	0.740	0.963
β_{51}	**0.153**	0.060	0.262	0.109	-0.431	0.968	**0.199**	0.087	0.318	0.284	-0.130	1.127
β_{71}	**0.212**	0.068	0.362	0.044	-0.590	0.483	**0.261**	0.112	0.404	0.012	-0.680	0.695
β_{32}	**0.545**	0.441	0.653	**0.892**	0.675	0.950	**0.612**	0.507	0.697	**0.880**	0.736	0.959
β_{42}	0.066	-0.095	0.243	0.026	-0.644	0.795	0.037	-0.105	0.210	-0.115	-0.762	0.749
β_{52}	0.037	-0.050	0.139	-0.124	-0.573	0.505	0.035	-0.067	0.134	-0.120	-0.687	0.412
β_{43}	**0.540**	0.357	0.706	0.655	-0.093	1.236	**0.596**	0.416	0.746	0.801	-0.053	1.403
β_{53}	**0.544**	0.408	0.651	**0.833**	0.094	1.264	**0.517**	0.399	0.645	0.669	-0.023	1.042
β_{54}	**0.200**	0.081	0.317	0.191	-0.116	0.358	**0.198**	0.091	0.308	0.177	-0.028	0.306
β_{65}	**0.540**	0.424	0.643	**0.609**	0.483	0.703	**0.563**	0.454	0.657	**0.624**	0.509	0.722
β_{75}	**0.465**	0.290	0.617	**0.867**	0.346	1.472	**0.493**	0.331	0.651	**0.917**	0.226	1.540
β_{76}	0.050	-0.061	0.179	-0.068	-0.221	0.076	0.043	-0.075	0.156	-0.065	-0.178	0.104

Bold printed values are the coefficient estimates whose corresponding CI does not cover the zero.
Percentile confidence intervals are calculated at a 95% confidence level.
^{a} based on 500 bootstrap samples. ^{b} based on 317 bootstrap samples.
^{c} based on 270 bootstrap samples.

The results show that OrdPLSc produces significant path coefficient estimates for β_{21}, β_{32}, β_{65}, and β_{75}, while the other approaches produce a larger number of significant path coefficient estimates. Under the approaches considered, PLS and OrdPLS yield the most path coefficients that are significantly different from zero. Comparing the magnitude of the significant estimates, the consistent versions of PLS and OrdPLS lead to larger absolute path coefficient estimates. However, the path coefficient estimates for PLS and OrdPLS are known to be inconsistent for common factor models (Schneeweiss, 1993; Schuberth et al., 2016). Therefore, it is recommended to rely on the OrdPLSc estimates since they have been corrected for attenuation and take the scale of the ordinal indicators into account. Moreover, estimates obtained from PLS and OrdPLS as well as PLSc and OrdPLSc are quite similar for most path coefficients. Such a result is expected since the discrepancy between the polychoric and the BP correlation is reduced by the large number of categories per indicator (here: 10).

As all constructs are modeled as common factors, estimated factor loadings $\hat{\boldsymbol{\lambda}}_j$ instead of weights are of main interest in the measurement model. Considering the factor loadings (see Table 4.2), PLS and OrdPLS mostly produce larger estimates than their consistent counterparts. Moreover, all factor loading estimates are significantly different from zero, except the factor loading of indicator loy2, which is not significant for OrdPLSc, OrdPLS, and PLSc. The factor loading estimates of PLS and OrdPLS as well as of PLSc and OrdPLSc are not comparable, since we report the standardized estimates of OrdPLS and OrdPLSc and the non-standardized factor loadings of PLS

and PLSc[28]. The difference in the magnitude of PLS and PLSc as well as OrdPLS and OrdPLSc factor loading estimates is not surprising as PLS as well as OrdPLS estimates suffers from attenuation in the case of a common factor model. The consistent versions controlling for the attenuation bias lead, in general, to smaller factor loading estimates.

Table 4.2: Factor loading and confidence interval estimates

	PLS	CI[a]		PLSc	CI[b]		OrdPLS	CI[a]		OrdPLSc	CI[c]	
ima1	**1.216**	0.931	1.462	**1.036**	0.814	1.251	**0.764**	0.690	0.818	**0.662**	0.555	0.760
ima2	**0.953**	0.665	1.209	**0.905**	0.649	1.169	**0.648**	0.525	0.734	**0.592**	0.471	0.691
ima3	**1.399**	1.015	1.698	**0.975**	0.653	1.256	**0.602**	0.463	0.695	**0.483**	0.318	0.610
ima4	**1.455**	1.203	1.669	**1.262**	0.989	1.483	**0.799**	0.729	0.854	**0.720**	0.604	0.818
ima5	**1.085**	0.854	1.359	**1.028**	0.821	1.232	**0.780**	0.724	0.826	**0.710**	0.623	0.791
exp1	**1.111**	0.808	1.367	**0.809**	0.562	1.106	**0.780**	0.654	0.848	**0.556**	0.426	0.686
exp2	**1.153**	0.724	1.547	**0.786**	0.518	1.198	**0.743**	0.589	0.832	**0.539**	0.391	0.707
exp3	**1.523**	1.022	1.931	**0.885**	0.585	1.242	**0.623**	0.476	0.738	**0.479**	0.360	0.620
qua1	**1.104**	0.916	1.281	**1.147**	0.969	1.337	**0.828**	0.779	0.875	**0.835**	0.761	0.895
qua2	**1.228**	0.929	1.529	**0.997**	0.751	1.306	**0.647**	0.531	0.737	**0.553**	0.447	0.683
qua3	**1.456**	1.199	1.685	**1.373**	1.131	1.564	**0.801**	0.747	0.852	**0.769**	0.679	0.849
qua4	**1.253**	1.051	1.428	**1.103**	0.894	1.294	**0.809**	0.744	0.871	**0.733**	0.656	0.819
qua5	**1.062**	0.874	1.237	**0.980**	0.777	1.142	**0.782**	0.718	0.837	**0.720**	0.616	0.821
qua6	**1.246**	1.069	1.402	**1.109**	0.940	1.294	**0.826**	0.752	0.889	**0.758**	0.684	0.849
qua7	**1.477**	1.252	1.738	**1.502**	1.276	1.732	**0.799**	0.735	0.849	**0.822**	0.758	0.891
val1	**2.032**	1.823	2.226	**1.646**	1.412	1.950	**0.914**	0.869	0.944	**0.771**	0.674	0.864
val2	**1.674**	1.413	1.907	**1.704**	1.504	1.965	**0.943**	0.925	0.958	**0.943**	0.881	0.996
sat1	**0.875**	0.715	1.031	**0.854**	0.694	0.981	**0.825**	0.768	0.870	**0.734**	0.644	0.813
sat2	**1.536**	1.329	1.751	**1.247**	1.035	1.445	**0.858**	0.814	0.893	**0.724**	0.656	0.802
sat3	**1.543**	1.319	1.774	**1.422**	1.246	1.653	**0.867**	0.830	0.901	**0.834**	0.780	0.910
loy1	**2.268**	1.936	2.538	**1.559**	1.257	2.002	**0.849**	0.766	0.903	**0.641**	0.524	0.739
loy2	**0.775**	0.037	1.396	0.513	-0.065	0.867	0.193	-0.056	0.393	0.163	-0.013	0.274
loy3	**1.923**	1.611	2.205	**1.893**	1.704	2.205	**0.924**	0.898	0.942	**0.903**	0.856	0.989

Bold printed values are the coefficient estimates where the corresponding CI does not cover the zero.
Percentile confidence intervals are calculated on a 95% confidence level.
[a] based on 500 bootstrap samples.   [b] based on 317 bootstrap samples.
[c] based on 270 bootstrap samples.

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[28]Non-standardized factor loading estimates are easier to interpret. For standardized factor loading estimates, we refer to Table 4.18 in the Appendix.

In the following, we investigate the convergent validity. On the main diagonals in the Tables 4.3a to 4.3d, we provide the AVEs that are commonly used to assess convergent validity.

Table 4.3: Average variance extracted and shared variance estimates

(a) PLS

	IMA	EXP	QUA	VAL	SAT	LOY
IMA	**0.476**	0.243	0.535	0.258	0.450	0.300
EXP	0.493	**0.471**	0.297	0.130	0.231	0.134
QUA	0.731	0.545	**0.574**	0.332	0.626	0.275
VAL	0.508	0.360	0.576	**0.850**	0.365	0.267
SAT	0.671	0.481	0.791	0.604	**0.683**	0.403
LOY	0.548	0.366	0.524	0.517	0.635	**0.520**

(b) PLSc

	IMA	EXP	QUA	VAL	SAT	LOY
IMA	**0.356**	0.786	0.835	0.433	0.786	0.600
EXP	0.887	**0.207**	0.796	0.373	0.693	0.460
QUA	0.914	0.892	**0.505**	0.460	0.906	0.455
VAL	0.658	0.611	0.679	**0.715**	0.567	0.475
SAT	0.886	0.833	0.952	0.753	**0.549**	0.747
LOY	0.775	0.678	0.674	0.689	0.864	**0.370**

(c) OrdPLS

	IMA	EXP	QUA	VAL	SAT	LOY
IMA	**0.522**	0.342	0.636	0.309	0.550	0.421
EXP	0.584	**0.517**	0.375	0.161	0.300	0.218
QUA	0.797	0.612	**0.619**	0.383	0.672	0.371
VAL	0.556	0.402	0.619	**0.862**	0.413	0.359
SAT	0.742	0.547	0.820	0.643	**0.723**	0.505
LOY	0.649	0.467	0.609	0.600	0.711	**0.537**

(d) OrdPLSc

	IMA	EXP	QUA	VAL	SAT	LOY
IMA	**0.409**	0.814	0.898	0.455	0.863	0.681
EXP	0.902	**0.276**	0.775	0.348	0.688	0.516
QUA	0.947	0.880	**0.557**	0.489	0.914	0.520
VAL	0.675	0.590	0.699	**0.742**	0.586	0.526
SAT	0.929	0.830	0.956	0.766	**0.586**	0.787
LOY	0.825	0.718	0.721	0.725	0.887	**0.417**

Correlations are below the diagonal, squared correlations are above the diagonal, and AVE estimates are presented on the diagonal (in boldface).

It is obvious that OrdPLS and PLS as well as OrdPLSc and PLSc lead to similar results, which is expected as the AVEs are based on the standardized factor loading estimates that only slightly differ because of the large number of categories per indicator (see Table 4.18). It is noteworthy that the AVEs obtained from PLS and OrdPLS estimates are not trustworthy if the common factor model holds, since the factor loading estimates are biased. Since only the AVEs for the constructs QUA, VAL, and SAT are larger than the recommended threshold of 0.5 (Fornell and Larcker, 1981) using OrdPLSc, convergent validity cannot be established for the remaining common factors.

To assess discriminant validity, we first consider the standardized cross-factor loadings, see the Table 4.19 to 4.22 in the Appendix. For PLS and OrdPLS, all factor loading estimates are larger than the estimated cross-loadings, which leads to the belief that discriminant validity is achieved. In contrast, OrdPLSc as well as PLSc lead to a different conclusion. In almost every block, there is at least one indicator where a cross-loading exceeds the corresponding factor loading, except for the construct VAL. This finding is supported by the Fornell-Larcker criterion. Using PLS and OrdPLS estimates respectively, the Fornell-Larcker criterion indicates that discriminant validity is established for all constructs except for IMG and QUA. While the Fornell-Larcker

criterion based on the PLSc and OrdPLSc estimates shows that discriminant validity can be established only for the construct VAL. Following Henseler et al. (2015), we recommend a cautious interpretation of the Fornell-Larcker criterion when it is based on PLS or OrdPLS factor loading estimates, as these are known to be upward-biased.

Moreover, the HTMT further supports the suspicion that some indicators are incorrectly assigned. The lower triangular of Table 4.4 represents the results based on the BP correlations, while the upper triangular contains the results based on the polychoric correlations. Since the HTMT is solely based on indicator correlations, it leads to the same results for PLS and PLSc as well as for OrdPLS and OrdPLSc.

Table 4.4: HTMT results for PLS(c) and OrdPLS(c)

	IMA	EXP	QUA	VAL	SAT	LOY
IMA		0.917	0.949	**0.681**	0.929	0.943
EXP	**0.888**		0.888	**0.602**	0.843	0.824
QUA	0.929	**0.878**		**0.699**	0.958	0.802
VAL	**0.652**	**0.589**	**0.673**		0.765	0.865
SAT	0.910	**0.865**	0.954	**0.741**		1.001
LOY	**0.867**	**0.770**	**0.723**	**0.797**	0.957	

The HTMT based on the polychoric correlation indicates that the constructs IMA and EXP, IMA and QUA, IMA and SAT, IMA and LOY, QUAL and SAT, and SAT and LOY cannot be adequately distinguished since it is above the recommended threshold of 0.9 (Gold et al., 2001).[29] The use of the HTMT based on the BP correlation in case of ordinal categorical indicators is not recommended because it does not take into account the qualitative character of the indicators. For a tutorial on how to proceed if the discriminant validity is not satisfied, see Farrell (2010) and Henseler et al. (2015).

Furthermore, we assess internal consistency. In doing so, we consider Cronbach's alpha and ordinal alpha respectively, which are lower-bound estimates for the reliability. Moreover, we refer to Dijkstra & Henseler's ρ_A and Dillon-Goldstein's ρ_c in order to examine the internal consistency. Tables 4.5c to 4.5a provide the results of the three measures for the various PLS approaches.

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[29]Furthermore, the HTMT correlation can be used in a bootstrap procedure that allows for the construction of confidence intervals (Henseler et al., 2015), which is not done here.

Table 4.5: Internal consistency reliability

(a) Cronbach's α and ordinal alpha

	Cronbach's α	ordinal alpha
IMA	**0.723**	**0.768**
EXP	0.452	0.526
QUA	**0.877**	**0.896**
VAL	**0.824**	**0.842**
SAT	**0.779**	**0.809**
LOY	0.472	0.497

(b) Dijkstra-Henseler's ρ_A

	PLS(c)	OrdPLS(c)
IMA	**0.728**	**0.784**
EXP	0.425	0.536
QUA	**0.879**	**0.903**
VAL	**0.820**	**0.866**
SAT	**0.786**	**0.813**
LOY	0.687	**0.789**

(c) Dillon-Goldstein's ρ_c

	PLS	PLSc	OrdPLS	OrdPLSc
IMA	**0.818**	**0.731**	**0.844**	**0.772**
EXP	**0.727**	0.437	**0.761**	0.533
QUA	**0.904**	**0.876**	**0.919**	**0.897**
VAL	**0.919**	**0.832**	**0.926**	**0.850**
SAT	**0.865**	**0.784**	**0.887**	**0.809**
LOY	**0.735**	0.582	**0.736**	0.625

Results for COM are not reported, as it is measured by only one indicator.

The results for Dillon-Goldstein's ρ_c (Table 4.5c) for PLS and OrdPLS as well as their consistent version are again very similar, which can, again, be explained by the large number of indicators categories. Although the results for PLS and OrdPLS are more desirable, it is recommended to employ them with caution as they are based on attenuated factor loading estimates (Zumbo et al., 2007). Comparing the values of Dillon-Goldstein's ρ_c for OrdPLSc with the recommended threshold of 0.7 (Henseler et al., 2016a), we conclude that construct scores are reliable except for the constructs EXP and LOY. This conclusion is fully supported by Cronbach's α and by ordinal alpha (see Table 4.5a). However, it is well-known that the use of Cronbach's α should be done with circumspection as it can only be appropriately interpreted if the assumption of tau-equivalence holds. If this assumption is violated, Cronbach's α underestimates the reliability (Raykov, 2004). Moreover, drawing conclusion from Cronbach's α in the case of ordinal categorical indicators is not recommended (Zumbo et al., 2007), as it is based on the BP correlation.

Finally, we consider Dijkstra-Henseler's ρ_A (Table 4.5b), which also largely supports our conclusion since most reliability estimates exceed the threshold of 0.7, except for EXP. Even though Dijkstra-Henseler's ρ_A is quite similar for PLS and OrdPLS as well

as for PLSc and OrdPLSc in our example, ρ_A based on the BP correlation should be used cautiously in the context of ordinal categorical indicators as it does not take into account the qualitative scale of the indicators. Again, due to the large number of categories, ρ_A leads to quite similar results for PLS and OrdPLS as well as for PLSc and OrdPLSc.

Besides studying the significance levels of the path coefficients, it is a common practice to consider the coefficient of determination R^2 of the endogenous constructs (Table 4.6) to investigate the structural model.

Table 4.6: R^2 of the endogenous constructs

	PLS	PLSc	OrdPLS	OrdPLSc
IMA	0.000	0.000	0.000	0.000
EXP	0.243	0.786	0.342	0.814
QUA	0.297	0.796	0.374	0.773
VAL	0.335	0.461	0.384	0.490
SAT	0.672	0.931	0.719	0.936
COM	0.292	0.371	0.319	0.391
LOY	0.432	0.750	0.538	0.790

Table 4.6 illustrates that the consistent PLS versions result in larger R^2s, which means that more variance of the endogenous construct is explained by the explanatory constructs. The R^2s for OrdPLS and PLS as well as OrdPLSc and PLSc are again quite similar.

Finally, we investigate the construct scores for OrdPLSc. Figure 4.15 shows a comparison of the latent scores calculated with PLS(c) and OrdPLS(c).[30] Construct scores for the construct COM are not reported since it is connected to a single indicator.

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[30]As the weights are the same for PLS and PLSc as well as for OrdPLS and OrdPLSc, we only report the scores of PLS and OrdPLS.
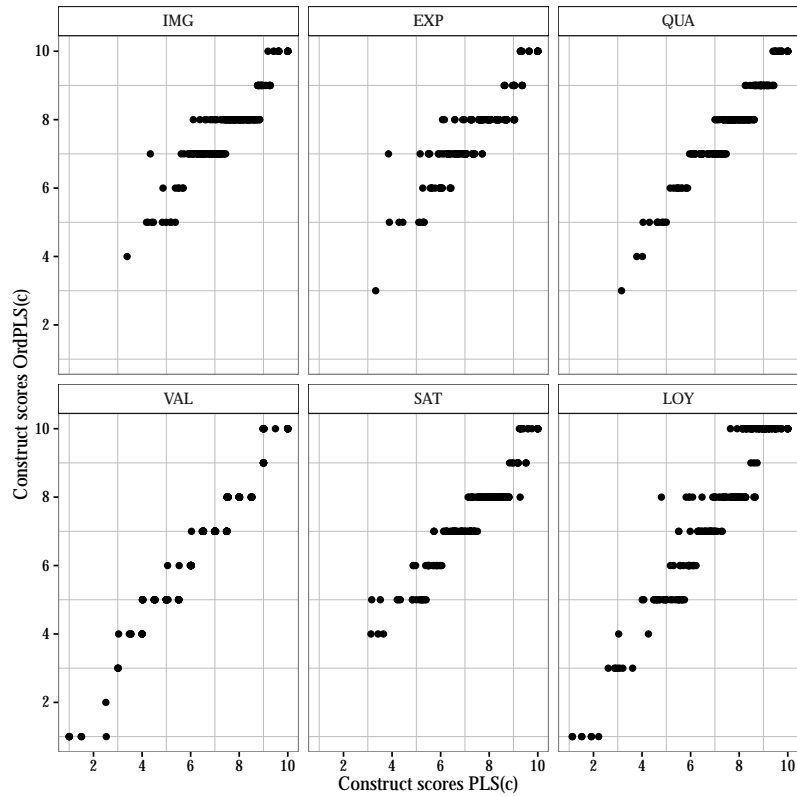
Figure 4.15: Construct scores for PLS(c) and OrdPLS(c) (Mode estimation)

According to the approaches described in Section 4.5, we obtain ordinal construct scores for OrdPLS(c). For PLS(c), we use rounded scores for a better comparison. Table 4.7 shows the degree of coherency between the construct scores obtained from PLS(c) and the three procedures for OrdPLS(c). Using the rounded scores for PLS(c), the percentages of exact concordance are reported in the first three rows, while the remaining rows contain the percentages of concordance with a difference between rounded values not larger than 1. We have at least 70% exact concordance except for the construct LOY. More than 90% of the cases for all constructs show a difference between rounded values lower than 1.

Table 4.7: Coherency of construct scores between PLS(c) and OrdPLS(c)

Method	IMG	EXP	QUA	VAL	SAT	LOY
Mode estimation[a]	70.4	71.2	79.2	84.4	71.6	48.0
Median estimation[a]	75.2	74.8	78.0	88.0	70.4	51.6
Mean estimation[a]	73.2	76.8	75.6	86.8	71.6	49.2
Mode estimation[b]	98.8	98.0	100.0	99.6	99.6	90.8
Median estimation[b]	99.2	98.4	100.0	100.0	99.6	94.0
Mean estimation[b]	99.2	98.4	100.0	99.6	100.0	91.6

[a] Percentages of exact concordance after having rounded PLS scores to integer values.
[b] Percentages of concordance with a difference between rounded values not larger than 1.

4.10 Discussion

The primary goal of our study is to propose a variance-based estimator for structural equation models that is able to consistently estimate models with common factors, composites, and ordinal categorical indicators. We develope OrdPLSc combining the approaches OrdPLS and PLSc, and thus, their favorable characteristics. Furthermore, due to the nature of the ordinal categorical indicators, point estimates of factor scores or composite scores should not be directly calculated from their observations. To overcome this shortcoming first attempts like the *mode estimation*, *median estimation*, or *mean estimation* can be used to obtain construct scores on the indicators scale (Cantaluppi, 2012). However, this issue currently limits the use of OrdPLSc for prediction.

Our Monte Carlo simulation results confirm that OrdPLSc fulfills its intended purpose. For a sample size of 500 observations, almost all OrdPLSc factor loading, weight, as well as path coefficient estimates are virtually unbiased under the conditions considered. As the combination of the polychoric correlation and PLSc leads to larger standard errors of parameter estimates, OrdPLSc produces a few improper solutions in terms of absolute factor loadings larger than 1. The number of inadmissible solutions is mainly driven by the estimates of the largest factor loading $\lambda_{y_{23}}$. However, the number of inadmissible solutions are in an acceptable range except for alternating extremely asymmetrically distributed threshold parameters. Compared to WLSMV, OrdPLSc produces very similar estimates but with larger standard errors and a few more inadmissible solutions. However, OrdPLSc outperforms PLS, OrdPLS, and PLSc in terms of parameter recovery for both models, which makes OrdPLSc the dominant approach under the considered variance-based estimators if ordinal categorical indica-

tors are included in the model. In case of model parameters that are not connected to a common factor, OrdPLSc and OrdPLS as well as PLSc and PLS produce almost the same estimates and standard errors. This is not surprising as no correction for attenuation is needed, which is the only difference between OrdPLSc and OrdPLS as well as between PLSc and PLS.

We investigate the behavior of PLSc, OrdPLS, and PLS in different scenarios using ordinal categorical indicators. Although PLSc uses the BP correlation and, therefore, does not account for the scale of ordinal categorical indicators, it performs surprisingly well in estimating the path coefficient of the model with only common factors in most conditions. This could be due to the use of identical threshold parameters for the indicators, however further research is needed.[31] Furthermore, PLSc behaves as expected and factor loadings are underestimated on average, which becomes more pronounced for more asymmetric threshold parameter distribution. This is due to the downward-bias of the BP correlation. This difference declines as the number of categories increases because the bias of the BP correlation decreases. Therefore, the use of PLSc for models with both common factors and composites is appropriate but only for indicators with a large number of categories.

Moreover, our findings support the results of Cantaluppi (2012), stating that OrdPLS path coefficient estimates are less biased than PLS estimates in the pure common factor model. Although OrdPLS takes account of the scale of ordinal categorical indicators, the problem of attenuation remains unaddressed which is illustrated by underestimated path coefficients and overestimated factor loadings. As this deviation is almost unaffected by the number of categories and the indicators' distribution, OrdPLS estimates seem to be constantly biased. However, OrdPLS consistently estimates the model parameters that are not connected to common factors because no correction for attenuation is needed. Therefore, OrdPLS is an appropriate estimator for models containing only constructs modeled as composites.

Traditional PLS suffers from the following two shortcomings: no correction for attenuation in case of common factors and no accounting for the scale of ordinal categorical indicators. For a small number of categories, the bias of attenuation and the

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[31]Since the BP correlation is about to be proportionally biased (for a certain range of correlations, see Kukuk (1991)), bias cancels out for path coefficients and only affects factor loading and correction factor estimates. Results may change for indicators with a different number of categories and different threshold parameter distribution.

bias of the BP correlation cancel out, which leads to factor loading means close to the population values. When the number of categories increases, the bias of the BP correlation decreases and average PLS factor loading estimates deviate more and more from the population values and converge to the OrdPLS means, which do not suffer from the bias of the BP correlation. Therefore, PLS should be cautiously used for models containing common factors regardless of whether ordinal categorical indicators are included.

Since OrdPLSc uses the polychoric correlation, which assumes normality for the latent variables underlying each ordinal categorical indicator, it cannot be declared as an approach that is free of distributional assumptions anymore. However, the assumption of joint normality of the underlying unobservable variables can be relaxed as the polychoric correlation produces fairly unbiased correlation estimates for elliptically symmetric distributed variables (Kukuk, 1999).

Furthermore, we present the assessment of common factor models with ordinal categorical indicators using OrdPLSc. For this purpose, we use a well-known empirical example from Tenenhaus et al. (2005). The results show that OrdPLS and OrdPLSc as well as PLS and PLSc produce quite similar estimates, which is not surprising as the large number of categories per indicator reduces the discrepancy between the BP and the polychoric correlation. However, in contrast to the original study where traditional PLS was applied, OrdPLSc lead to substantially different results. This is mainly due to the correction for attenuation of the estimates and to the use of validity and reliability measures based on the polychoric correlation. In general, we recommend the usage of OrdPLSc in case of common factor models containing ordinal categorical indicators, in particular, when indicators with a small number of categories are included in the model.

In our simulation study as well as in the empirical example, we only consider situations where all indicators are measured on an ordinal categorical scale. Of course, in practice, continuous indicators are also often part of the model. In such a context, the polyserial correlation can be used to adequately address the issue of ordinal categorical indicators. Hence, future research should investigate the behavior of OrdPLSc for models containing a mixture of both ordinal categorical and continuous indicators. Besides the use of the polyserial correlation as input, we further recommend the investigation of the behavior of OrdPLSc, in particular, for small sample sizes. Furthermore,

out-of-sample prediction plays an increasingly important role in PLS (Shmueli et al., 2016). Thus, the prediction power needs to be investigated for approaches dealing with ordinal categorical indicators, e.g., using k-fold cross-validation.[32] Moreover, we recommend the extension to the polychoric correlation for other variance-based estimators to deal with ordinal categorical indicators, e.g., generalized structural component analysis (Hwang and Takane, 2014). Of particular interest is also their comparison to OrdPLS(c). Finally, tests for overall-model fit in case of ordinal categorical indicators need to be developed.

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[32]This topic is the subject of a current research by Florian Schuberth & Gabriele Cantaluppi.

4.11 Appendix to Chapter 4

Threshold parameter distribution
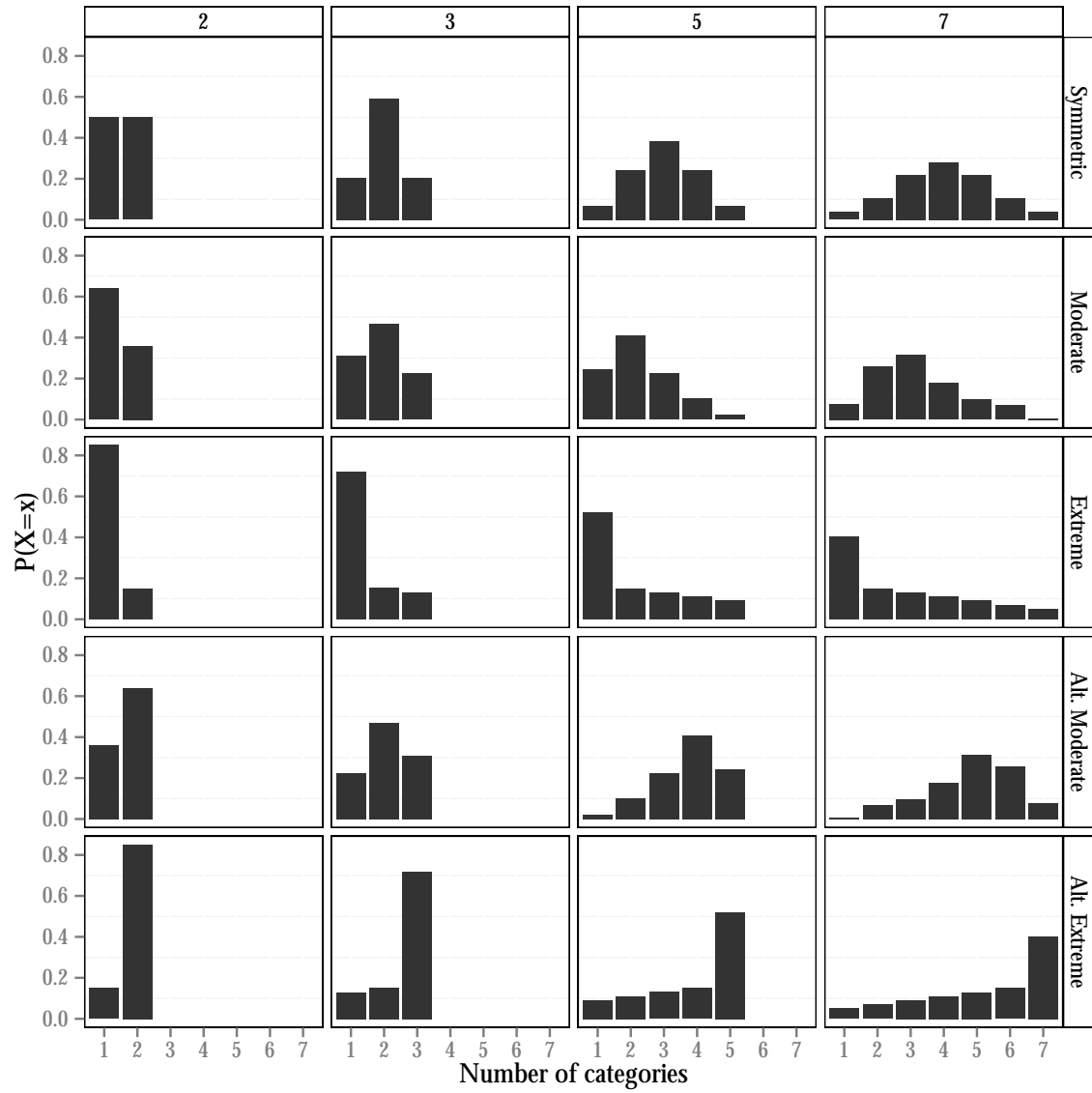
Figure 4.16: Threshold parameter distribution

Results of the Monte Carlo simulation

In the following, the results of the ADD approach for two categories and the results of the NONE approach for more than two categories are presented. These are the results used in the paper. Every second row contains the average standard deviations of the parameter estimates. The last four columns contain the source and the number of inadmissible results

- *Load*: At least one absolute factor loading is larger than 1.

- *CompCor*: Correlation matrix between the composites/common factors is non positive-definite.

- *notc*: Non-convergence of the PLS algorithm.

- *Boot*: Number of inadmissible solutions during the bootstrap procedure.

Table 4.8: Results for the model with three common factors: symmetrically distributed thresholds

Threshold dist.	Estimator	# cat	$\gamma_1=0.6$	$\gamma_2=0.0$	$\beta=0.6$	$\lambda_{x_1}=0.8$	$\lambda_{x_2}=0.7$	$\lambda_{x_3}=0.6$	$\lambda_{y_{11}}=0.7$	$\lambda_{y_{12}}=0.7$	$\lambda_{y_{13}}=0.7$	$\lambda_{y_{21}}=0.5$	$\lambda_{y_{22}}=0.7$	$\lambda_{y_{23}}=0.9$	Load.	CompCor	notc	Boot
Symmetric	PLS	2	0.3549	0.1053	0.3246	0.8005	0.7453	0.6645	0.7420	0.7408	0.7405	0.5784	0.7545	0.8514	0.00	0.00	0.00	0
			0.0395	0.0465	0.0436	0.0332	0.0417	0.0534	0.0348	0.0349	0.0350	0.0649	0.0406	0.0254				
		3	0.3996	0.1013	0.3684	0.8237	0.7720	0.6990	0.7678	0.7680	0.7680	0.6140	0.7829	0.8689	0.00	0.00	0.00	0
			0.0369	0.0451	0.0415	0.0237	0.0311	0.0410	0.0264	0.0264	0.0264	0.0517	0.0299	0.0176				
		5	0.4326	0.0973	0.4007	0.8474	0.7985	0.7259	0.7941	0.7946	0.7940	0.6443	0.8117	0.8898	0.00	0.00	0.00	0
			0.0359	0.0449	0.0409	0.0179	0.0247	0.0343	0.0215	0.0215	0.0215	0.0443	0.0236	0.0126				
		7	0.4415	0.0945	0.4116	0.8550	0.8079	0.7348	0.8025	0.8023	0.8020	0.6532	0.8211	0.8967	0.00	0.00	0.00	0
			0.0355	0.0447	0.0407	0.0164	0.0229	0.0323	0.0202	0.0203	0.0203	0.0424	0.0219	0.0113				
	OrdPLS	2	0.4582	0.0935	0.4251	0.8624	0.8170	0.7428	0.8126	0.8111	0.8111	0.6618	0.8310	0.9037	0.00	0.00	0.00	0
			0.0486	0.0685	0.0618	0.0270	0.0359	0.0487	0.0320	0.0321	0.0322	0.0626	0.0348	0.0195				
		3	0.4553	0.0900	0.4257	0.8635	0.8173	0.7459	0.8116	0.8115	0.8118	0.6619	0.8320	0.9042	0.00	0.00	0.00	0
			0.0412	0.0553	0.0502	0.0209	0.0286	0.0391	0.0255	0.0255	0.0255	0.0509	0.0273	0.0149				
		5	0.4543	0.0920	0.4235	0.8637	0.8170	0.7449	0.8121	0.8123	0.8119	0.6637	0.8319	0.9044	0.00	0.00	0.00	0
			0.0372	0.0484	0.0439	0.0170	0.0239	0.0335	0.0212	0.0212	0.0212	0.0439	0.0227	0.0117				
		7	0.4531	0.0916	0.4240	0.8639	0.8179	0.7451	0.8122	0.8119	0.8117	0.6637	0.8320	0.9045	0.00	0.00	0.00	0
			0.0361	0.0465	0.0422	0.0159	0.0225	0.0319	0.0200	0.0201	0.0201	0.0421	0.0214	0.0109				
	PLSc	2	0.5890	0.0068	0.5809	0.6512	0.5715	0.4844	0.5706	0.5708	0.5695	0.4043	0.5693	0.7417	0.00	0.00	0.00	6887
			0.0667	0.1226	0.1176	0.0668	0.0689	0.0738	0.0550	0.0550	0.0551	0.0788	0.0669	0.0643				
		3	0.6018	-0.0047	0.6045	0.7090	0.6207	0.5324	0.6203	0.6217	0.6198	0.4413	0.6198	0.7976	0.00	0.00	0.00	7525
			0.0549	0.0995	0.0938	0.0566	0.0596	0.0650	0.0466	0.0465	0.0466	0.0697	0.0565	0.0529				
		5	0.6024	0.0002	0.6013	0.7626	0.6669	0.5711	0.6681	0.6693	0.6673	0.4771	0.6663	0.8568	1.00	0.00	0.00	19029
			0.0487	0.0848	0.0792	0.0501	0.0537	0.0601	0.0418	0.0418	0.0418	0.0649	0.0506	0.0448				
		7	0.6012	-0.0008	0.6025	0.7793	0.6831	0.5838	0.6826	0.6826	0.6818	0.4870	0.6808	0.8764	3.00	0.00	0.00	30651
			0.0470	0.0811	0.0755	0.0482	0.0520	0.0586	0.0403	0.0403	0.0403	0.0632	0.0487	0.0421				
	OrdPLSc	2	0.6067	-0.0015	0.6111	0.7935	0.6998	0.5970	0.6992	0.6995	0.6972	0.5032	0.6996	0.8828	99.00	0.00	0.00	199431
			0.0662	0.1339	0.1253	0.0749	0.0810	0.0885	0.0643	0.0644	0.0645	0.0948	0.0776	0.0642				
		3	0.5971	-0.0018	0.6014	0.8006	0.7052	0.6064	0.7032	0.7054	0.7034	0.5079	0.7065	0.8911	48.00	0.00	0.00	83035
			0.0639	0.0997	0.1009	0.0600	0.0689	0.0779	0.0563	0.0558	0.0563	0.0844	0.0679	0.0490				
		5	0.6006	0.0013	0.5998	0.7999	0.7002	0.6007	0.7017	0.7027	0.7010	0.5031	0.7009	0.8948	19.00	0.00	0.00	55107
			0.0561	0.0856	0.0852	0.0518	0.0596	0.0678	0.0478	0.0478	0.0479	0.0741	0.0584	0.0427				
		7	0.5996	0.0001	0.6013	0.7998	0.7012	0.6003	0.7009	0.7013	0.7002	0.5012	0.7002	0.8966	14.00	0.00	0.00	48640
			0.0538	0.0817	0.0811	0.0492	0.0568	0.0650	0.0454	0.0454	0.0454	0.0710	0.0553	0.0406				
	WLSMV	2	0.6061	-0.0017	0.6069	0.7965	0.7024	0.5990	0.7031	0.7002	0.6998	0.5035	0.7042	0.8915	49.00	0.00	0.00	50.00
			0.0652	0.1177	0.1114	0.0578	0.0582	0.0607	0.0531	0.0532	0.0533	0.0622	0.0563	0.0575				
		3	0.6045	-0.0061	0.6074	0.7990	0.7018	0.6019	0.7001	0.7005	0.7001	0.5006	0.7011	0.8974	15.00	0.00	0.00	15.00
			0.0542	0.0944	0.0889	0.0459	0.0469	0.0494	0.0430	0.0429	0.0429	0.0516	0.0455	0.0458				
		5	0.6039	-0.0009	0.6025	0.7985	0.7005	0.5999	0.7006	0.7013	0.7000	0.5014	0.6996	0.8986	0.00	0.00	0.00	0.00
			0.0474	0.0808	0.0753	0.0373	0.0388	0.0420	0.0356	0.0357	0.0357	0.0442	0.0374	0.0363				
		7	0.6025	-0.0014	0.6033	0.7987	0.7019	0.6001	0.7005	0.7003	0.6996	0.5011	0.6995	0.8987	1.00	0.00	0.00	1.00
			0.0453	0.0765	0.0712	0.0346	0.0363	0.0396	0.0336	0.0336	0.0336	0.0420	0.0350	0.0335				

Table 4.9: Results for the model with three common factors: moderately asymmetrically distributed thresholds

Threshold dist.	Estimator	# cat	$\gamma_1=0.6$	$\gamma_2=0.0$	$\beta=0.6$	$\lambda_{x_1}=0.8$	$\lambda_{x_2}=0.7$	$\lambda_{x_3}=0.6$	$\lambda_{y_{11}}=0.7$	$\lambda_{y_{12}}=0.7$	$\lambda_{y_{13}}=0.7$	$\lambda_{y_{21}}=0.5$	$\lambda_{y_{22}}=0.7$	$\lambda_{y_{23}}=0.9$	Load.	CompCor	notc	Boot
Moderate	PLS	2	0.3463	0.1035	0.3186	0.7964	0.7424	0.6613	0.7380	0.7370	0.7356	0.5733	0.7518	0.8490	0.00	0.00	0.00	0
			0.0409	0.0476	0.0449	0.0358	0.0446	0.0567	0.0374	0.0375	0.0377	0.0686	0.0434	0.0273				
		3	0.4051	0.1013	0.3734	0.8299	0.7786	0.7042	0.7743	0.7755	0.7751	0.6209	0.7906	0.8754	0.00	0.00	0.00	0
			0.0370	0.0453	0.0418	0.0223	0.0298	0.0399	0.0254	0.0252	0.0253	0.0504	0.0286	0.0162				
		5	0.4238	0.0966	0.3950	0.8445	0.7949	0.7211	0.7904	0.7901	0.7894	0.6366	0.8087	0.8880	0.00	0.00	0.00	0
			0.0370	0.0456	0.0420	0.0193	0.0264	0.0365	0.0230	0.0230	0.0231	0.0470	0.0252	0.0135				
		7	0.4352	0.0953	0.4055	0.8516	0.8028	0.7306	0.7985	0.7980	0.7977	0.6472	0.8173	0.8941	0.00	0.00	0.00	0
			0.0364	0.0453	0.0416	0.0175	0.0245	0.0341	0.0214	0.0214	0.0215	0.0444	0.0232	0.0121				
	OrdPLS	2	0.4567	0.0923	0.4257	0.8611	0.8175	0.7439	0.8117	0.8103	0.8094	0.6619	0.8310	0.9032	0.00	0.00	0.00	0
			0.0506	0.0718	0.0645	0.0286	0.0375	0.0509	0.0337	0.0338	0.0340	0.0654	0.0365	0.0206				
		3	0.4547	0.0921	0.4236	0.8630	0.8168	0.7449	0.8115	0.8126	0.8124	0.6634	0.8316	0.9043	0.00	0.00	0.00	0
			0.0408	0.0542	0.0493	0.0201	0.0277	0.0382	0.0247	0.0244	0.0246	0.0496	0.0265	0.0141				
		5	0.4533	0.0913	0.4245	0.8636	0.8174	0.7454	0.8123	0.8121	0.8112	0.6629	0.8322	0.9044	0.00	0.00	0.00	0
			0.0381	0.0497	0.0451	0.0177	0.0247	0.0346	0.0220	0.0220	0.0220	0.0453	0.0234	0.0122				
		7	0.4534	0.0919	0.4236	0.8638	0.8169	0.7455	0.8122	0.8119	0.8117	0.6637	0.8321	0.9045	0.00	0.00	0.00	0
			0.0365	0.0471	0.0428	0.0163	0.0230	0.0324	0.0204	0.0204	0.0205	0.0427	0.0218	0.0111				
	PLSc	2	0.5829	0.0055	0.5785	0.6420	0.5653	0.4803	0.5630	0.5629	0.5605	0.3996	0.5647	0.7322	0.00	0.00	0.00	6114
			0.0700	0.1291	0.1241	0.0703	0.0725	0.0771	0.0578	0.0579	0.0579	0.0818	0.0701	0.0678				
		3	0.5972	0.0026	0.5938	0.7229	0.6328	0.5395	0.6330	0.6349	0.6329	0.4513	0.6309	0.8154	1.00	0.00	0.00	10166
			0.0541	0.0950	0.0896	0.0557	0.0588	0.0646	0.0460	0.0459	0.0460	0.0694	0.0558	0.0514				
		5	0.5965	-0.0007	0.5985	0.7555	0.6600	0.5654	0.6607	0.6616	0.6595	0.4692	0.6600	0.8513	1.00	0.00	0.00	20152
			0.0509	0.0876	0.0823	0.0528	0.0563	0.0626	0.0440	0.0440	0.0439	0.0673	0.0529	0.0471				
		7	0.5992	-0.0002	0.5997	0.7716	0.6743	0.5777	0.6758	0.6755	0.6739	0.4807	0.6739	0.8691	1.00	0.00	0.00	29261
			0.0488	0.0838	0.0784	0.0502	0.0540	0.0604	0.0420	0.0421	0.0420	0.0653	0.0507	0.0442				
	OrdPLSc	2	0.6061	-0.0040	0.6123	0.7891	0.7018	0.5964	0.6981	0.6981	0.6940	0.5024	0.7015	0.8799	88.00	0.00	0.00	202684
			0.0688	0.1421	0.1328	0.0780	0.0844	0.0928	0.0672	0.0674	0.0676	0.0992	0.0814	0.0670				
		3	0.5973	0.0029	0.5971	0.7996	0.7032	0.6021	0.7029	0.7055	0.7034	0.5073	0.7030	0.8926	37.00	0.00	0.00	78073
			0.0628	0.0970	0.0976	0.0586	0.0674	0.0768	0.0547	0.0545	0.0549	0.0830	0.0666	0.0476				
		5	0.5980	0.0003	0.6009	0.7997	0.7016	0.6035	0.7026	0.7037	0.7015	0.5049	0.7028	0.8942	29.00	0.00	0.00	58129
			0.0574	0.0878	0.0876	0.0534	0.0614	0.0695	0.0492	0.0490	0.0492	0.0757	0.0597	0.0435				
		7	0.6001	0.0004	0.6005	0.8000	0.7002	0.6001	0.7015	0.7016	0.7002	0.5017	0.7003	0.8965	15.00	0.00	0.00	51433
			0.0545	0.0829	0.0823	0.0502	0.0576	0.0660	0.0462	0.0462	0.0463	0.0721	0.0564	0.0412				
	WLSMV	2	0.6053	-0.0033	0.6088	0.7947	0.7034	0.6012	0.7007	0.6994	0.6980	0.5024	0.7046	0.8897	49.00	0.00	0.00	49.00
			0.0679	0.1231	0.1165	0.0600	0.0604	0.0629	0.0554	0.0555	0.0555	0.0647	0.0585	0.0598				
		3	0.6037	-0.0007	0.6023	0.7970	0.7003	0.6010	0.7001	0.7021	0.7011	0.5019	0.7005	0.8979	11.00	0.00	0.00	11.00
			0.0533	0.0921	0.0863	0.0440	0.0452	0.0481	0.0415	0.0414	0.0415	0.0502	0.0436	0.0432				
		5	0.6025	-0.0023	0.6044	0.7987	0.7013	0.6006	0.7006	0.7011	0.6989	0.5004	0.7005	0.8980	6.00	0.00	0.00	6.00
			0.0484	0.0826	0.0772	0.0385	0.0399	0.0431	0.0369	0.0368	0.0368	0.0454	0.0385	0.0376				
		7	0.6028	-0.0009	0.6026	0.7988	0.7002	0.6005	0.7008	0.7004	0.6992	0.5011	0.6998	0.8987	2.00	0.00	0.00	2.00
			0.0455	0.0771	0.0718	0.0354	0.0369	0.0400	0.0340	0.0340	0.0341	0.0423	0.0355	0.0343				

Table 4.10: Results for the model with three common factors: extremely asymmetrically distributed thresholds

Threshold dist.	Estimator	# cat	$\gamma_1=0.6$	$\gamma_2=0.0$	$\beta=0.6$	$\lambda_{x_1}=0.8$	$\lambda_{x_2}=0.7$	$\lambda_{\xi_3}=0.6$	$\lambda_{y_{11}}=0.7$	$\lambda_{y_{12}}=0.7$	$\lambda_{y_{13}}=0.7$	$\lambda_{y_{21}}=0.5$	$\lambda_{y_{22}}=0.7$	$\lambda_{y_{23}}=0.9$	Load.	CompCor	notc	Boot
Ext. Asymm.	PLS	2	0.2966	0.0902	0.2842	0.7817	0.7124	0.6269	0.7114	0.7113	0.7121	0.5240	0.7228	0.8409	0.00	0.00	0.00	0
			0.0517	0.0568	0.0555	0.0613	0.0754	0.0910	0.0608	0.0610	0.0607	0.1041	0.0722	0.0468				
		3	0.3539	0.0957	0.3321	0.8119	0.7523	0.6701	0.7477	0.7482	0.7486	0.5760	0.7667	0.8639	0.00	0.00	0.00	0
			0.0451	0.0509	0.0493	0.0354	0.0460	0.0593	0.0387	0.0387	0.0386	0.0719	0.0437	0.0257				
		5	0.3991	0.0967	0.3708	0.8345	0.7819	0.7036	0.7767	0.7758	0.7766	0.6139	0.7972	0.8817	0.00	0.00	0.00	0
			0.0401	0.0476	0.0450	0.0237	0.0320	0.0434	0.0277	0.0279	0.0276	0.0552	0.0306	0.0167				
		7	0.4159	0.0959	0.3872	0.8443	0.7932	0.7166	0.7881	0.7875	0.7879	0.6296	0.8088	0.8894	0.00	0.00	0.00	0
			0.0387	0.0468	0.0437	0.0204	0.0282	0.0390	0.0246	0.0247	0.0246	0.0502	0.0269	0.0142				
	OrdPLS	2	0.4586	0.0801	0.4416	0.8620	0.8126	0.7421	0.8080	0.8078	0.8092	0.6529	0.8291	0.9028	0.00	0.00	0.00	0
			0.0676	0.1087	0.0910	0.0439	0.0582	0.0768	0.0486	0.0487	0.0483	0.0994	0.0571	0.0344				
		3	0.4564	0.0888	0.4293	0.8623	0.8157	0.7443	0.8099	0.8102	0.8109	0.6603	0.8312	0.9035	0.00	0.00	0.00	0
			0.0514	0.0720	0.0642	0.0275	0.0373	0.0510	0.0331	0.0331	0.0329	0.0660	0.0356	0.0194				
		5	0.4556	0.0914	0.4247	0.8630	0.8169	0.7447	0.8118	0.8108	0.8112	0.6615	0.8321	0.9040	0.00	0.00	0.00	0
			0.0423	0.0561	0.0509	0.0203	0.0280	0.0391	0.0250	0.0251	0.0250	0.0515	0.0268	0.0140				
		7	0.4540	0.0923	0.4235	0.8633	0.8169	0.7447	0.8117	0.8112	0.8114	0.6625	0.8319	0.9041	0.00	0.00	0.00	0
			0.0393	0.0513	0.0466	0.0180	0.0253	0.0356	0.0225	0.0226	0.0225	0.0468	0.0241	0.0124				
	PLSc	2	0.5514	-0.0144	0.5726	0.5990	0.5135	0.4325	0.5145	0.5140	0.5130	0.3485	0.5124	0.6939	3.00	0.00	0.00	42061
			0.0980	0.1930	0.1873	0.1004	0.1021	0.1059	0.0811	0.0813	0.0815	0.1074	0.0990	0.0961				
		3	0.5669	0.0005	0.5694	0.6763	0.5846	0.4946	0.5838	0.5851	0.5836	0.4072	0.5858	0.7733	0.00	0.00	0.00	18581
			0.0723	0.1232	0.1196	0.0754	0.0782	0.0840	0.0622	0.0622	0.0622	0.0880	0.0749	0.0702				
		5	0.5835	0.0025	0.5803	0.7302	0.6374	0.5427	0.6368	0.6357	0.6363	0.4482	0.6377	0.8299	1.00	0.00	0.00	21914
			0.0580	0.0971	0.0926	0.0602	0.0635	0.0698	0.0501	0.0502	0.0501	0.0751	0.0605	0.0546				
		7	0.5881	0.0026	0.5859	0.7535	0.6568	0.5602	0.6571	0.6567	0.6566	0.4650	0.6571	0.8531	2.00	0.00	0.00	27152
			0.0537	0.0900	0.0852	0.0555	0.0593	0.0658	0.0465	0.0466	0.0465	0.0707	0.0561	0.0494				
	OrdPLSc	2	0.6072	-0.0388	0.6550	0.7894	0.6937	0.5934	0.6971	0.6951	0.6909	0.4927	0.6971	0.8638	212.00	1.00	0.00	465423
			0.0930	0.2345	0.2140	0.1062	0.1195	0.1332	0.0933	0.0932	0.0939	0.1446	0.1166	0.0938				
		3	0.5926	-0.0027	0.6038	0.8009	0.7069	0.6055	0.7060	0.7054	0.7048	0.5125	0.7082	0.8845	76.00	0.00	0.00	119120
			0.0783	0.1322	0.1319	0.0721	0.0844	0.0973	0.0693	0.0696	0.0694	0.1049	0.0831	0.0586				
		5	0.6000	-0.0019	0.6025	0.7980	0.7029	0.6021	0.7019	0.7013	0.7022	0.5037	0.7023	0.8924	33.00	0.00	0.00	77407
			0.0643	0.1010	0.1008	0.0593	0.0685	0.0779	0.0555	0.0556	0.0554	0.0852	0.0673	0.0479				
		7	0.5994	0.0009	0.6000	0.7993	0.7014	0.6018	0.7022	0.7021	0.7012	0.5044	0.7020	0.8937	28.00	0.00	0.00	59205
			0.0589	0.0909	0.0905	0.0543	0.0625	0.0713	0.0501	0.0502	0.0504	0.0777	0.0609	0.0442				
	WLSMV	2	0.6054	-0.0265	0.6404	0.7972	0.7003	0.6023	0.6991	0.6979	0.7006	0.5022	0.7073	0.8822	115.00	1.00	0.00	130.00
			0.0902	0.1781	0.1681	0.0799	0.0800	0.0828	0.0730	0.0730	0.0729	0.0850	0.0770	0.0791				
		3	0.6055	-0.0108	0.6150	0.7971	0.7003	0.6013	0.6983	0.6985	0.7001	0.5019	0.7038	0.8927	33.00	0.00	0.00	34.00
			0.0677	0.1217	0.1144	0.0573	0.0583	0.0615	0.0536	0.0537	0.0535	0.0638	0.0559	0.0560				
		5	0.6057	-0.0042	0.6064	0.7973	0.7007	0.6005	0.7001	0.6992	0.6992	0.5002	0.7012	0.8963	12.00	0.00	0.00	12.00
			0.0545	0.0947	0.0885	0.0437	0.0452	0.0487	0.0418	0.0418	0.0417	0.0511	0.0435	0.0425				
		7	0.6040	-0.0015	0.6036	0.7980	0.7003	0.6000	0.6999	0.6998	0.6993	0.5008	0.7001	0.8973	6.00	0.00	0.00	6.00
			0.0500	0.0856	0.0799	0.0391	0.0408	0.0442	0.0377	0.0377	0.0377	0.0466	0.0392	0.0379				

Table 4.11: Results for the model with three common factors: alternating moderately asymmetrically distributed thresholds

Threshold dist.	Estimator	# cat	$\gamma_1 = 0.6$	$\gamma_2 = 0.0$	$\beta = 0.6$	$\lambda_{x_1} = 0.8$	$\lambda_{x_2} = 0.7$	$\lambda_{x_3} = 0.6$	$\lambda_{y_{11}} = 0.7$	$\lambda_{y_{12}} = 0.7$	$\lambda_{y_{13}} = 0.7$	$\lambda_{y_{21}} = 0.5$	$\lambda_{y_{22}} = 0.7$	$\lambda_{y_{23}} = 0.9$	Load.	CompCor	notc	Boot
Alt. Mod. Asym.	PLS	2	0.3443	0.1062	0.3166	0.7904	0.7279	0.6600	0.7325	0.7277	0.7311	0.5788	0.7320	0.8387	0.00	0.00	0.00	0
			0.0392	0.0467	0.0430	0.0360	0.0457	0.0561	0.0366	0.0373	0.0368	0.0671	0.0445	0.0285				
		3	0.4048	0.1013	0.3733	0.8299	0.7780	0.7045	0.7747	0.7745	0.7742	0.6208	0.7897	0.8746	0.00	0.00	0.00	0
			0.0370	0.0453	0.0417	0.0223	0.0297	0.0398	0.0253	0.0253	0.0254	0.0504	0.0286	0.0163				
		5	0.4235	0.0992	0.3923	0.8403	0.7863	0.7199	0.7872	0.7827	0.7872	0.6388	0.7977	0.8820	0.00	0.00	0.00	0
			0.0359	0.0450	0.0408	0.0192	0.0263	0.0357	0.0225	0.0225	0.0225	0.0459	0.0251	0.0137				
		7	0.4353	0.0967	0.4041	0.8495	0.7980	0.7296	0.7970	0.7936	0.7962	0.6484	0.8107	0.8907	0.00	0.00	0.00	0
			0.0356	0.0448	0.0407	0.0173	0.0241	0.0336	0.0209	0.0210	0.0210	0.0437	0.0231	0.0121				
	OrdPLS	2	0.4564	0.0907	0.4276	0.8624	0.8175	0.7433	0.8119	0.8115	0.8105	0.6636	0.8294	0.9035	0.00	0.00	0.00	0
			0.0500	0.0712	0.0640	0.0288	0.0384	0.0509	0.0338	0.0345	0.0341	0.0646	0.0375	0.0213				
		3	0.4545	0.0920	0.4236	0.8633	0.8170	0.7453	0.8121	0.8122	0.8117	0.6631	0.8314	0.9040	0.00	0.00	0.00	0
			0.0407	0.0542	0.0493	0.0201	0.0277	0.0381	0.0245	0.0246	0.0247	0.0496	0.0265	0.0142				
		5	0.4538	0.0912	0.4241	0.8638	0.8179	0.7447	0.8121	0.8122	0.8122	0.6632	0.8320	0.9045	0.00	0.00	0.00	0
			0.0379	0.0496	0.0450	0.0178	0.0247	0.0347	0.0220	0.0221	0.0220	0.0452	0.0236	0.0123				
		7	0.4536	0.0919	0.4234	0.8641	0.8173	0.7450	0.8124	0.8118	0.8117	0.6638	0.8318	0.9045	0.00	0.00	0.00	0
			0.0364	0.0471	0.0427	0.0162	0.0230	0.0324	0.0204	0.0204	0.0205	0.0427	0.0218	0.0111				
	PLSc	2	0.5977	-0.0031	0.6041	0.6253	0.5512	0.4670	0.5465	0.5566	0.5454	0.3904	0.5445	0.7045	0.00	0.00	0.00	4461
			0.0696	0.1380	0.1316	0.0679	0.0699	0.0750	0.0554	0.0555	0.0555	0.0785	0.0673	0.0658				
		3	0.5973	0.0022	0.5951	0.7231	0.6317	0.5401	0.6323	0.6340	0.6316	0.4505	0.6307	0.8127	0.00	0.00	0.00	9615
			0.0540	0.0951	0.0897	0.0554	0.0588	0.0645	0.0458	0.0459	0.0460	0.0693	0.0558	0.0515				
		5	0.6045	-0.0029	0.6074	0.7434	0.6541	0.5575	0.6503	0.6582	0.6502	0.4641	0.6510	0.8345	0.00	0.00	0.00	11732
			0.0502	0.0895	0.0836	0.0514	0.0550	0.0610	0.0424	0.0428	0.0425	0.0655	0.0517	0.0467				
		7	0.6038	-0.0019	0.6052	0.7653	0.6712	0.5729	0.6702	0.6733	0.6684	0.4778	0.6686	0.8591	1.00	0.00	0.00	21020
			0.0481	0.0843	0.0785	0.0493	0.0530	0.0594	0.0409	0.0412	0.0409	0.0641	0.0498	0.0439				
	OrdPLSc	2	0.6073	-0.0095	0.6198	0.7926	0.6967	0.5980	0.6975	0.6994	0.6976	0.5057	0.6993	0.8800	119.00	0.00	0.00	233367
			0.0685	0.1433	0.1344	0.0786	0.0862	0.0923	0.0677	0.0681	0.0679	0.0978	0.0826	0.0679				
		3	0.5964	0.0031	0.5973	0.8011	0.7027	0.6030	0.7035	0.7045	0.7034	0.5073	0.7034	0.8907	39.00	0.00	0.00	75784
			0.0625	0.0966	0.0971	0.0584	0.0676	0.0764	0.0545	0.0545	0.0547	0.0828	0.0663	0.0480				
		5	0.5986	-0.0002	0.6005	0.7995	0.7028	0.6019	0.7017	0.7039	0.7013	0.5035	0.7015	0.8948	24.00	0.00	0.00	61201
			0.0577	0.0881	0.0882	0.0537	0.0616	0.0701	0.0497	0.0495	0.0498	0.0764	0.0604	0.0439				
		7	0.5999	0.0011	0.5996	0.8003	0.7018	0.5996	0.7021	0.7016	0.7006	0.5022	0.7011	0.8958	18.00	0.00	0.00	49995
			0.0544	0.0828	0.0821	0.0501	0.0573	0.0659	0.0461	0.0460	0.0462	0.0719	0.0561	0.0412				
	WLSMV	2	0.6039	-0.0076	0.6117	0.7965	0.7036	0.6009	0.7025	0.7025	0.6992	0.5052	0.7028	0.8922	52.00	0.00	0.00	56.00
			0.0673	0.1224	0.1163	0.0616	0.0621	0.0630	0.0557	0.0567	0.0559	0.0642	0.0603	0.0626				
		3	0.6035	-0.0007	0.6023	0.7981	0.7009	0.6013	0.7011	0.7014	0.6998	0.5016	0.7000	0.8975	5.00	0.00	0.00	5.00
			0.0532	0.0919	0.0863	0.0440	0.0452	0.0481	0.0414	0.0415	0.0416	0.0502	0.0437	0.0434				
		5	0.6023	-0.0020	0.6028	0.7990	0.7020	0.5996	0.7004	0.7014	0.7006	0.5007	0.7002	0.8985	7.00	0.00	0.00	7.00
			0.0483	0.0825	0.0771	0.0388	0.0402	0.0431	0.0369	0.0370	0.0369	0.0453	0.0388	0.0380				
		7	0.6032	-0.0011	0.6026	0.7993	0.7008	0.5998	0.7010	0.7002	0.6994	0.5014	0.6996	0.8984	3.00	0.00	0.00	3.00
			0.0455	0.0771	0.0719	0.0353	0.0369	0.0400	0.0340	0.0341	0.0340	0.0423	0.0356	0.0343				

Table 4.12: Results for the model with three common factors: alternating extremely asymmetrically distributed thresholds

Threshold dist.	Estimator	# cat	$\gamma_1=0.6$	$\gamma_2=0.0$	$\beta=0.6$	$\lambda_{x_1}=0.8$	$\lambda_{x_2}=0.7$	$\lambda_{x_3}=0.6$	$\lambda_{y_{11}}=0.7$	$\lambda_{y_{12}}=0.7$	$\lambda_{y_{13}}=0.7$	$\lambda_{y_{21}}=0.5$	$\lambda_{y_{22}}=0.7$	$\lambda_{y_{23}}=0.9$	Load.	CompCor	notc	Boot
Alt. Ext. Asym.	PLS	2	0.2783	0.1093	0.2586	0.7366	0.6447	0.6230	0.6731	0.6724	0.6722	0.5431	0.6450	0.7748	0.00	0.00	0.00	0
			0.0413	0.0505	0.0443	0.0670	0.0862	0.0849	0.0596	0.0700	0.0599	0.0971	0.0861	0.0617				
		3	0.3461	0.1122	0.3182	0.7806	0.6946	0.6665	0.7246	0.7072	0.7245	0.5919	0.6969	0.8179	0.00	0.00	0.00	0
			0.0379	0.0469	0.0415	0.0378	0.0507	0.0555	0.0367	0.0407	0.0368	0.0663	0.0497	0.0324				
		5	0.3963	0.1057	0.3644	0.8190	0.7505	0.7016	0.7662	0.7513	0.7654	0.6220	0.7581	0.8592	0.00	0.00	0.00	0
			0.0367	0.0458	0.0412	0.0242	0.0332	0.0417	0.0264	0.0274	0.0266	0.0526	0.0321	0.0188				
		7	0.4145	0.1025	0.3825	0.8332	0.7711	0.7149	0.7808	0.7690	0.7802	0.6351	0.7808	0.8736	0.00	0.00	0.00	0
			0.0362	0.0454	0.0410	0.0206	0.0285	0.0377	0.0236	0.0241	0.0237	0.0482	0.0275	0.0152				
	OrdPLS	2	0.4573	0.0692	0.4508	0.8824	0.8509	0.7379	0.8175	0.8279	0.8176	0.6423	0.8699	0.9258	0.00	0.00	0.00	0
			0.0808	0.1222	0.1201	0.0502	0.0656	0.0808	0.0582	0.0667	0.0584	0.0987	0.0627	0.0400				
		3	0.4578	0.0885	0.4323	0.8641	0.8171	0.7434	0.8125	0.8121	0.8123	0.6628	0.8309	0.9041	0.00	0.00	0.00	0
			0.0489	0.0697	0.0627	0.0290	0.0396	0.0502	0.0336	0.0358	0.0337	0.0633	0.0387	0.0224				
		5	0.4552	0.0914	0.4249	0.8637	0.8179	0.7442	0.8126	0.8116	0.8121	0.6621	0.8312	0.9043	0.00	0.00	0.00	0
			0.0411	0.0550	0.0498	0.0207	0.0287	0.0389	0.0250	0.0258	0.0252	0.0505	0.0276	0.0148				
		7	0.4542	0.0921	0.4235	0.8635	0.8181	0.7447	0.8120	0.8116	0.8120	0.6630	0.8317	0.9042	0.00	0.00	0.00	0
			0.0387	0.0507	0.0460	0.0183	0.0255	0.0355	0.0225	0.0229	0.0226	0.0464	0.0245	0.0128				
	PLSc	2	0.6663	-0.0886	0.7702	0.4806	0.4366	0.3620	0.4106	0.4654	0.4099	0.2905	0.4222	0.5171	0.00	31.00	0.00	157661
			0.0992	0.3259	0.3071	0.0845	0.0789	0.0869	0.0662	0.0659	0.0663	0.0867	0.0755	0.0839				
		3	0.6380	-0.0329	0.6783	0.5912	0.5303	0.4423	0.5111	0.5527	0.5115	0.3642	0.5200	0.6461	0.00	0.00	0.00	5627
			0.0709	0.1706	0.1611	0.0660	0.0658	0.0727	0.0528	0.0533	0.0528	0.0751	0.0627	0.0642				
		5	0.6125	-0.0072	0.6219	0.6891	0.6110	0.5156	0.6010	0.6216	0.5998	0.4272	0.6042	0.7674	0.00	0.00	0.00	4047
			0.0564	0.1079	0.1012	0.0564	0.0591	0.0652	0.0459	0.0467	0.0460	0.0695	0.0561	0.0533				
		7	0.6080	-0.0034	0.6126	0.7241	0.6399	0.5409	0.6321	0.6468	0.6307	0.4503	0.6344	0.8092	0.00	0.00	0.00	7477
			0.0525	0.0958	0.0897	0.0530	0.0563	0.0626	0.0434	0.0442	0.0435	0.0670	0.0533	0.0491				
	OrdPLSc	2	0.5858	-0.0287	0.6369	0.7962	0.7153	0.6311	0.7271	0.7087	0.7229	0.5413	0.7212	0.8535	967.00	15.00	0.00	4484252
			0.1122	0.3018	0.2912	0.1188	0.1384	0.1421	0.1134	0.1160	0.1121	0.1570	0.1403	0.1094				
		3	0.5863	0.0030	0.5976	0.8060	0.7116	0.6152	0.7136	0.7119	0.7143	0.5260	0.7135	0.8819	117.00	0.00	0.00	146370
			0.0771	0.1286	0.1315	0.0712	0.0867	0.0937	0.0698	0.0718	0.0695	0.1009	0.0857	0.0602				
		5	0.5957	0.0026	0.5976	0.8016	0.7059	0.6047	0.7070	0.7047	0.7054	0.5090	0.7044	0.8921	53.00	0.00	0.00	84468
			0.0637	0.0984	0.0995	0.0592	0.0696	0.0775	0.0556	0.0564	0.0558	0.0842	0.0684	0.0487				
		7	0.5981	0.0024	0.5986	0.8003	0.7032	0.6016	0.7038	0.7023	0.7027	0.5057	0.7016	0.8940	31.00	0.00	0.00	64161
			0.0590	0.0900	0.0902	0.0547	0.0634	0.0719	0.0507	0.0511	0.0507	0.0778	0.0621	0.0449				
	WLSMV	2	0.6217	-0.0424	0.6785	0.7846	0.6861	0.6087	0.7016	0.6860	0.6941	0.5148	0.6850	0.8495	175.00	7.00	0.00	207.00
			0.1016	0.2187	0.2208	0.1030	0.1123	0.0911	0.0831	0.0953	0.0831	0.0902	0.1171	0.1159				
		3	0.6032	-0.0051	0.6142	0.8001	0.7029	0.6013	0.7035	0.7034	0.7023	0.5051	0.7030	0.8903	80.00	0.00	0.00	84.00
			0.0658	0.1182	0.1131	0.0628	0.0646	0.0618	0.0551	0.0583	0.0553	0.0626	0.0634	0.0659				
		5	0.6041	-0.0035	0.6053	0.7987	0.7028	0.5999	0.7020	0.7008	0.7004	0.5007	0.7003	0.8969	22.00	0.00	0.00	22.00
			0.0533	0.0928	0.0872	0.0454	0.0469	0.0484	0.0420	0.0430	0.0421	0.0505	0.0456	0.0460				
		7	0.6037	-0.0010	0.6031	0.7981	0.7025	0.6004	0.7008	0.7005	0.7004	0.5013	0.6999	0.8977	9.00	0.00	0.00	9.00
			0.0493	0.0846	0.0792	0.0399	0.0415	0.0440	0.0378	0.0383	0.0378	0.0462	0.0402	0.0396				

Table 4.13: Results for the model with two composites and one common factor: symmetrically distributed thresholds

Threshold dist.	Estimator	# cat	γ_1=0.6	γ_2=0.0	β=0.6	λ_{y21}=0.5	λ_{y22}=0.7	λ_{y23}=0.9	w_{x1}=0.3	w_{x2}=0.5	w_{x3}=0.6	w_{y11}=0.4	w_{y12}=0.5	w_{y13}=0.5	Load.	CompCor	notc	Boot
Symmetric	PLS	2	0.4451	0.0757	0.3767	0.5796	0.7553	0.8515	0.2995	0.5556	0.6051	0.4552	0.5094	0.5204	0.00	0.00	0.00	0
			0.0364	0.0484	0.0443	0.0605	0.0376	0.0227	0.0927	0.0869	0.0832	0.0707	0.0666	0.0681				
		3	0.5107	0.0601	0.4368	0.6160	0.7830	0.8686	0.3014	0.5310	0.6026	0.4353	0.5040	0.5095	0.00	0.00	0.00	0
			0.0327	0.0474	0.0425	0.0483	0.0277	0.0158	0.0785	0.0756	0.0712	0.0592	0.0553	0.0568				
		5	0.5670	0.0290	0.4953	0.6443	0.8120	0.8897	0.3005	0.5113	0.5994	0.4134	0.5019	0.5029	0.00	0.00	0.00	0
			0.0301	0.0478	0.0425	0.0417	0.0219	0.0112	0.0701	0.0700	0.0654	0.0530	0.0485	0.0506				
		7	0.5830	0.0171	0.5146	0.6542	0.8212	0.8962	0.2985	0.5062	0.5987	0.4078	0.4995	0.5013	0.00	0.00	0.00	0
			0.0294	0.0480	0.0424	0.0399	0.0203	0.0101	0.0680	0.0686	0.0641	0.0513	0.0468	0.0490				
	OrdPLS	2	0.6104	-0.0059	0.5485	0.6636	0.8314	0.9035	0.2980	0.4963	0.5936	0.3924	0.5019	0.4992	0.00	0.00	0.00	0
			0.0465	0.0907	0.0804	0.0600	0.0332	0.0185	0.1056	0.1173	0.1055	0.0930	0.0761	0.0853				
		3	0.6055	0.0029	0.5413	0.6639	0.8318	0.9042	0.2994	0.4942	0.5980	0.3971	0.5001	0.4984	0.00	0.00	0.00	0
			0.0370	0.0672	0.0597	0.0483	0.0260	0.0138	0.0844	0.0916	0.0829	0.0706	0.0598	0.0656				
		5	0.6048	0.0017	0.5405	0.6638	0.8321	0.9042	0.3001	0.4957	0.5983	0.3973	0.5005	0.4990	0.00	0.00	0.00	0
			0.0313	0.0548	0.0485	0.0417	0.0213	0.0107	0.0720	0.0756	0.0695	0.0568	0.0500	0.0536				
		7	0.6032	0.0015	0.5396	0.6648	0.8320	0.9041	0.2981	0.4979	0.5980	0.3990	0.4988	0.4993	0.00	0.00	0.00	0
			0.0299	0.0515	0.0455	0.0397	0.0200	0.0098	0.0688	0.0714	0.0661	0.0532	0.0475	0.0504				
	PLSc	2	0.4451	0.0942	0.4685	0.4056	0.5712	0.7406	0.2995	0.5556	0.6051	0.4552	0.5094	0.5204	0.00	0.00	0.00	2137
			0.0364	0.0602	0.0567	0.0712	0.0607	0.0580	0.0927	0.0870	0.0832	0.0707	0.0666	0.0680				
		3	0.5107	0.0717	0.5199	0.4452	0.6207	0.7951	0.3013	0.5311	0.6025	0.4353	0.5040	0.5096	1.00	0.00	0.00	2483
			0.0327	0.0565	0.0514	0.0622	0.0507	0.0468	0.0786	0.0757	0.0712	0.0593	0.0553	0.0568				
		5	0.5670	0.0332	0.5666	0.4784	0.6665	0.8558	0.3005	0.5113	0.5994	0.4134	0.5019	0.5029	0.00	0.00	0.00	7010
			0.0300	0.0547	0.0493	0.0573	0.0445	0.0391	0.0701	0.0699	0.0654	0.0529	0.0485	0.0506				
		7	0.5830	0.0193	0.5822	0.4900	0.6816	0.8732	0.2985	0.5062	0.5987	0.4078	0.4995	0.5013	0.00	0.00	0.00	12623
			0.0293	0.0544	0.0487	0.0558	0.0428	0.0368	0.0680	0.0685	0.0640	0.0512	0.0469	0.0490				
	OrdPLSc	2	0.6101	-0.0065	0.6138	0.5030	0.6999	0.8846	0.2976	0.4963	0.5943	0.3917	0.5024	0.4996	62.00	0.00	0.00	118064
			0.0467	0.1023	0.0920	0.0877	0.0718	0.0601	0.1058	0.1176	0.1057	0.0933	0.0764	0.0856				
		3	0.6054	0.0038	0.6036	0.5077	0.7035	0.8906	0.2998	0.4940	0.5982	0.3970	0.4998	0.4988	29.00	0.00	0.00	54083
			0.0370	0.0748	0.0684	0.0758	0.0610	0.0456	0.0842	0.0917	0.0829	0.0705	0.0598	0.0655				
		5	0.6049	0.0020	0.6035	0.5025	0.6985	0.8947	0.3003	0.4953	0.5986	0.3974	0.5006	0.4989	5.00	0.00	0.00	31682
			0.0313	0.0611	0.0555	0.0645	0.0506	0.0385	0.0719	0.0757	0.0695	0.0567	0.0499	0.0535				
		7	0.6033	0.0016	0.6028	0.5040	0.6995	0.8937	0.2983	0.4978	0.5979	0.3993	0.4988	0.4991	7.00	0.00	0.00	21461
			0.0299	0.0575	0.0520	0.0607	0.0468	0.0364	0.0689	0.0715	0.0661	0.0532	0.0474	0.0504				

Table 4.14: Results for the model with two composites and one common factor: moderately asymmetrically distributed thresholds

Threshold dist.	Estimator	# cat	γ_1=0.6	γ_2=0.0	β=0.6	λ_{y21}=0.5	λ_{y22}=0.7	λ_{y23}=0.9	w_{x_1}=0.3	w_{x_2}=0.5	w_{x_3}=0.6	$w_{y_{11}}$=0.4	$w_{y_{12}}$=0.5	$w_{y_{13}}$=0.5	Load.	CompCor	notc	Boot
Moderate	PLS	2	0.4338	0.0768	0.3695	0.5715	0.7520	0.8497	0.2962	0.5560	0.6093	0.4611	0.5077	0.5208	0.00	0.00	0.00	0
			0.0379	0.0493	0.0455	0.0644	0.0400	0.0244	0.0971	0.0915	0.0873	0.0741	0.0705	0.0715				
		3	0.5242	0.0521	0.4488	0.6215	0.7914	0.8752	0.2990	0.5271	0.6024	0.4297	0.5046	0.5077	0.00	0.00	0.00	0
			0.0322	0.0479	0.0429	0.0472	0.0263	0.0144	0.0766	0.0748	0.0703	0.0583	0.0540	0.0558				
		5	0.5554	0.0334	0.4842	0.6377	0.8088	0.8875	0.2988	0.5156	0.6009	0.4176	0.5015	0.5051	0.00	0.00	0.00	0
			0.0315	0.0486	0.0435	0.0442	0.0234	0.0121	0.0729	0.0727	0.0682	0.0556	0.0512	0.0532				
		7	0.5737	0.0225	0.5045	0.6479	0.8178	0.8937	0.2979	0.5090	0.6000	0.4107	0.5003	0.5029	0.00	0.00	0.00	0
			0.0304	0.0486	0.0433	0.0417	0.0216	0.0109	0.0701	0.0707	0.0659	0.0534	0.0488	0.0510				
	OrdPLS	2	0.6084	-0.0044	0.5487	0.6610	0.8311	0.9032	0.2964	0.4916	0.5982	0.3951	0.4996	0.4981	0.00	0.00	0.00	0
			0.0488	0.0956	0.0844	0.0633	0.0349	0.0194	0.1119	0.1242	0.1109	0.0979	0.0806	0.0898				
		3	0.6069	0.0014	0.5411	0.6642	0.8320	0.9041	0.2986	0.4942	0.5988	0.3960	0.5014	0.4981	0.00	0.00	0.00	0
			0.0358	0.0647	0.0576	0.0471	0.0249	0.0130	0.0817	0.0881	0.0799	0.0675	0.0577	0.0629				
		5	0.6043	0.0020	0.5404	0.6634	0.8324	0.9041	0.3002	0.4954	0.5989	0.3973	0.4999	0.4992	0.00	0.00	0.00	0
			0.0324	0.0568	0.0504	0.0431	0.0220	0.0111	0.0743	0.0783	0.0718	0.0590	0.0519	0.0556				
		7	0.6039	0.0019	0.5399	0.6642	0.8326	0.9042	0.2989	0.4964	0.5986	0.3984	0.4993	0.4992	0.00	0.00	0.00	0
			0.0304	0.0526	0.0465	0.0404	0.0204	0.0101	0.0698	0.0729	0.0672	0.0544	0.0483	0.0515				
	PLSc	2	0.4338	0.0963	0.4624	0.3968	0.5650	0.7329	0.2962	0.5560	0.6093	0.4611	0.5077	0.5208	0.00	0.00	0.00	2112
			0.0379	0.0619	0.0585	0.0743	0.0637	0.0611	0.0970	0.0913	0.0872	0.0740	0.0705	0.0715				
		3	0.5242	0.0613	0.5277	0.4535	0.6326	0.8135	0.2990	0.5271	0.6024	0.4297	0.5046	0.5077	0.00	0.00	0.00	3544
			0.0322	0.0563	0.0514	0.0616	0.0498	0.0453	0.0767	0.0748	0.0703	0.0583	0.0540	0.0558				
		5	0.5554	0.0384	0.5563	0.4718	0.6604	0.8491	0.2988	0.5156	0.6009	0.4176	0.5015	0.5051	0.00	0.00	0.00	7114
			0.0315	0.0559	0.0508	0.0597	0.0469	0.0413	0.0730	0.0728	0.0683	0.0555	0.0512	0.0531				
		7	0.5737	0.0256	0.5733	0.4835	0.6757	0.8655	0.2980	0.5088	0.6001	0.4108	0.5004	0.5029	1.00	0.00	0.00	10344
			0.0305	0.0553	0.0499	0.0576	0.0447	0.0387	0.0701	0.0707	0.0660	0.0534	0.0488	0.0510				
	OrdPLSc	2	0.6096	-0.0020	0.6127	0.4983	0.7018	0.8820	0.2977	0.4922	0.5969	0.3956	0.4994	0.4975	68.00	0.00	0.00	125118
			0.0489	0.1082	0.0968	0.0922	0.0751	0.0626	0.1119	0.1243	0.1112	0.0982	0.0807	0.0900				
		3	0.6070	0.0017	0.6038	0.5080	0.7013	0.8918	0.2989	0.4948	0.5982	0.3957	0.5013	0.4985	21.00	0.00	0.00	46862
			0.0359	0.0720	0.0658	0.0734	0.0590	0.0441	0.0816	0.0882	0.0801	0.0676	0.0577	0.0630				
		5	0.6046	0.0021	0.6034	0.5033	0.7005	0.8937	0.3001	0.4955	0.5988	0.3975	0.4998	0.4991	12.00	0.00	0.00	33044
			0.0324	0.0634	0.0576	0.0665	0.0521	0.0396	0.0743	0.0783	0.0719	0.0589	0.0518	0.0555				
		7	0.6039	0.0022	0.6031	0.5035	0.7001	0.8939	0.2992	0.4962	0.5987	0.3984	0.4989	0.4995	6.00	0.00	0.00	24475
			0.0303	0.0587	0.0531	0.0618	0.0479	0.0371	0.0698	0.0728	0.0671	0.0544	0.0483	0.0514				

Table 4.15: Results for the model with two composites and one common factor: extremely asymmetrically distributed thresholds

Threshold dist.	Estimator	# cat	$\gamma_1=0.6$	$\gamma_2=0.0$	$\beta=0.6$	$\lambda_{y21}=0.5$	$\lambda_{y22}=0.7$	$\lambda_{y23}=0.9$	$w_{x_1}=0.3$	$w_{x_2}=0.5$	$w_{x_3}=0.6$	$w_{y_{11}}=0.4$	$w_{y_{12}}=0.5$	$w_{y_{13}}=0.5$	Load.	CompCor	notc	Boot
Ext. Asymm.	PLS	2	0.3681	0.0779	0.3193	0.5310	0.7267	0.8392	0.2765	0.5774	0.6123	0.4792	0.5072	0.5320	0.00	0.00	0.00	0
			0.0500	0.0585	0.0561	0.0971	0.0658	0.0420	0.1331	0.1281	0.1244	0.1069	0.1033	0.1036				
		3	0.4523	0.0659	0.3869	0.5779	0.7673	0.8642	0.2870	0.5545	0.6052	0.4520	0.5064	0.5213	0.00	0.00	0.00	0
			0.0416	0.0530	0.0501	0.0676	0.0405	0.0229	0.0996	0.0970	0.0932	0.0787	0.0745	0.0759				
		5	0.5194	0.0457	0.4480	0.6155	0.7969	0.8820	0.2912	0.5304	0.6026	0.4303	0.5038	0.5099	0.00	0.00	0.00	0
			0.0352	0.0503	0.0460	0.0518	0.0285	0.0149	0.0814	0.0807	0.0764	0.0631	0.0587	0.0605				
		7	0.5461	0.0339	0.4752	0.6313	0.8089	0.8892	0.2939	0.5215	0.6000	0.4211	0.5024	0.5061	0.00	0.00	0.00	0
			0.0331	0.0498	0.0450	0.0470	0.0250	0.0126	0.0759	0.0762	0.0719	0.0587	0.0540	0.0562				
	OrdPLS	2	0.6153	-0.0155	0.5629	0.6596	0.8306	0.9023	0.2897	0.4894	0.5950	0.3884	0.4992	0.5014	0.00	0.00	0.00	0
			0.0708	0.1784	0.1515	0.1005	0.0602	0.0398	0.1813	0.1942	0.1761	0.1565	0.1247	0.1410				
		3	0.6077	-0.0021	0.5459	0.6622	0.8314	0.9040	0.2960	0.4948	0.5956	0.3932	0.4998	0.5012	0.00	0.00	0.00	0
			0.0476	0.0919	0.0805	0.0631	0.0338	0.0180	0.1117	0.1205	0.1088	0.0941	0.0790	0.0866				
		5	0.6050	-0.0004	0.5418	0.6631	0.8320	0.9041	0.2969	0.4950	0.5990	0.3958	0.5007	0.4996	0.00	0.00	0.00	0
			0.0367	0.0660	0.0584	0.0487	0.0252	0.0129	0.0846	0.0896	0.0818	0.0683	0.0593	0.0640				
		7	0.6042	0.0010	0.5403	0.6644	0.8321	0.9038	0.2991	0.4958	0.5983	0.3978	0.5002	0.4989	0.00	0.00	0.00	0
			0.0333	0.0585	0.0518	0.0442	0.0225	0.0113	0.0765	0.0804	0.0738	0.0606	0.0532	0.0571				
	PLSc	2	0.3680	0.1017	0.4165	0.3569	0.5198	0.6896	0.2766	0.5772	0.6125	0.4789	0.5071	0.5324	2.00	0.00	0.00	11492
			0.0500	0.0769	0.0753	0.0999	0.0911	0.0886	0.1331	0.1280	0.1242	0.1069	0.1031	0.1035				
		3	0.4523	0.0801	0.4701	0.4101	0.5877	0.7730	0.2870	0.5545	0.6052	0.4520	0.5064	0.5213	0.00	0.00	0.00	8396
			0.0415	0.0646	0.0618	0.0799	0.0680	0.0630	0.0997	0.0971	0.0933	0.0786	0.0744	0.0758				
		5	0.5194	0.0533	0.5221	0.4510	0.6374	0.8299	0.2912	0.5304	0.6026	0.4303	0.5038	0.5099	0.00	0.00	0.00	10865
			0.0351	0.0588	0.0546	0.0669	0.0539	0.0481	0.0815	0.0808	0.0766	0.0631	0.0587	0.0605				
		7	0.5461	0.0390	0.5454	0.4674	0.6578	0.8523	0.2939	0.5215	0.6000	0.4211	0.5024	0.5061	0.00	0.00	0.00	12985
			0.0331	0.0572	0.0525	0.0628	0.0497	0.0433	0.0760	0.0762	0.0719	0.0586	0.0540	0.0562				
	OrdPLSc	2	0.6138	-0.0187	0.6352	0.5050	0.7024	0.8608	0.2942	0.4871	0.5953	0.3897	0.4973	0.5004	134.00	0.00	0.00	192388
			0.0711	0.1970	0.1696	0.1416	0.1136	0.0950	0.1813	0.1949	0.1765	0.1568	0.1251	0.1413				
		3	0.6073	-0.0051	0.6108	0.5119	0.7060	0.8860	0.2966	0.4939	0.5959	0.3944	0.4997	0.5000	50.00	0.00	0.00	79697
			0.0476	0.1021	0.0916	0.0962	0.0766	0.0553	0.1117	0.1209	0.1090	0.0938	0.0789	0.0865				
		5	0.6050	-0.0010	0.6049	0.5057	0.7015	0.8919	0.2985	0.4943	0.5992	0.3957	0.5009	0.4996	22.00	0.00	0.00	48922
			0.0367	0.0734	0.0666	0.0757	0.0594	0.0439	0.0845	0.0897	0.0819	0.0683	0.0592	0.0639				
		7	0.6042	0.0012	0.6031	0.5036	0.6999	0.8932	0.2998	0.4954	0.5985	0.3980	0.5004	0.4987	10.00	0.00	0.00	37311
			0.0333	0.0652	0.0592	0.0687	0.0536	0.0401	0.0765	0.0805	0.0738	0.0606	0.0533	0.0572				

Table 4.16: Results for the model with two composites and one common factor: alternating moderately asymmetrically distributed thresholds

Threshold dist.	Estimator	# cat	$\gamma_1=0.6$	$\gamma_2=0.0$	$\beta=0.6$	$\lambda_{y21}=0.5$	$\lambda_{y22}=0.7$	$\lambda_{y23}=0.9$	$w_{x1}=0.3$	$w_{x2}=0.5$	$w_{x3}=0.6$	$w_{y11}=0.4$	$w_{y12}=0.5$	$w_{y13}=0.5$	Load.	CompCor	notc	Boot
	PLS	2	0.4278 (0.0367)	0.0845 (0.0481)	0.3608 (0.0436)	0.5773 (0.0630)	0.7353 (0.0406)	0.8378 (0.0258)	0.2968 (0.0958)	0.5676 (0.0883)	0.6062 (0.0849)	0.4600 (0.0721)	0.5174 (0.0688)	0.5164 (0.0699)	0.00	0.00	0.00	0
		3	0.5233 (0.0322)	0.0529 (0.0477)	0.4480 (0.0427)	0.6211 (0.0473)	0.7899 (0.0264)	0.8751 (0.0144)	0.3008 (0.0766)	0.5281 (0.0747)	0.6013 (0.0703)	0.4291 (0.0582)	0.5054 (0.0540)	0.5082 (0.0558)	0.00	0.00	0.00	0
		5	0.5520 (0.0306)	0.0413 (0.0478)	0.4758 (0.0422)	0.6394 (0.0433)	0.7983 (0.0231)	0.8812 (0.0123)	0.2969 (0.0719)	0.5253 (0.0706)	0.5971 (0.0666)	0.4177 (0.0541)	0.5068 (0.0499)	0.5020 (0.0519)	0.00	0.00	0.00	0
		7	0.5716 (0.0298)	0.0279 (0.0479)	0.4984 (0.0424)	0.6491 (0.0411)	0.8109 (0.0214)	0.8902 (0.0109)	0.2976 (0.0693)	0.5145 (0.0692)	0.5977 (0.0649)	0.4107 (0.0522)	0.5036 (0.0480)	0.5014 (0.0500)	0.00	0.00	0.00	0
	OrdPLS	2	0.6109 (0.0494)	-0.0048 (0.0974)	0.5493 (0.0866)	0.6634 (0.0627)	0.8309 (0.0358)	0.9030 (0.0205)	0.2952 (0.1120)	0.4939 (0.1265)	0.5978 (0.1125)	0.3964 (0.0993)	0.5001 (0.0811)	0.4970 (0.0909)	0.00	0.00	0.00	0
		3	0.6063 (0.0359)	0.0019 (0.0646)	0.5407 (0.0574)	0.6637 (0.0473)	0.8314 (0.0251)	0.9044 (0.0130)	0.3003 (0.0818)	0.4948 (0.0882)	0.5977 (0.0801)	0.3954 (0.0675)	0.5016 (0.0578)	0.4990 (0.0630)	0.00	0.00	0.00	0
		5	0.6053 (0.0323)	0.0027 (0.0569)	0.5395 (0.0505)	0.6636 (0.0430)	0.8321 (0.0221)	0.9039 (0.0113)	0.2984 (0.0741)	0.4969 (0.0788)	0.5981 (0.0723)	0.3981 (0.0591)	0.4995 (0.0519)	0.4988 (0.0556)	0.00	0.00	0.00	0
Alt. Mod. Asym.		7	0.6040 (0.0304)	0.0024 (0.0527)	0.5388 (0.0466)	0.6644 (0.0404)	0.8318 (0.0205)	0.9042 (0.0101)	0.2987 (0.0699)	0.4970 (0.0730)	0.5982 (0.0672)	0.3980 (0.0544)	0.4997 (0.0483)	0.4995 (0.0514)	0.00	0.00	0.00	0
	PLSc	2	0.4278 (0.0367)	0.1082 (0.0617)	0.4623 (0.0575)	0.3878 (0.0718)	0.5498 (0.0610)	0.7016 (0.0595)	0.2968 (0.0958)	0.5676 (0.0884)	0.6062 (0.0850)	0.4600 (0.0722)	0.5174 (0.0687)	0.5164 (0.0699)	0.00	0.00	0.00	1024
		3	0.5233 (0.0322)	0.0624 (0.0563)	0.5270 (0.0514)	0.4521 (0.0618)	0.6310 (0.0497)	0.8131 (0.0452)	0.3008 (0.0766)	0.5281 (0.0747)	0.6013 (0.0704)	0.4291 (0.0582)	0.5054 (0.0539)	0.5082 (0.0558)	0.00	0.00	0.00	2971
		5	0.5520 (0.0306)	0.0479 (0.0555)	0.5523 (0.0499)	0.4654 (0.0583)	0.6530 (0.0459)	0.8308 (0.0410)	0.2969 (0.0720)	0.5253 (0.0707)	0.5971 (0.0666)	0.4177 (0.0540)	0.5068 (0.0500)	0.5020 (0.0518)	0.00	0.00	0.00	2996
		7	0.5716 (0.0298)	0.0319 (0.0548)	0.5695 (0.0492)	0.4799 (0.0567)	0.6697 (0.0441)	0.8562 (0.0384)	0.2976 (0.0693)	0.5145 (0.0691)	0.5977 (0.0648)	0.4107 (0.0523)	0.5036 (0.0480)	0.5014 (0.0501)	0.00	0.00	0.00	6490
	OrdPLSc	2	0.6115 (0.0497)	-0.0061 (0.1104)	0.6165 (0.0995)	0.5052 (0.0924)	0.6971 (0.0775)	0.8828 (0.0642)	0.2954 (0.1125)	0.4943 (0.1270)	0.5978 (0.1131)	0.3961 (0.0995)	0.5002 (0.0816)	0.4962 (0.0912)	75.00	0.00	0.00	145346
		3	0.6065 (0.0359)	0.0026 (0.0719)	0.6027 (0.0659)	0.5062 (0.0742)	0.6997 (0.0597)	0.8934 (0.0441)	0.3000 (0.0818)	0.4948 (0.0883)	0.5980 (0.0801)	0.3950 (0.0675)	0.5020 (0.0579)	0.4991 (0.0629)	17.00	0.00	0.00	51479
		5	0.6053 (0.0324)	0.0029 (0.0635)	0.6026 (0.0579)	0.5023 (0.0670)	0.6991 (0.0529)	0.8939 (0.0401)	0.2986 (0.0741)	0.4967 (0.0788)	0.5983 (0.0722)	0.3981 (0.0590)	0.4994 (0.0518)	0.4990 (0.0556)	7.00	0.00	0.00	36472
		7	0.6041 (0.0303)	0.0028 (0.0588)	0.6017 (0.0532)	0.5038 (0.0618)	0.6987 (0.0481)	0.8943 (0.0371)	0.2993 (0.0698)	0.4972 (0.0727)	0.5979 (0.0672)	0.3981 (0.0544)	0.4994 (0.0483)	0.4996 (0.0513)	8.00	0.00	0.00	24188

Table 4.17: Results for the model with two composites and one common factor: alternating extremely asymmetrically distributed thresholds

Threshold dist.	Estimator	# cat	$\gamma_1=-0.6$	$\gamma_2=0.0$	$\beta=0.6$	$\lambda_{y21}=0.5$	$\lambda_{y22}=0.7$	$\lambda_{y23}=0.9$	$w_{x1}=0.3$	$w_{x2}=0.5$	$w_{x3}=0.6$	$w_{y11}=0.4$	$w_{y12}=0.5$	$w_{y13}=0.5$	Load.	CompCor	note	Boot
Alt. Ext. Asym.	PLS	2	0.3240	0.1059	0.2691	0.5489	0.6523	0.7686	0.2933	0.6288	0.5983	0.4696	0.5626	0.5101	0.00	0.00	0.00	0
			0.0421	0.0513	0.0457	0.0931	0.0847	0.0610	0.1274	0.1164	0.1147	0.0978	0.1028	0.0956				
		3	0.4224	0.0964	0.3494	0.5929	0.7024	0.8145	0.2929	0.5964	0.5958	0.4493	0.5421	0.5047	0.00	0.00	0.00	0
			0.0365	0.0482	0.0425	0.0627	0.0464	0.0306	0.0952	0.0876	0.0855	0.0718	0.0711	0.0697				
		5	0.5047	0.0674	0.4251	0.6233	0.7602	0.8580	0.2929	0.5548	0.5961	0.4285	0.5227	0.5015	0.00	0.00	0.00	0
			0.0328	0.0479	0.0422	0.0493	0.0295	0.0169	0.0791	0.0753	0.0721	0.0598	0.0562	0.0577				
		7	0.5338	0.0480	0.4601	0.6342	0.7834	0.8737	0.2893	0.5400	0.5956	0.4232	0.5143	0.4994	0.00	0.00	1.00	0
			0.0314	0.0479	0.0420	0.0455	0.0251	0.0135	0.0749	0.0725	0.0686	0.0562	0.0521	0.0540				
	OrdPLS	2	0.6554	-0.1850	0.7143	0.6479	0.8649	0.9195	0.2799	0.4442	0.5991	0.4026	0.4591	0.4896	0.00	0.00	0.00	0
			0.1258	0.8609	0.8002	0.1732	0.1485	0.1356	0.3040	0.5921	0.5213	0.3042	0.2826	0.2511				
		3	0.6130	-0.0055	0.5502	0.6652	0.8323	0.9040	0.2946	0.4933	0.5982	0.3978	0.4943	0.5005	0.00	0.00	0.00	0
			0.0502	0.1009	0.0899	0.0618	0.0378	0.0220	0.1135	0.1329	0.1172	0.1004	0.0836	0.0910				
		5	0.6043	-0.0024	0.5444	0.6624	0.8328	0.9049	0.2918	0.4966	0.5991	0.4013	0.4968	0.4994	0.00	0.00	0.00	0
			0.0370	0.0667	0.0591	0.0483	0.0259	0.0136	0.0852	0.0930	0.0838	0.0692	0.0600	0.0643				
		7	0.6052	0.0009	0.5403	0.6646	0.8315	0.9040	0.2983	0.4971	0.5976	0.3976	0.4988	0.5003	0.00	0.00	0.00	0
			0.0333	0.0589	0.0522	0.0439	0.0230	0.0118	0.0764	0.0817	0.0747	0.0610	0.0537	0.0571				
	PLSc	2	0.3240	0.1653	0.4212	0.2931	0.4302	0.5075	0.2933	0.6288	0.5983	0.4696	0.5626	0.5101	0.00	0.00	0.00	1432
			0.0421	0.0806	0.0759	0.0837	0.0742	0.0810	0.1275	0.1165	0.1146	0.0979	0.1027	0.0956				
		3	0.4207	0.1240	0.4749	0.3616	0.5322	0.6370	0.2885	0.5964	0.5948	0.4558	0.5405	0.5004	0.00	0.00	0.00	253
			0.0365	0.0646	0.0588	0.0699	0.0587	0.0593	0.0956	0.0881	0.0859	0.0716	0.0709	0.0698				
		5	0.5047	0.0818	0.5162	0.4285	0.6088	0.7637	0.2929	0.5548	0.5961	0.4285	0.5227	0.5015	0.00	0.00	0.00	1104
			0.0328	0.0582	0.0525	0.0625	0.0508	0.0475	0.0792	0.0753	0.0720	0.0598	0.0561	0.0576				
		7	0.5338	0.0564	0.5419	0.4492	0.6401	0.8074	0.2893	0.5400	0.5956	0.4232	0.5143	0.4994	0.00	0.00	0.00	1769
			0.0314	0.0565	0.0506	0.0600	0.0475	0.0431	0.0749	0.0724	0.0686	0.0562	0.0521	0.0540				
	OrdPLSc	2	0.6505	-0.1900	0.7851	0.5623	0.7094	0.8522	0.2817	0.4362	0.6057	0.3909	0.4813	0.4914	681.00	35.00	2.00	1030941
			0.1300	0.8872	0.8251	0.2236	0.1828	0.1594	0.3089	0.5995	0.5311	0.3035	0.2797	0.2499				
		3	0.6123	-0.0059	0.6102	0.5220	0.7100	0.8861	0.2964	0.4913	0.5994	0.3966	0.4963	0.4998	90.00	0.00	0.00	111322
			0.0502	0.1105	0.1015	0.0979	0.0835	0.0598	0.1138	0.1330	0.1170	0.1002	0.0832	0.0908				
		5	0.6040	-0.0021	0.6056	0.5064	0.7023	0.8946	0.2927	0.4953	0.5999	0.4007	0.4973	0.4993	28.00	0.00	0.00	64260
			0.0370	0.0740	0.0678	0.0765	0.0626	0.0453	0.0851	0.0928	0.0836	0.0693	0.0601	0.0644				
		7	0.6051	0.0008	0.6029	0.5046	0.6994	0.8938	0.2985	0.4975	0.5973	0.3980	0.4987	0.5000	14.00	0.00	0.00	42613
			0.0333	0.0655	0.0598	0.0693	0.0550	0.0412	0.0764	0.0817	0.0748	0.0608	0.0536	0.0571				

Standardized loading and cross-loading estimates

Table 4.18: Standardized factor loading estimates

	PLS	PLSc	OrdPLS	OrdPLSc
ima1	0.717	0.611	0.764	0.662
ima2	0.566	0.537	0.648	0.592
ima3	0.658	0.458	0.602	0.483
ima4	0.792	0.686	0.799	0.720
ima5	0.698	0.662	0.780	0.710
exp1	0.687	0.500	0.780	0.556
exp2	0.644	0.439	0.743	0.539
exp3	0.726	0.422	0.623	0.479
qua1	0.778	0.808	0.828	0.835
qua2	0.651	0.528	0.647	0.553
qua3	0.801	0.755	0.801	0.769
qua4	0.760	0.669	0.809	0.733
qua5	0.732	0.676	0.782	0.720
qua6	0.766	0.682	0.826	0.758
qua7	0.803	0.816	0.799	0.822
val1	0.933	0.756	0.914	0.771
val2	0.911	0.927	0.943	0.943
sat1	0.711	0.693	0.825	0.734
sat2	0.872	0.708	0.858	0.724
sat3	0.885	0.815	0.867	0.834
loy1	0.855	0.587	0.849	0.641
loy2	0.273	0.181	0.193	0.163
loy3	0.869	0.855	0.924	0.903

Table 4.19: Standardized cross-loading estimates of PLS

	IMA	EXP	QUA	VAL	SAT	COM	LOY
ima1	**0.717**	0.347	0.571	0.393	0.540	0.423	0.338
ima2	**0.566**	0.387	0.492	0.269	0.398	0.188	0.293
ima3	**0.658**	0.272	0.368	0.332	0.339	0.207	0.309
ima4	**0.792**	0.374	0.571	0.459	0.542	0.440	0.461
ima5	**0.698**	0.340	0.544	0.260	0.501	0.337	0.485
exp1	0.349	**0.687**	0.437	0.293	0.362	0.183	0.268
exp2	0.404	**0.644**	0.343	0.175	0.345	0.225	0.320
exp3	0.285	**0.726**	0.357	0.273	0.300	0.126	0.190
qua1	0.622	0.534	**0.778**	0.454	0.661	0.380	0.461
qua2	0.405	0.308	**0.651**	0.295	0.474	0.300	0.319
qua3	0.621	0.423	**0.801**	0.467	0.651	0.472	0.461
qua4	0.480	0.389	**0.760**	0.390	0.587	0.379	0.353
qua5	0.598	0.406	**0.732**	0.455	0.517	0.389	0.373
qua6	0.551	0.447	**0.766**	0.405	0.539	0.418	0.333
qua7	0.596	0.411	**0.803**	0.547	0.707	0.465	0.446
val1	0.405	0.314	0.477	**0.933**	0.495	0.287	0.435
val2	0.542	0.354	0.594	**0.911**	0.629	0.360	0.525
sat1	0.558	0.495	0.637	0.403	**0.711**	0.334	0.484
sat2	0.524	0.395	0.672	0.480	**0.872**	0.416	0.484
sat3	0.612	0.382	0.684	0.588	**0.885**	0.547	0.609
loy1	0.430	0.281	0.393	0.407	0.455	0.237	**0.855**
loy2	0.109	0.095	0.065	0.148	0.115	0.122	**0.273**
loy3	0.528	0.351	0.537	0.481	0.658	0.448	**0.869**

The bold printed value in each row shows on which construct the indicator loads most.

Table 4.20: Standardized cross-loading estimates of PLSc

	IMA	EXP	QUA	VAL	SAT	COM	LOY
ima1	**0.611**	0.533	0.608	0.434	0.609	0.423	0.408
ima2	0.537	**0.594**	0.524	0.297	0.449	0.188	0.353
ima3	**0.458**	0.417	0.392	0.367	0.382	0.207	0.373
ima4	**0.686**	0.574	0.609	0.507	0.612	0.440	0.556
ima5	**0.662**	0.522	0.580	0.287	0.565	0.337	0.586
exp1	0.409	**0.500**	0.466	0.324	0.409	0.183	0.324
exp2	**0.473**	0.439	0.366	0.193	0.389	0.225	0.386
exp3	0.334	**0.422**	0.381	0.301	0.338	0.126	0.229
qua1	0.729	**0.819**	0.808	0.501	0.745	0.380	0.556
qua2	0.474	0.473	0.528	0.326	**0.535**	0.300	0.385
qua3	0.728	0.649	**0.755**	0.516	0.734	0.472	0.556
qua4	0.563	0.596	**0.669**	0.430	0.662	0.379	0.426
qua5	**0.701**	0.623	0.676	0.503	0.583	0.389	0.450
qua6	0.646	**0.686**	0.682	0.448	0.608	0.418	0.402
qua7	0.698	0.631	**0.816**	0.604	0.797	0.465	0.538
val1	0.475	0.482	0.509	**0.756**	0.558	0.287	0.525
val2	0.635	0.543	0.633	**0.927**	0.710	0.360	0.633
sat1	0.654	**0.760**	0.679	0.445	0.693	0.334	0.584
sat2	0.614	0.606	**0.717**	0.530	0.708	0.416	0.584
sat3	0.718	0.587	0.729	0.649	**0.815**	0.547	0.735
loy1	0.504	0.431	0.419	0.450	0.514	0.237	**0.587**
loy2	0.128	0.146	0.069	0.164	0.130	0.122	**0.181**
loy3	0.618	0.539	0.572	0.531	0.742	0.448	**0.855**

The bold printed value in each row shows on which construct the indicator loads most.

Table 4.21: Cross-loading estimates of OrdPLS

	IMA	EXP	QUA	VAL	SAT	COM	LOY
ima1	**0.765**	0.423	0.620	0.453	0.614	0.458	0.440
ima2	**0.647**	0.445	0.559	0.324	0.474	0.253	0.399
ima3	**0.602**	0.325	0.408	0.362	0.378	0.247	0.376
ima4	**0.799**	0.453	0.652	0.517	0.609	0.491	0.545
ima5	**0.780**	0.456	0.610	0.346	0.570	0.389	0.559
exp1	0.415	**0.779**	0.475	0.334	0.407	0.245	0.336
exp2	0.490	**0.747**	0.428	0.240	0.421	0.273	0.400
exp3	0.348	**0.621**	0.415	0.293	0.346	0.164	0.263
qua1	0.688	0.559	**0.828**	0.522	0.719	0.416	0.563
qua2	0.460	0.351	**0.647**	0.329	0.511	0.314	0.398
qua3	0.671	0.474	**0.801**	0.509	0.678	0.502	0.531
qua4	0.593	0.466	**0.809**	0.457	0.658	0.435	0.435
qua5	0.664	0.495	**0.781**	0.495	0.564	0.435	0.453
qua6	0.642	0.534	**0.826**	0.482	0.620	0.458	0.445
qua7	0.641	0.466	**0.799**	0.577	0.731	0.495	0.505
val1	0.429	0.343	0.511	**0.912**	0.523	0.322	0.480
val2	0.589	0.397	0.627	**0.944**	0.661	0.385	0.620
sat1	0.633	0.526	0.691	0.473	**0.820**	0.379	0.575
sat2	0.572	0.440	0.696	0.524	**0.859**	0.451	0.549
sat3	0.681	0.435	0.705	0.633	**0.871**	0.592	0.677
loy1	0.524	0.383	0.461	0.492	0.513	0.275	**0.855**
loy2	0.095	0.066	0.076	0.138	0.114	0.123	**0.178**
loy3	0.625	0.445	0.610	0.563	0.726	0.496	**0.922**

The bold printed value in each row shows on which construct the indicator loads most.

Table 4.22: Cross-loading estimates of OrdPLSc

	IMA	EXP	QUA	VAL	SAT	COM	LOY
ima1	0.666	0.578	0.653	0.486	**0.679**	0.458	0.497
ima2	0.587	**0.608**	0.588	0.348	0.525	0.253	0.451
ima3	**0.482**	0.443	0.429	0.388	0.419	0.247	0.425
ima4	**0.722**	0.619	0.686	0.554	0.674	0.491	0.615
ima5	**0.709**	0.623	0.641	0.371	0.630	0.389	0.631
exp1	0.469	**0.554**	0.500	0.358	0.450	0.245	0.379
exp2	**0.554**	0.545	0.450	0.257	0.466	0.273	0.452
exp3	0.393	**0.476**	0.436	0.314	0.383	0.164	0.297
qua1	0.777	0.764	**0.834**	0.559	0.795	0.416	0.635
qua2	0.519	0.480	0.557	0.353	**0.566**	0.314	0.449
qua3	0.758	0.648	**0.772**	0.546	0.750	0.502	0.599
qua4	0.670	0.637	**0.737**	0.490	0.729	0.435	0.491
qua5	**0.749**	0.676	0.713	0.531	0.624	0.435	0.512
qua6	0.725	0.729	**0.753**	0.516	0.685	0.458	0.502
qua7	0.724	0.637	**0.825**	0.619	0.808	0.495	0.570
val1	0.485	0.469	0.538	**0.764**	0.579	0.322	0.542
val2	0.665	0.543	0.660	**0.951**	0.731	0.385	0.700
sat1	0.714	0.719	**0.727**	0.507	0.713	0.379	0.649
sat2	0.646	0.601	**0.732**	0.561	0.725	0.451	0.619
sat3	0.769	0.595	0.742	0.678	**0.854**	0.592	0.764
loy1	0.591	0.524	0.485	0.527	0.567	0.275	**0.660**
loy2	0.108	0.090	0.080	**0.148**	0.127	0.123	0.142
loy3	0.705	0.609	0.641	0.603	0.804	0.496	**0.891**

The bold printed value in each row shows on which construct the indicator loads most.

Results of PLS and PLSc for the mobile phone industry customer satisfaction model based on the indicator correlation matrix

A reviewer suggested to estimate the model using the indicator correlation matrix instead of the indicator covariance matrix in case where ordinal categorical indicators are treated as continuous. In the following, the results based on the Bravais-Pearson correlations are reported.

Table 4.23: Path coefficient estimates of the mobile phone customer satisfaction model based on the correlation matrix

	PLS	CI^a		PLSc	CI^b	
β_{21}	**0.505**	0.398	0.622	**0.864**	0.694	0.946
β_{51}	**0.179**	0.075	0.305	0.148	-0.275	0.841
β_{71}	**0.195**	0.051	0.345	-0.114	-0.721	0.594
β_{32}	**0.557**	0.459	0.663	**0.872**	0.707	0.951
β_{42}	0.051	-0.085	0.235	-0.051	-0.694	0.644
β_{52}	0.064	-0.040	0.157	0.036	-0.471	0.504
β_{43}	**0.557**	0.385	0.691	0.721	-0.012	1.291
β_{53}	**0.513**	0.376	0.626	0.667	-0.082	1.095
β_{54}	**0.192**	0.089	0.304	0.177	-0.029	0.311
β_{65}	**0.526**	0.405	0.632	**0.594**	0.472	0.690
β_{75}	**0.483**	0.314	0.633	**0.983**	0.208	1.517
β_{76}	0.071	-0.040	0.194	-0.036	-0.175	0.114

Bold printed values are the coefficient estimates whose corresponding CI does not cover the zero.
Percentile confidence intervals are calculated at a 95% confidence level.
^{a} based on 500 bootstrap samples. ^{b} based on 483 bootstrap samples.

Table 4.24: Factor loading and confidence interval estimates based on the correlation matrix

	PLS	CI[a]		PLSc	CI[b]	
ima1	**0.743**	0.636	0.807	**0.612**	0.439	0.746
ima2	**0.601**	0.474	0.696	**0.538**	0.375	0.657
ima3	**0.578**	0.438	0.686	**0.451**	0.305	0.581
ima4	**0.768**	0.665	0.838	**0.673**	0.515	0.797
ima5	**0.744**	0.675	0.802	**0.667**	0.576	0.776
exp1	**0.771**	0.663	0.845	**0.511**	0.365	0.673
exp2	**0.687**	0.454	0.818	**0.458**	0.303	0.644
exp3	**0.612**	0.450	0.746	**0.440**	0.317	0.572
qua1	**0.803**	0.752	0.847	**0.807**	0.748	0.879
qua2	**0.637**	0.517	0.734	**0.542**	0.419	0.651
qua3	**0.784**	0.714	0.833	**0.753**	0.669	0.831
qua4	**0.769**	0.674	0.849	**0.673**	0.570	0.779
qua5	**0.756**	0.674	0.821	**0.683**	0.560	0.783
qua6	**0.775**	0.629	0.868	**0.682**	0.551	0.811
qua7	**0.779**	0.705	0.836	**0.810**	0.740	0.877
val1	**0.904**	0.856	0.936	**0.754**	0.661	0.856
val2	**0.938**	0.922	0.951	**0.928**	0.860	0.986
sat1	**0.799**	0.744	0.849	**0.693**	0.616	0.778
sat2	**0.846**	0.798	0.885	**0.701**	0.630	0.773
sat3	**0.852**	0.813	0.886	**0.810**	0.754	0.880
loy1	**0.814**	0.701	0.877	**0.594**	0.486	0.721
loy2	**0.219**	0.010	0.413	0.173	-0.013	0.301
loy3	**0.917**	0.890	0.937	**0.869**	0.801	0.971

Bold printed values are the coefficient estimates where the corresponding CI does not cover the zero.
Percentile confidence intervals are calculated on a 95% confidence level.
[a] based on 500 bootstrap samples.   [b] based on 483 bootstrap samples.

Table 4.25: Average variance extracted and shared variance estimates based on the correlation matrix

(a) PLS

	IMA	EXP	QUA	VAL	SAT	LOY
IMAG	**0.478**	0.255	0.561	0.258	0.480	0.318
EXPE	0.505	**0.480**	0.311	0.131	0.260	0.144
QUAL	0.749	0.557	**0.577**	0.343	0.632	0.289
VAL	0.508	0.361	0.586	**0.849**	0.367	0.281
SAT	0.693	0.510	0.795	0.606	**0.693**	0.431
LOY	0.564	0.380	0.538	0.530	0.656	**0.517**

(b) PLSc

	IMA	EXP	QUA	VAL	SAT	LOY
IMAG	**0.353**	0.746	0.858	0.412	0.826	0.577
EXPE	0.864	**0.221**	0.761	0.333	0.716	0.419
QUAL	0.926	0.872	**0.507**	0.457	0.910	0.438
VAL	0.642	0.577	0.676	**0.715**	0.551	0.443
SAT	0.909	0.846	0.954	0.742	**0.542**	0.736
LOY	0.760	0.647	0.662	0.666	0.858	**0.379**

Correlations are below the diagonal, squared correlations are above the diagonal, and AVE estimates are presented on the diagonal (in boldface).

Since the HTMT is based on the indicator correlations it is the same as is observed in Table 4.4.

Table 4.26: Internal consistency reliability using the correlation matrix

(a) Dijkstra-Henseler's ρ_A

	PLS(c)
IMA	**0.740**
EXP	0.462
QUA	**0.884**
VAL	**0.849**
SAT	**0.785**
LOY	**0.746**

(b) Dillon-Goldstein's ρ_c

	PLS	PLSc
IMA	**0.819**	**0.720**
EXP	**0.733**	0.459
QUA	**0.905**	**0.877**
VAL	**0.918**	**0.833**
SAT	**0.871**	**0.780**
LOY	**0.724**	0.590

Values larger than 0.7 are printed in bold.
Results for COM are not reported, as it is connected to one indicator only.

Table 4.27: R^2 of the endogenous constructs

	PLS	PLSc
IMA	0.000	0.000
EXP	0.255	0.746
QUA	0.311	0.761
VAL	0.345	0.457
SAT	0.680	0.931
COM	0.277	0.353
LOY	0.457	0.739

Table 4.28: Cross-loading estimates of PLS based on the correlation matrix

	IMAG	EXPE	QUAL	VAL	SAT	COMP	LOY
ima1	**0.743**	0.350	0.571	0.396	0.549	0.423	0.354
ima2	**0.601**	0.380	0.497	0.274	0.418	0.188	0.304
ima3	**0.578**	0.284	0.368	0.338	0.331	0.207	0.308
ima4	**0.768**	0.370	0.573	0.475	0.548	0.440	0.460
ima5	**0.744**	0.359	0.552	0.271	0.514	0.337	0.493
exp1	0.352	**0.771**	0.436	0.294	0.372	0.183	0.271
exp2	0.408	**0.687**	0.348	0.179	0.366	0.225	0.321
exp3	0.288	**0.612**	0.370	0.274	0.320	0.126	0.196
qua1	0.634	0.514	**0.803**	0.469	0.680	0.380	0.476
qua2	0.430	0.319	**0.637**	0.307	0.490	0.300	0.342
qua3	0.628	0.434	**0.784**	0.473	0.645	0.472	0.473
qua4	0.496	0.391	**0.769**	0.395	0.601	0.379	0.368
qua5	0.609	0.419	**0.756**	0.464	0.524	0.389	0.377
qua6	0.568	0.445	**0.775**	0.410	0.549	0.418	0.343
qua7	0.586	0.417	**0.779**	0.553	0.698	0.465	0.452
val1	0.395	0.312	0.474	**0.904**	0.486	0.287	0.431
val2	0.530	0.351	0.595	**0.938**	0.619	0.360	0.536
sat1	0.577	0.492	0.642	0.411	**0.799**	0.334	0.504
sat2	0.523	0.398	0.670	0.491	**0.846**	0.416	0.497
sat3	0.624	0.391	0.673	0.598	**0.852**	0.547	0.627
loy1	0.434	0.294	0.394	0.413	0.455	0.237	**0.814**
loy2	0.100	0.093	0.063	0.139	0.107	0.122	**0.219**
loy3	0.539	0.356	0.534	0.494	0.663	0.448	**0.917**

The largest loading of each indicator is printed in bold.

Table 4.29: Cross-loading estimates of PLSc based on the correlation matrix

	IMAG	EXPE	QUAL	VAL	SAT	COMP	LOY
ima1	0.612	0.515	0.607	0.430	**0.619**	0.423	0.410
ima2	0.538	**0.560**	0.529	0.298	0.472	0.188	0.352
ima3	**0.451**	0.418	0.391	0.367	0.374	0.207	0.357
ima4	**0.673**	0.545	0.610	0.516	0.619	0.440	0.532
ima5	**0.667**	0.529	0.587	0.294	0.580	0.337	0.571
exp1	0.410	**0.511**	0.464	0.319	0.420	0.183	0.313
exp2	**0.475**	0.458	0.370	0.195	0.413	0.225	0.372
exp3	0.334	**0.440**	0.393	0.298	0.361	0.126	0.227
qua1	0.738	0.756	**0.807**	0.509	0.768	0.380	0.551
qua2	0.500	0.470	0.542	0.333	**0.553**	0.300	0.396
qua3	0.730	0.639	**0.753**	0.514	0.727	0.472	0.548
qua4	0.577	0.575	0.673	0.428	**0.678**	0.379	0.426
qua5	**0.708**	0.617	0.683	0.504	0.591	0.389	0.437
qua6	0.660	0.655	**0.682**	0.445	0.620	0.418	0.397
qua7	0.681	0.613	**0.810**	0.600	0.788	0.465	0.523
val1	0.459	0.458	0.504	**0.754**	0.549	0.287	0.499
val2	0.616	0.517	0.632	**0.928**	0.698	0.360	0.620
sat1	0.671	**0.724**	0.683	0.446	0.693	0.334	0.584
sat2	0.608	0.585	**0.712**	0.533	0.701	0.416	0.575
sat3	0.726	0.575	0.716	0.649	**0.810**	0.547	0.726
loy1	0.505	0.433	0.419	0.448	0.514	0.237	**0.594**
loy2	0.116	0.136	0.067	0.151	0.120	0.122	**0.173**
loy3	0.627	0.525	0.567	0.536	0.748	0.448	**0.869**

The largest loading of each indicator is printed in bold.

Chapter 5

Polynomial factor models: non-iterative estimation via method-of-moments

5.1 Introduction[1]

Structural equation modeling with latent variables (SEM) (Jöreskog, 1969, 1970; Bollen, 1989) is an established method, in particular, in social and behavioral sciences, but also beyond. Its capability to model linear relationships among observed and latent variables, to deal with various forms of measurement errors, and to test entire theories makes it a prime candidate for confirmatory purposes. However, in its original appearance, it faces limitations inherent in its linearity assumptions.

Over the last three decades, there has been a growing interest in modeling non-linear relationships among the latent variables in SEM (Schumacker and Marcoulides, 1998). In particular, the incorporation of quadratic and interaction terms has gained more and more attraction. As a result, a large variety of approaches were developed that can be grouped into the following: product indicator approaches, (e.g., the constrained

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[1]This chapter is based on joint work with Rebecca Büchner, Karin Schermelleh-Engel, and Theo K. Dijkstra.

product indicator approach (Jöreskog and Yang, 1996), or the unconstrained product indicator approach (Marsh et al., 2004)), distribution analytic approaches (e.g., quasi-maximum likelihood estimator (QML) (Klein and Muthén, 2007), or latent moderated structural equations (LMS) (Klein and Moosbrugger, 2000)), moment based approaches (e.g., two-stage method-of-moments estimator (2SMM) (Wall and Amemiya, 2003), or consistent partial least squares for nonlinear structural equation models (PLSc) (Dijkstra and Schermelleh-Engel, 2014)), and Bayesian approaches (e.g., the approach by Arminger and Muthén (1998), or the approach by Kelava and Nagengast (2012)). For a more detailed overview, we referred to Brandt et al. (2015).

In the following Chapter, we introduce a new estimator for recursive nonlinear factor models. It is based on the method-of-moments and is similar to PLSc for nonlinear factor models. However, instead of relying on an iterative procedure to obtain the weights, so-called *one-step weights* are used to build proxies for the latent variables and to estimate the model parameters. Due to its simplicity and less strict assumptions, our approach can be advantageous in complex situations, e.g., where endogenous latent variables are part of higher-order terms.

The remainder of the Chapter is structured as follows: In Section 5.2, we present our new approach. Section 5.3 shows the setup of a Monte Carlo simulation to investigate the performance of our approach. In Section 5.4, we present the results of our simulation study. The Chapter closes with a discussion of the results and an outlook for future research.

5.2 The non-iterative method-of-moments for polynomial factor models

Starting point is a system of q recursive equations with p exogenous and q endogenous latent variables (LVs). The i-th equation can be generally written in the following form:

$$\eta_{p+i} = L_i(\eta_{1:p+i-1}) + \zeta_i, \text{ for } i = 1, ..., q, \tag{5.1}$$

where L_i is a linear function of the preceeding $p+i-1$ LVs. The structural error term ζ_i is assumed to be independent of the LVs from the right-hand side of its equation. Each LV is standardized to have mean of zero and unit variance. Moreover, it is connected

to at least two indicators[2] and each block of indicators $\boldsymbol{y}_i$ is connected to only one LV. The linear measurement model has the typical following form:

$$\boldsymbol{y}_i = \boldsymbol{\lambda}_i \eta_i + \boldsymbol{\epsilon}_i, \tag{5.2}$$

where the vector $\boldsymbol{\lambda}_i$ contains the factor loadings, the vector $\boldsymbol{y}_i$ contains the continuous indicators, and the vector $\boldsymbol{\epsilon}_i$ contains the measurement errors. All of the vectors are of the same length. The measurement errors are mutually independent[3] and independent of all LVs, including the structural error terms. All indicators have a mean of zero and a unit variance, and it is assumed that finite moments of the required order exist. Thus, the correlation matrix $\boldsymbol{\Sigma}_{ii}$ of the indicators of block i is calculated as follows:

$$\mathrm{E}(\boldsymbol{y}_i \boldsymbol{y}_i') = \boldsymbol{\Sigma}_{ii} = \boldsymbol{\lambda}_i \boldsymbol{\lambda}_i' + \boldsymbol{\Theta}_i, \tag{5.3}$$

where the variance-covariance matrix of the measurement errors $\boldsymbol{\Theta}_i$ is a diagonal matrix with the variances of the measurement errors on its diagonal. The correlations between the indicators of two blocks i and j are captured in the matrix $\boldsymbol{\Sigma}_{ij}$ which is given by the following:

$$\mathrm{E}(\boldsymbol{y}_i \boldsymbol{y}_j') = \boldsymbol{\Sigma}_{ij} = \rho_{ij} \boldsymbol{\lambda}_i \boldsymbol{\lambda}_j', \tag{5.4}$$

where $\boldsymbol{\lambda}_i$ and $\boldsymbol{\lambda}_j$ denote the vectors containing the factor loadings of block i and j, respectively, and ρ_{ij} is the correlation between the LVs η_i and η_j. In the following, the matrices $\boldsymbol{S}_{ii}$ and $\boldsymbol{S}_{ij}$ denote the sample counterparts of $\boldsymbol{\Sigma}_{ii}$ and $\boldsymbol{\Sigma}_{ij}$ and represent consistent estimates. Since we assume continuous indicators, the correlations are estimated by the Bravais-Pearson correlation coefficient.

5.2.1 Factor loadings

The parameters of the measurement model and the structural model are estimated separately. For the estimation of both, we use composites that serve as proxies for the LVs. A composite is defined as a weighted linear combination of its connected indicators. To build the proxies we refer to *all-adjacent one-step weights* that are

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[2]The *MoMpoly* function can also treat single-indicator LVs. In this case, the LV equals the indicator.

[3]This assumption is not necessary for measurements errors of one block of indicators and the MoMpoly package is capable of dealing with correlated measurement errors within a block, see (Dijkstra, 2013b).

calculated for block i as follows:

$$\hat{\boldsymbol{w}}_i \propto \sum_{j \neq i} e_{ij} \boldsymbol{S}_{ij} \boldsymbol{w}_j, \tag{5.5}$$

where $\boldsymbol{w}_j$ is an arbitrary weight vector of the same length as the vector $\boldsymbol{y}_j$ and the inner weight is defined as the sign of the correlation between proxy i and proxy j, $e_{ij} = \text{sign}(\boldsymbol{w}_i' \boldsymbol{S}_{ij} \boldsymbol{w}_j)$. The arbitrary weight vector $\boldsymbol{w}_j$ as well as $\hat{\boldsymbol{w}}_i$ are normalized to ensure a unit variance of each composite, $\boldsymbol{w}_j' \boldsymbol{S}_{jj} \boldsymbol{w}_j = 1$, and $\hat{\boldsymbol{w}}_i' \boldsymbol{S}_{ii} \hat{\boldsymbol{w}}_i = 1$. In contrast to the *all-adjacent one-step weights*, where all LVs except the i-th LV are taken into account ($j \neq i$) for the calculation of $\hat{\boldsymbol{w}}_i$, it can be useful to calculate the weights based on the adjacent LVs only, $j \in C(i)$, where $C(i)$ contains the indices of the LVs connected directly via the structural model. We call the latter approach *adjacent-only one-step weights*.

The probability limit of $\hat{\boldsymbol{w}}_i$ is given by the following:[4]

$$\bar{\boldsymbol{w}}_i = \text{plim}(\hat{\boldsymbol{w}}_i) = \frac{\boldsymbol{\lambda}_i}{\sqrt{\boldsymbol{\lambda}_i' \boldsymbol{\Sigma}_{ii} \boldsymbol{\lambda}_i}}. \tag{5.6}$$

It is obvious that the weights are not equal, but proportional to the factor loadings and that they are distorted by the factor $(\boldsymbol{\lambda}_i' \boldsymbol{\Sigma}_{ii} \boldsymbol{\lambda}_i)^{-\frac{1}{2}}$. However, consistent factor loading estimates can be obtained by rescaling the estimated weights. A straightforward way of obtaining a scaling factor $\hat{c}_i$ with $\text{plim}(\hat{c}_i) = \sqrt{\boldsymbol{\lambda}_i' \boldsymbol{\Sigma}_{ii} \boldsymbol{\lambda}_i}$ is the minimization of the squared difference between off-diagonal elements[5] of

$$\boldsymbol{S}_{ii} \quad \text{and} \quad \hat{c}_i^2 \hat{\boldsymbol{w}}_i \hat{\boldsymbol{w}}_i' \tag{5.7}$$

with respect to $\hat{c}_i^2$. As a result, we obtain the correction factor as

$$\hat{c}_i = \sqrt{\frac{\hat{\boldsymbol{w}}_i'(\boldsymbol{S}_{ii} - \text{diag}(\boldsymbol{S}_{ii}))\hat{\boldsymbol{w}}_i}{\hat{\boldsymbol{w}}_i'(\hat{\boldsymbol{w}}_i \hat{\boldsymbol{w}}_i' - \text{diag}(\hat{\boldsymbol{w}}_i \hat{\boldsymbol{w}}_i'))\hat{\boldsymbol{w}}_i}}, \tag{5.8}$$

where $\text{diag}(\boldsymbol{S}_{ii})$ and $\text{diag}(\hat{\boldsymbol{w}}_i \hat{\boldsymbol{w}}_i'))$ return a diagonal matrix containing the main diagonal elements of $\boldsymbol{S}_{ii}$ and $\hat{\boldsymbol{w}}_i \hat{\boldsymbol{w}}_i'$, respectively on its diagonal. The factor loadings can be consistently estimated by $\hat{\boldsymbol{\lambda}}_i = \hat{c}_i \hat{\boldsymbol{w}}_i$.

5.2.2 Correlations between the latent variables

Since we consider a recursive system of equations where the structural error term of each equation is independent of the LVs on the right-hand side of the equation, each

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[4] See the Appendix for a derivation of the $\text{plim}(\hat{\boldsymbol{w}}_i)$.

[5] Other ways of obtaining the correction factor $\hat{c}_i$ are conceivable (Dijkstra, 2013b) and are implemented in the MoMpoly package.

equation can be treated as an ordinary regression equation. Thus, the path coefficients are determined by the moments of the LVs and consistent estimates of the moments are required for their estimation. For this purpose, we define a population proxy $\bar{\eta}_i$ for each LV η_i by $\bar{\eta}_i = \bar{\boldsymbol{w}}_i'\boldsymbol{y}_i$. Replacing the vector of indicators $\boldsymbol{y}_i$ by the measurement model, we obtain the following:

$$\bar{\eta}_i = \bar{\boldsymbol{w}}_i'\boldsymbol{y}_i = \bar{\boldsymbol{w}}_i'\boldsymbol{\lambda}_i\eta_i + \bar{\boldsymbol{w}}_i'\boldsymbol{\epsilon}_i = Q_i\eta_i + \delta_i, \tag{5.9}$$

where Q_i is the correlation between the proxy and the LV, which is usually denoted as *quality* of proxy $\bar{\eta}_i$ (Dijkstra and Henseler, 2015b). Hence, the squared correlation between the proxy and its LV is obtained as follows:

$$Q_i^2 = r^2(\eta_i, \bar{\eta}_i) = (\bar{\boldsymbol{w}}_i'\boldsymbol{\lambda}_i)^2 = \bar{c}_i^2(\bar{\boldsymbol{w}}_i'\bar{\boldsymbol{w}}_i)^2. \tag{5.10}$$

Moreover, the squared correlation between two population proxies $\bar{\eta}_i$ and $\bar{\eta}_j$ is given by the following:

$$r^2(\bar{\eta}_i, \bar{\eta}_j) = (\bar{\boldsymbol{w}}_i'\boldsymbol{\Sigma}_{ij}\bar{\boldsymbol{w}}_j)^2. \tag{5.11}$$

From Equation 5.11, an important relationship between the correlations of two proxies and the correlation between two LVs can be deduced as follows:

$$r^2(\bar{\eta}_i, \bar{\eta}_j) = (\rho_{ij}\bar{\boldsymbol{w}}_i'\boldsymbol{\lambda}_i\bar{\boldsymbol{w}}_j'\boldsymbol{\lambda}_j)^2 = \rho_{ij}^2(\bar{\boldsymbol{w}}_i'\boldsymbol{\lambda}_i)^2(\bar{\boldsymbol{w}}_j'\boldsymbol{\lambda}_j)^2 = \rho_{ij}^2 Q_i^2 Q_j^2. \tag{5.12}$$

Since the qualities of the proxies are smaller than 1, it is obvious that the correlation between the two LVs is underestimated by the correlation of the proxies. However, the correlation can be consistently estimated by solving Equation 5.12 for the correlation ρ_{ij} and by replacing the theoretical quantities by their sample counterparts,

$$\hat{\rho}_{ij} = \frac{\hat{\boldsymbol{w}}_i'\boldsymbol{S}_{ij}\hat{\boldsymbol{w}}_j}{\hat{Q}_i\hat{Q}_j}. \tag{5.13}$$

As, we obtain consistent LV correlation estimates, it is straightforward to calculate the path coefficient estimates.

Something similar was already done by Dijkstra and Schermelleh-Engel (2014) for polynomial factor models and by Dijkstra and Henseler (2015a,b) for linear models using PLS weights. In contrast to PLS weights, our proposed weights are not obtained by iteration until a certain fix point is reached. Evidentially, for the proportionality of the weights to the factor loadings, the iterative procedure from PLS is not required.

5.2.3 Model with interaction terms

To illustrate our approach for polynomial factor models, we extend the initial model by two-way interaction terms. Again, equation i of a system of q recursive equations containing linear and two-way interaction terms can be generally written as follows:

$$\eta_{p+i} = L_i(\eta_{1:p+i-1}) + I_i(\eta_{1:p+i-1}) + \zeta_i, \text{ for } i = 1, ..., q. \tag{5.14}$$

$L(\eta_{1:p+i-1})$ is a linear function of the $p + i - 1$ preceding LVs and $I(\eta_{1:p+i-1})$ is a linear function of their centered cross-products $\eta_k \eta_l - \rho_{kl}$, where the indices k and l refer to different LVs. Again, each structural error term is independent of the LVs on the right-hand side of its equation leading to q regression equations. Therefore, the path coefficients of each equation are determined by the covariances among the explanatory LVs on the right-hand side and the covariances between the explanatory LVs and the dependent LV. To calculate these covariances, the following moments are required:[6]

$$\text{E}(\bar{\eta}_i^2 \bar{\eta}_j) = Q_i^2 Q_j \, \text{E}(\eta_i^2 \eta_j), \tag{5.15}$$

$$\text{E}(\bar{\eta}_i \bar{\eta}_j \bar{\eta}_k) = Q_i Q_j Q_k \, \text{E}(\eta_i \eta_j \eta_k), \tag{5.16}$$

$$\text{E}(\bar{\eta}_i^2 \bar{\eta}_j^2) = Q_i^2 Q_j^2 (\text{E}(\eta_i^2 \eta_j^2) - 1) + 1, \text{ and} \tag{5.17}$$

$$\text{E}(\bar{\eta}_i^2 \bar{\eta}_j \bar{\eta}_k) = Q_i^2 Q_j Q_k \, \text{E}(\eta_i^2 \eta_j \eta_k) + \text{E}(\eta_j \eta_k) Q_j Q_k (1 - Q_i^2), \tag{5.18}$$

where the different subscripts indicate different proxies and their corresponding LVs.

To obtain estimates of the moments of the LVs, and thus, the path coefficient estimates, each Equation from 5.15 to 5.18 is solved for the moment of the LVs and the qualities Q are replaced by their estimates. Furthermore, the theoretical moments of the proxies need to be replaced by their sample counterparts, i.e, by the average product of the sample proxies.

For a further illustration, we consider a single equation with two exogenous LVs η_1 and η_2 and a two-way interaction term, which is as follows:

$$\eta_3 = \gamma_1 \eta_1 + \gamma_2 \eta_2 + \gamma_{12}(\eta_1 \eta_2 - \rho_{12}) + \zeta_1, \tag{5.19}$$

where the γ's satisfy the following moment equations:

$$\begin{pmatrix} \text{E}(\eta_3 \eta_1) \\ \text{E}(\eta_3 \eta_2) \\ \text{E}(\eta_3 \eta_1 \eta_2) \end{pmatrix} = \begin{pmatrix} 1 & \text{E}(\eta_1 \eta_2) & \text{E}(\eta_1^2 \eta_2) \\ \text{E}(\eta_1 \eta_2) & 1 & \text{E}(\eta_1 \eta_2^2) \\ \text{E}(\eta_1^2 \eta_2) & \text{E}(\eta_1 \eta_2^2) & \text{E}(\eta_1^2 \eta_2^2) - \text{E}(\eta_1 \eta_2)^2 \end{pmatrix} \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_{12} \end{pmatrix}. \tag{5.20}$$

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[6] See the Appendix for their derivation.

The path coefficient estimates are obtained by replacing the theoretical moments by their estimates and by solving Equation 5.20 for $\boldsymbol{\gamma}$.

It is important to mention here that besides the existence of the finite moments and the usual independence assumptions of certain variables, no distributional assumptions are needed to estimate the path coefficients. However, if we add higher-order terms, making assumptions on the higher-order moments of the δ's from Equation 5.9 cannot be avoided.

5.2.4 Model with higher-order terms

To highlight this issue, we additionally include quadratic terms to the initial system of equations. However, following the same logic, it is straightforward to include cubic $(\eta_i^3 - \mathrm{E}(\eta_i^3))$, quartic $(\eta_i^4 - \mathrm{E}(\eta_i^4))$, or even higher-order terms and interaction terms consisting of more than two LVs. Again, we consider the i-th equation of a system of q recursive equations, containing $q + p$ LVs, evident below:

$$\eta_{p+i} = L_i(\eta_{1:p+i-1}) + I_i(\eta_{1:p+i-1}) + Sq_i(\eta_{1:p+i-1}) + \zeta_i. \tag{5.21}$$

The functions L_i and I_i are defined as above. The function Sq_i is a linear function of the centered squares $\eta^2 - 1$ of the proceeding $p + i - 1$ LVs. Since each structural error term ζ_i is independent of the LVs of the right-hand side of its equation, each equation can be treated separately and the path coefficients are determined by the covariances among the explanatory variables and those between the explanatory LVs and the dependent LV. While the covariances between the dependent LV and the explanatory LVs can be estimated by the moments presented in Section 5.2.3, higher-order moments are required for the calculation of the covariance matrix of the explanatory variables of each equation, which are as follows:

$$\mathrm{E}(\bar{\eta}_i^3 \bar{\eta}_j) = Q_i^3 Q_j \, \mathrm{E}(\eta_i^3 \eta_j) + 3 \, \mathrm{E}(\bar{\eta}_i \bar{\eta}_j)(1 - Q_i^2) \tag{5.22}$$

$$\mathrm{E}(\bar{\eta}_i^3) = Q_i^3 \, \mathrm{E}(\eta_i^3) + \mathrm{E}(\delta_i^3) \tag{5.23}$$

$$\mathrm{E}(\bar{\eta}_i^4) = Q_i^4 \, \mathrm{E}(\eta_i^4) + 6 Q_i^2 (1 - Q_i^2) + \mathrm{E}(\delta_i^4). \tag{5.24}$$

Obviously, assumptions on the higher-order moments of the δ's are required for the calculation of the moments of the LVs in Equation 5.23 and 5.24, i.e., $\mathrm{E}(\delta_i^3)$ and $\mathrm{E}(\delta_i^4)$.

In the following, we adopt the moments of the normal distribution, i.e., a skewness of zero, $E(\delta_i^3) = 0$, and a kurtosis of $3(1 - Q_i^2)^2 = E(\delta_i^4)$.[7]

In principle, adding further higher-order terms or interaction terms consisting of more than two LVs is not a problem; however, the estimation of the required moments becomes more and more challenging as further higher-order moments are needed. To our knowledge, there exist no general formula to obtain the higher-order moments without making distributional assumptions. Therefore, for simplicity, we assume joint normality of all exogenous variables, i.e., $\eta_{1:p}$, the ζ's, and the ϵ's. It is well-known that the moments of joint normally distributed random variables are solely determined by their moments up to the second-order. Since all LVs are standardized, the moments of the exogenous LVs simplify as follows:

$$E(\eta_i^2 \eta_j) = 0 \tag{5.25}$$

$$E(\eta_i \eta_j \eta_k) = 0 \tag{5.26}$$

$$E(\eta_i^2 \eta_j^2) = 1 + 2\rho_{ij}^2 \tag{5.27}$$

$$E(\eta_i^2 \eta_j \eta_k) = \rho_{jk} + 2\rho_{ij}\rho_{ik}. \tag{5.28}$$

The estimated moments are obtained by replacing ρ_{ij} by its estimate from Equation 5.13.

Of course, the moments of endogenous LVs as well as the moments of a mixture of endogenous and exogenous LVs require some attention, since the moments of the normal distribution can only be applied if the explanatory endogenous and exogenous LVs considered are indeed jointly normally distributed. This is for example not the case if the endogenous LV is explained in a previous equation by a higher-order or an interaction term, even if every LV, which is part of the higher-order or the interaction term, itself is normally distributed. In particular, in systems of several equations, endogenous latent variables often appear on the right-hand side of the equation, which violates the assumption of joint normality of the explanatory variable if the endogenous LV is not normally distributed. However, as we only consider recursive models, each endogenous LV can be expressed by exogenous LVs solely, which are, by assumption, jointly normally distributed. Therefore, the path coefficients can be retrieved from the 'replaced' equations.[8]

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[7]The kurtosis of a normally distributed random variable, $X \sim N(\mu, \sigma^2)$ is given by $E((X^4 - E(X))^4) = 3\sigma^4$.

[8]In the MoMpoly package, this approach is called *approach.replace*.

5.3 Monte Carlo simulation

To investigate the performance of our approach, in particular, parameter recovery and standard deviations of the parameter estimates, we run a Monte Carlo simulation. We consider two models, one single structural equation model consisting of two exogenous LVs, their quadratic and interaction terms, which is given by the following:

$$\eta_3 = \gamma_1\eta_1 + \gamma_2\eta_2 + \gamma_{11}(\eta_1^2 - 1) + \gamma_{12}(\eta_1\eta_2 - \rho_{12}) + \gamma_{22}(\eta_2^2 - 1) + \zeta_1. \tag{5.29}$$

The structural error term ζ_1 is independent of the explanatory variables and the correlation between the two exogenous LVs η_1 and η_2 is set to 0.3. The population path coefficients are set to $\gamma_1 = 0.3$, $\gamma_2 = 0.4$, $\gamma_{11} = 0.12$, $\gamma_{12} = 0.15$, and $\gamma_{22} = 0.1$.

Furthermore, we consider a second, more complex model consisting of the following recursive equations:

$$\begin{aligned}
\eta_3 &= \gamma_{31}\eta_1 + \gamma_{32}\eta_2 + \zeta_1 \\
\eta_4 &= \gamma_{41}\eta_1 + \gamma_{43}\eta_3 + \gamma_{433}(\eta_3^2 - 1) + \zeta_2 \\
\eta_5 &= \gamma_{52}\eta_2 + \gamma_{54}\eta_4 + \gamma_{534}(\eta_3\eta_4 - \mathrm{E}(\eta_3\eta_4)) + \zeta_3.
\end{aligned} \tag{5.30}$$

The structural errors are mutually independent and independent of the exogenous latent variables. The population path coefficients are set to $\gamma_{31} = 0.5$, $\gamma_{32} = -0.4$, $\gamma_{41} = 0.35$, $\gamma_{43} = 0.2$, $\gamma_{433} = -0.1$, $\gamma_{52} = 0.3$, $\gamma_{54} = -0.25$, and $\gamma_{534} = 0.3$ The correlation between the two exogenous LVs is set to $\rho_{12} = 0.3$. The correlation between η_3 and η_4 yield 0.333.

The measurement model has the following form: $\boldsymbol{y}_i = \boldsymbol{\lambda}_i\eta_i + \boldsymbol{\epsilon}_i$, where each standardized LV η_i is connected to 3 standardized indicators captured in the vector $\boldsymbol{y}_i$. For each of the three blocks, the factor loadings are set to $\boldsymbol{\lambda}_i' = \begin{pmatrix} 0.9 & 0.85 & 0.8 \end{pmatrix}$. Moreover, all measurement errors are mutually independent and independent of the LVs.

For each model, 500 data sets with $N = 400$ observations each are generated from the multivariate normal distribution with means zero and the corresponding variance-covariance matrix of the exogenous variables (exogenous LVs, measurement and structural errors). Using the generated values of the exogenous LVs, it is straightforward to obtain the values of the endogenous LVs and the indicators. Each sample is standardized before the analysis.

As a benchmark comparison, for the first model, we compare our approach to latent moderated structural equations (LMS), a maximum likelihood estimator that is known

to be asymptotically efficient under normality of the exogenous variables (Klein and Moosbrugger, 2000). Due to the model complexity, the second model is only estimated by MoMpoly.

The whole simulation is conducted in R (R Core Team, 2016), except the estimation of the first model using LMS, which is conducted in Mplus (Muthén and Muthén, 1998-2015). The results of our approach are obtained by the MoMpoly function from the MoMpoly package[9]. As starting weights, we use unit weights for every estimation. Moreover, we use the *all-adjacent one-step weights* to build the proxies for the latent variables. The data sets for the exogenous variables are generated in R using the mvrnorm function from the MASS package (Venables and Ripley, 2002). To compare all estimation in a fair way, we drop all Heywood cases from the results. Based on the remaining estimates, averages and standard deviations are calculated.

5.4 Results

This section provides the results of our simulation. The results for the single-equation model from Equation 5.29 are shown in Table 5.1. It contains the average parameter estimates obtained from MoMpoly and LMS and their corresponding standard deviations. Due to space constraints, not all parameters are presented but can be found in the Appendix.

Table 5.1: Results for the first model

Para.	true	mean MoMpoly[1]	mean LMS[2]	sd MoMpoly[1]	sd LMS[2]
γ_1	0.30	0.298	0.297	0.048	0.047
γ_2	0.40	0.403	0.402	0.047	0.045
γ_{11}	0.12	0.118	0.117	0.044	0.041
γ_{12}	0.15	0.147	0.147	0.062	0.059
γ_{22}	0.10	0.104	0.101	0.042	0.039
ρ_{12}	0.30	0.300	0.299	0.052	0.052
λ_{11}	0.90	0.898	0.899	0.044	0.017
λ_{12}	0.85	0.854	0.852	0.052	0.018
λ_{13}	0.80	0.795	0.800	0.058	0.022

[1]Inadmissible results are removed, and therefore, the results are based on 484 estimations.
[2]No inadmissible results were produced.

While LMS produces no improper solutions (Heywood cases), MoMpoly produces 16 estimations where at least one absolute factor loading is larger than 1. The results

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[9]The package is provided by the first author upon request.

show that the mean path coefficient estimates from MoMpoly are very similar to those from LMS, which are close to the values of the population parameters. The standard deviations of path coefficient estimates from MoMpoly are only slightly larger compared to those from LMS. However, although both methods produce similar average factor loading estimates, it is salient that the factor loading estimates from MoMpoly show larger standard deviations than those from LMS.

The results for the second model are presented in Table 5.2. Again, the average estimates and their standard deviations are shown.

Table 5.2: Results for the second model

Para.	true	mean[1]	sd[1]
γ_{31}	0.50	0.502	0.049
γ_{32}	-0.40	-0.395	0.053
γ_{41}	0.35	0.347	0.056
γ_{43}	0.20	0.201	0.058
γ_{433}	-0.10	-0.099	0.038
γ_{52}	0.30	0.301	0.050
γ_{54}	-0.25	-0.247	0.052
γ_{534}	0.30	0.298	0.052
ρ_{12}	0.30	0.299	0.051
λ_{51}	0.90	0.895	0.054
λ_{51}	0.85	0.846	0.061
λ_{51}	0.80	0.803	0.068

[1]Inadmissible results are removed, and therefore, the results are based on 475 estimations.

In 15 out 500 estimations, at least one absolute factor loading is estimated larger than one. Also, for the more complex model, both average path coefficient and factor loading estimates are close to the true value.

5.5   Discussion and future research

We introduce a new estimator based on non-iterative method-of-moments (MoMpoly), which is capable of consistently estimating recursive polynomial factor models. The results of our Monte Carlo simulation show that MoMpoly produces average estimates for path coefficients and factor loadings close to the population values. However, MoMpoly estimates show larger standard deviations than those from LMS. This is particularly the case for factor loading estimates. This is not surprising as the circumstances of our simulation study favors LMS, which is a maximum likelihood estimator and known to be asymptotically efficient and consistent if the underlying assumptions hold. More-

over, in contrast to LMS, MoMpoly is a partial information method, i.e., the proxies are built without taking into account the detailed specification of the structural model. Thus, MoMpoly cannot be expected to be as asymptotically efficient as LMS. However, due to its simplicity, MoMpoly is an estimator with tremendous potential, in particular for complex models and situations where LMS faces its limitations.

In this context, an important issue is the investigation of MoMpolys' robustness to non-normally distributed samples and its performance for misspecified models. Due to the nature of MoMpoly (partial information approach), it might be more robust to erroneous model specifications. To further leverage the capabilities of MoMpoly, future research needs to address the issue of correlated structural error terms inducing the problem of endogeneity and the resulting consequences for the parameter estimates. A possible way out could be the combination of MoMpoly with the two-stage least squares estimator. Moreover, we want to investigate the use of other moments for the δ's than those from the normal distribution. Finally, the MoMpoly approach can be easily modified to estimate non-linear composite models.

5.6 Appendix to Chapter 5

Probability limit of the estimated weight vector $\hat{\boldsymbol{w}}_i$

We assume that $\text{plim}(\boldsymbol{S}_{ij}) = \boldsymbol{\Sigma}_{ij} = \rho_{ij}\boldsymbol{\lambda}_i\boldsymbol{\lambda}_j'$. The probability limit (plim) of the estimated weights can be calculated by replacing the empirical covariance matrix $\boldsymbol{S}_{ij}$ by its theoretical counterpart $\boldsymbol{\Sigma}_{ij}$ in Equation 5.6, which leads to the following:

$$\bar{\boldsymbol{w}}_i = \text{plim}(\hat{\boldsymbol{w}}_i) \propto \sum_{j\neq i} e_{ij}\boldsymbol{\Sigma}_{ij}\boldsymbol{w}_j = \sum_{j\neq i} e_{ij}\rho_{ij}\boldsymbol{\lambda}_i\boldsymbol{\lambda}_j'\boldsymbol{w}_j = \boldsymbol{\lambda}_i\sum_{j\neq i} e_{ij}\rho_{ij}\boldsymbol{\lambda}_j'\boldsymbol{w}_j. \tag{5.31}$$

The expression $\sum_{j\neq i} e_{ij}\rho_{ij}\boldsymbol{\lambda}_j'\boldsymbol{w}_j$ is a constant term, and therefore, $\bar{\boldsymbol{w}}_i$ is proportional to the population loading vector $\boldsymbol{\lambda}_i$:

$$\bar{\boldsymbol{w}}_i = a_i\boldsymbol{\lambda}_i, \tag{5.32}$$

where a_i is a constant term. Since the weights are scaled to ensure that the proxy has a unit variance, the following holds:

$$\bar{\boldsymbol{w}}_i'\boldsymbol{\Sigma}_{ii}\bar{\boldsymbol{w}}_i = 1 = a_i^2\boldsymbol{\lambda}_i\boldsymbol{\Sigma}_{ii}\boldsymbol{\lambda}_i. \tag{5.33}$$

This leads to $a_i = 1/\sqrt{\boldsymbol{\lambda}_i'\boldsymbol{\Sigma}_{ii}\boldsymbol{\lambda}_i}$ and $\bar{\boldsymbol{w}}_i = \boldsymbol{\lambda}_i/\sqrt{\boldsymbol{\lambda}_i'\boldsymbol{\Sigma}_{ii}\boldsymbol{\lambda}_i}$ and shows that the weights cannot be directly used to estimate the factor loadings, since the weights are distorted by the factor $\sqrt{\boldsymbol{\lambda}_i'\boldsymbol{\Sigma}_{ii}\boldsymbol{\lambda}_i}$.

Probability limit of the correction factor $\hat{c}_i$

A correction factor to control for this distortion can be obtained by minimizing the squared difference between the off-diagonal elements of $\boldsymbol{S}_{ii}$ and $\hat{c}_i^2\hat{\boldsymbol{w}}_i\hat{\boldsymbol{w}}_i'$. The resultant correction factor is given by the following:

$$\hat{c}_i = \sqrt{\frac{\hat{\boldsymbol{w}}_i'(\boldsymbol{S}_{ii} - \text{diag}(\boldsymbol{S}_{ii}))\hat{\boldsymbol{w}}_i}{\hat{\boldsymbol{w}}_i'(\hat{\boldsymbol{w}}_i\hat{\boldsymbol{w}}_i' - \text{diag}(\hat{\boldsymbol{w}}_i\hat{\boldsymbol{w}}_i'))\hat{\boldsymbol{w}}_i}}. \tag{5.34}$$

The plim of $\hat{c}_i$ can be obtained by replacing $\hat{\boldsymbol{w}}_i$ and $\boldsymbol{S}_{ii}$ by their theoretical counterparts (see Equation 5.32 and 5.3):

$$c_i = \text{plim}(\hat{c}_i) = \sqrt{\frac{\bar{\boldsymbol{w}}_i'(\boldsymbol{\Sigma}_{ii} - \text{diag}(\boldsymbol{\Sigma}_{ii}))\bar{\boldsymbol{w}}_i}{\bar{\boldsymbol{w}}_i'(\bar{\boldsymbol{w}}_i\bar{\boldsymbol{w}}_i' - \text{diag}(\bar{\boldsymbol{w}}_i\bar{\boldsymbol{w}}_i'))\bar{\boldsymbol{w}}_i}} = \tag{5.35}$$

$$= \sqrt{\frac{a_i\boldsymbol{\lambda}_i'(\boldsymbol{\lambda}_i\boldsymbol{\lambda}_i' + \boldsymbol{\Theta}_{ii} - \text{diag}(\boldsymbol{\lambda}_i\boldsymbol{\lambda}_i' + \boldsymbol{\Theta}_{ii}))a_i\boldsymbol{\lambda}_i}{a_i\boldsymbol{\lambda}_i'(a_i\boldsymbol{\lambda}_i a_i\boldsymbol{\lambda}_i' - \text{diag}(a_i\boldsymbol{\lambda}_i a_i\boldsymbol{\lambda}_i'))a_i\boldsymbol{\lambda}_i}} = \tag{5.36}$$

$$= \sqrt{\frac{a_i\boldsymbol{\lambda}_i'(\boldsymbol{\lambda}_i\boldsymbol{\lambda}_i' - \text{diag}(\boldsymbol{\lambda}_i\boldsymbol{\lambda}_i'))a_i\boldsymbol{\lambda}_i}{a_i\boldsymbol{\lambda}_i'(a_i\boldsymbol{\lambda}_i a_i\boldsymbol{\lambda}_i' - \text{diag}(a_i\boldsymbol{\lambda}_i a_i\boldsymbol{\lambda}_i'))a_i\boldsymbol{\lambda}_i}} = \tag{5.37}$$

$$= \sqrt{\frac{1}{a^2}} = \sqrt{\frac{1}{1/\boldsymbol{\lambda}_i'\boldsymbol{\Sigma}_{ii}\boldsymbol{\lambda}_i}} = \sqrt{\boldsymbol{\lambda}_i'\boldsymbol{\Sigma}_{ii}\boldsymbol{\lambda}_i}. \tag{5.38}$$

Derivation of the moments of the explanatory variables in case of one-way interaction terms

In the following, we derive the moments required for the calculation of the covariances of the model with two-way interaction terms presented in Section 5.2.3. It is important to keep in mind, that the LVs are assumed to be standardized having means of zero and unit variances. Furthermore, the measurement errors are mutually independent and they are independent of the LVs. The mean and the variance of δ_i can be calculated as follows:

$$\text{E}(\delta_i) = \text{E}(\bar{\boldsymbol{w}}_i'\boldsymbol{\epsilon}_i) = \bar{\boldsymbol{w}}_i'\text{E}(\boldsymbol{\epsilon}_i) = \bar{\boldsymbol{w}}_i'\boldsymbol{0} = 0 \tag{5.39}$$

$$\bar{\eta}_i = Q_i\eta_i + \delta_i \Leftrightarrow \delta_i = \bar{\eta}_i - Q_i\eta_i \tag{5.40}$$

$$\text{var}(\delta_i) = \text{E}(\delta_i^2) - \text{E}(\delta_i)^2 = \text{E}((\bar{\eta}_i - Q_i\eta_i)^2) - 0^2 = \tag{5.41}$$

$$\text{E}(\bar{\eta}_i^2 - 2Q_i\bar{\eta}_i\eta_i + Q_i^2\eta_i^2) = 1 - 2Q_i^2 + Q_i^2 = 1 - Q_i^2. \tag{5.42}$$

We start with the moment presented in Equation 5.15, which can be derived as follows:

$$\text{E}(\bar{\eta}_i^2\bar{\eta}_j) = \text{E}((Q_i\eta_i + \delta_i)^2(Q_j\eta_j + \delta_j)) = \tag{5.43}$$

$$\text{E}(Q_i^2\eta_i^2 + 2Q_i\eta_i\delta_i + \delta_i^2)(Q_j\eta_j + \delta_j)) = \tag{5.44}$$

$$Q_i^2Q_j\text{E}(\eta_i^2\eta_j) + 2Q_iQ_j\text{E}(\eta_i\eta_j)\text{E}(\delta_i) + Q_j\text{E}(\delta_i^2)\text{E}(\eta_j) + \tag{5.45}$$

$$Q_i^2\text{E}(\eta_i^2)\text{E}(\delta_j) + 2Q_i\text{E}(\eta_i)\text{E}(\delta_i)\text{E}(\delta_j) + \text{E}(\delta_i^2)\text{E}(\delta_j) = \tag{5.46}$$

$$Q_i^2Q_j\text{E}(\eta_i^2\eta_j) + 2Q_iQ_j\rho_{ij}\cdot 0 + Q_j(1 - Q_i^2)\cdot 0 + Q_i^2\cdot 1\cdot 0 + \tag{5.47}$$

$$2Q_i\cdot 0\cdot 0\cdot 0 + (1 - Q_i^2)\cdot 0 = \tag{5.48}$$

$$Q_i^2Q_j\text{E}(\eta_i^2\eta_j). \tag{5.49}$$

The moment presented in Equation 5.16 can be calculated as follows:

$$\mathrm{E}(\bar{\eta}_i \bar{\eta}_j \bar{\eta}_k) = \mathrm{E}((Q_i \eta_i + \delta_i)(Q_j \eta_j + \delta_j)(Q_k \eta_k + \delta_k)). \tag{5.50}$$

Since $\mathrm{E}(\delta_i) = \mathrm{E}(\delta_j) = \mathrm{E}(\delta_k) = 0$ and the error terms are mutually independent, it is obvious that the above equation reduces to the following:

$$\mathrm{E}(\bar{\eta}_i \bar{\eta}_j \bar{\eta}_k) = Q_i Q_j Q_k \, \mathrm{E}(\eta_i \eta_j \eta_k). \tag{5.51}$$

Next, we derive the moment from Equation 5.17:

$$\mathrm{E}(\bar{\eta}_i^2 \bar{\eta}_j^2) = \mathrm{E}((Q_i \eta_i + \delta_i)^2 (Q_j \eta_j + \delta_j)^2) = \tag{5.52}$$

$$\mathrm{E}((Q_i^2 \eta_i^2 + 2Q_i \eta_i \delta_i + \delta_i^2)(Q_j^2 \eta_j^2 + 2Q_j \eta_j \delta_j + \delta_j^2)) = \tag{5.53}$$

$$\mathrm{E}((Q_i^2 \eta_i^2 + 2Q_i \eta_i \delta_i + \delta_i^2)Q_j^2 \eta_j^2) + \tag{5.54}$$

$$\mathrm{E}((Q_i^2 \eta_i^2 + 2Q_i \eta_i \delta_i + \delta_i^2)2Q_j \eta_j \delta_j) + \tag{5.55}$$

$$\mathrm{E}((Q_i^2 \eta_i^2 + 2Q_i \eta_i \delta_i + \delta_i^2)\delta_j^2) = \tag{5.56}$$

$$Q_i^2 Q_j^2 \, \mathrm{E}(\eta_i^2 \eta_j^2) + 0 + (1 - Q_i^2)Q_j^2 + \tag{5.57}$$

$$0 + 0 + 0 + \tag{5.58}$$

$$Q_i^2(1 - Q_j^2) + 0 + (1 - Q_i^2)(1 - Q_j^2) = \tag{5.59}$$

$$Q_i^2 Q_j^2 \, \mathrm{E}(\eta_i^2 \eta_j^2) + Q_j^2 - Q_i^2 Q_j^2 + Q_i^2 - Q_i^2 Q_j^2 + \tag{5.60}$$

$$1 - Q_j^2 - Q_i^2 + Q_i^2 Q_j^2 = \tag{5.61}$$

$$Q_i^2 Q_j^2 \, \mathrm{E}(\eta_i^2 \eta_j^2) + 1 - Q_i^2 Q_j^2. \tag{5.62}$$

The last moment from Equation 5.18 $\mathrm{E}(\bar{\eta}_i^2 \bar{\eta}_j \bar{\eta}_k)$ is not derived here, but can be obtained in a similar way.

Derivation of the moments in case of two-way interaction and quadratic terms

In the following, we derive the additional moments required to estimate a model with two-way interaction and quadratic terms (Equations 5.22 to 5.24):

$$E(\bar{\eta}_i^3 \bar{\eta}_j) = E((Q_i\eta_i + \delta_i)^3(Q_j\eta_j + \delta_j)) \tag{5.63}$$

$$E((Q_i^3\eta_i^3 + 2Q_i^2\eta_i^2\delta_i + Q_i\eta_i\delta_i^2 + Q_i^2\eta_i^2\delta_i + 2Q_i\eta_i\delta_i^2 + \delta_i^3)(Q_j\eta_j + \delta_j)) = \tag{5.64}$$

$$E((Q_i^3\eta_i^3 + 2Q_i^2\eta_i^2\delta_i + Q_i\eta_i\delta_i^2 + Q_i^2\eta_i^2\delta_i + 2Q_i\eta_i\delta_i^2 + \delta_i^3)Q_j\eta_j) + \tag{5.65}$$

$$E((Q_i^3\eta_i^3 + 2Q_i^2\eta_i^2\delta_i + Q_i\eta_i\delta_i^2 + Q_i^2\eta_i^2\delta_i + 2Q_i\eta_i\delta_i^2 + \delta_i^3)\delta_j) = \tag{5.66}$$

$$Q_i^3 Q_j E(\eta_i^3\eta_j) + 0 + Q_i Q_j(1 - Q_i^2) E(\eta_i\eta_j) + 0+ \tag{5.67}$$

$$2Q_i Q_j(1 - Q_i^2) E(\eta_i\eta_j) + 0 + 0 + 0 + 0 + 0 + 0 + 0 = \tag{5.68}$$

$$Q_i^3 Q_j E(\eta_i^3\eta_j) + 3Q_i Q_j(1 - Q_i^2) E(\eta_i\eta_j) = \tag{5.69}$$

$$Q_i^3 Q_j E(\eta_i^3\eta_j) + 3(1 - Q_i^2) E(\bar{\eta}_i\bar{\eta}_j). \tag{5.70}$$

$$E(\bar{\eta}_i^3) = E((Q_i\eta_i + \delta_i)^3) = \tag{5.71}$$

$$E(Q_i^3\eta_i^3 + 2Q_i^2\eta_i^2\delta_i + Q_i\eta_i\delta_i^2 + Q_i^2\eta_i^2\delta_i + 2Q_i\eta_i\delta_i^2 + \delta_i^3) = \tag{5.72}$$

$$Q_i^3 E(\eta_i^3) + 0 + 0 + 0 + 0 + E(\delta_i^3) = \tag{5.73}$$

$$Q_i^3 E(\eta_i^3) + 0 = Q_i^3 E(\eta_i^3). \tag{5.74}$$

In the last step, we assume that the error terms are symmetrically distributed, i.e., $E(\delta_i^3) = 0$.

$$E(\bar{\eta}_i^4) = E((Q_i\eta_i + \delta_i)^4) = \tag{5.75}$$

$$E(Q_i^4\eta_i^4 + 2Q_i^3\eta_i^3\delta_i + Q_i^2\eta_i^2\delta_i^2 + Q_i^3\eta_i^3\delta_i + 2Q_i^2\eta_i^2\delta_i^2 + Q_i\eta_i\delta_i^3) + \tag{5.76}$$

$$E(Q_i^3\eta_i^3\delta_i + 2Q_i^2\eta_i^2\delta_i^2 + Q_i\eta_i\delta_i^3 + Q_i^2\eta_i^2\delta_i^2 + 2Q_i\eta_i\delta_i^3 + \delta_i^4) = \tag{5.77}$$

$$Q_i^4 E(\eta_i^4) + 0 + Q_i^2(1 - Q_i^2) + 0 + 2Q_i^2(1 - Q_i^2) + 0+ \tag{5.78}$$

$$0 + 2Q_i^2(1 - Q_i^2) + 0 + Q_i^2(1 - Q_i^2) + 0 + E(\delta_i^4) = \tag{5.79}$$

$$Q_i^4 E(\eta_i^4) + 6Q_i(1 - Q_i^2) + E(\delta_i^4) = \tag{5.80}$$

$$Q_i^4 E(\eta_i^4) + 6Q_i(1 - Q_i^2) + 3(1 - Q_i^2)^2. \tag{5.81}$$

In the last step, we adopt the kurtosis of the normal distribution for δ_i.

Results of the Monte Carlo simulation

Table 5.3: Results for the model containing a single equation

Para.	true	mean	sd
γ_1	0.300	0.298	0.048
γ_{11}	0.120	0.118	0.044
γ_{12}	0.150	0.147	0.062
γ_2	0.400	0.403	0.047
γ_{22}	0.100	0.104	0.042
ρ_{12}	0.300	0.300	0.052
λ_{31}	0.900	0.896	0.034
λ_{32}	0.850	0.850	0.039
λ_{33}	0.800	0.797	0.041
λ_{11}	0.900	0.898	0.044
λ_{12}	0.850	0.854	0.052
λ_{13}	0.800	0.795	0.058
λ_{21}	0.900	0.898	0.037
λ_{22}	0.850	0.850	0.044
λ_{23}	0.800	0.800	0.049

Table 5.4: Results for the model containing a set of recursive equations

Para.	true	mean	sd	Para	true	mean	sd
γ_{31}	0.500	0.502	0.049	λ_{41}	0.900	0.898	0.040
γ_{32}	-0.400	-0.395	0.053	λ_{42}	0.850	0.850	0.043
γ_{41}	0.350	0.347	0.056	λ_{43}	0.800	0.800	0.048
γ_{43}	0.200	0.201	0.058	λ_{51}	0.900	0.895	0.054
γ_{433}	-0.100	-0.099	0.038	λ_{52}	0.850	0.846	0.061
γ_{52}	0.300	0.301	0.050	λ_{53}	0.800	0.803	0.068
γ_{534}	0.300	0.298	0.052	λ_{11}	0.900	0.897	0.035
γ_{54}	-0.250	-0.247	0.052	λ_{12}	0.850	0.851	0.040
ρ_{12}	0.300	0.299	0.051	λ_{13}	0.800	0.799	0.042
λ_{31}	0.900	0.904	0.036	λ_{21}	0.900	0.897	0.041
λ_{32}	0.850	0.847	0.040	λ_{22}	0.850	0.848	0.046
λ_{33}	0.800	0.797	0.045	λ_{23}	0.800	0.803	0.049

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