Structural Equation Modelling with Latent Variables

Evidence from a Monte Carlo Study

Dissertation

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List of Abbreviations

ADF:	Asymptotic Distribution-Free method
boot.:	bootstrapped
CBSEM:	covariance-based structural equation modelling
CB-SEM:	covariance-based structural equation modelling
cent.:	centroid scheme
Coeff.:	Coefficient
cont. unif.:	continuous uniform
e.g.:	for example
fact.:	factorial scheme
f.i.:	for instance
fMM:	formative measurement model
GLS:	Generalised Least Squares method
i.a.:	inter alia
inner est.:	inner estimation
K:	number of Monte Carlo simulation loops
KR:	number of bootstrap replications
LV:	latent variable
MC:	Multicollinearity
md:	mean deviation
miss. res.:	missing results
ML:	Maximum Likelihood
MS:	Misspecification
MSE:	Mean Squared Error
no.:	number
OLS:	Ordinary Least Squares
path:	path weighting scheme
PLS:	Partial Least Squares
rMM:	reflective measurement model

rmse:	root mean squared error
RSS:	residual sum of squares
sd:	standard deviation
SEM:	structural equation model
SM:	structural model
TSS:	total sum of squares

Chapter 1

Introduction

1.1 Structural Equation Models

Structural equation modelling with latent variables is a multivariate statistical technique. It has been very prominent in the social sciences for many decades to the effect that a great number of studies has been published applying this technique, f.i. in the fields of housing and earnings, scholastic achievement and racial discrimination in employment, among many other fields (Jöreskog, 1982, p. 81). Traditionally those models are estimated mainly with the Maximum Likelihood (ML) approach. Recently, structural equation models with latent variables are more and more frequently estimated with the Partial Least Squares (PLS) approach. These studies can be found especially in the field of marketing and management. A list of examples is given in Appendix A.[1]

Structural equation models with latent variables play such an important role for several reasons (Haenlein/Kaplan, 2004, p. 283 et seqq.): firstly, structural equation modelling allows to model complex dependencies simultaneously and offers great flexibility. Secondly, causalities between unobservable variables can be modelled. All variables that are not directly corresponding to anything observable / measurable must be treated as unobservable. They are called either latent variables or constructs. Such latent variables get operationalised by measurable variables, which are named indicators, manifest

[1] In section 2.3 I refer more in detail to the respective table.

variables or items. Examples for latent variables are satisfaction, service or product quality, perceived price, or image of a soccer team. Structural equation models allow the estimation of causalities between latent variables. Thirdly, in this technique measurement errors can be modelled. A measurement error occurs when an item is not perfectly measuring what it is supposed to measure, but it is influenced by other components. These extra influences can occur in particular in the context of psychological variables.

The purpose of structural equation modelling with latent variables might be the examination of the dependencies between latent variables. But, it can as well be the examination of the individual impact of manifest driver variables, i.e. the identification of the impact of a specific success factor on an outcome variable. For the latter purpose the research interest extends to the role of the individual indicators.

The relations between all dependent and all independent latent variables build the so-called inner model or structural model. In the field of covariance-based structural equation modelling, to which the ML approach appertains, the name "structural model" is used whereas in the field of PLS especially the name "inner model" is used. In this thesis I do not distinguish and use both expressions equivalently. The inner model shows the causal relations between the not directly measurable constructs. The latent variables get operationalised by measurable variables, i.e. by the indicators. This is done individually for each construct with a so-called measurement model, also named outer model. The latter name is only found in PLS studies. The expression "measurement model" can be found especially in ML studies, but also in the field of PLS. I will call the relationship between a latent variable and its indicators mainly "measurement model", but use in the context of PLS (section 2.2.2) the expression "outer model" equivalently.
In this section the notation of structural equation models will be illustrated only briefly. A detailed explanation of the notation will be given for each individual approach in the respective section, because the notations differ slightly.

Traditionally the inner model is

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

where $\boldsymbol{\eta}$ is a vector with all latent endogenous variables. The matrix $\mathbf{B}$ consists of the coefficients which connect all latent endogenous variables. Certainly, it has only zeros on its main diagonal - otherwise a variable would explain itself, i.e. it would function as dependent and independent variable at the same time. Besides, $\mathbf{B}$ does not necessarily need to be a lower triangular matrix because models with interdependencies can be estimated, for example with the ML approach. But, in this thesis exclusively recursive models are regarded (i.e. models where the causality strictly flows in one direction) - only this kind of models can be estimated with PLS (Wold, 1982, p. 40).[2] $\boldsymbol{\xi}$ is the latent exogenous variable vector. The matrix $\boldsymbol{\Gamma}$ contains the coefficients for the effects of the latent exogenous on the latent endogenous variables. The vector $\boldsymbol{\zeta}$ consists of the error terms.

There are two main different ways of operationalising a latent variable: either in a reflective or in a formative measurement model.[3] The following paragraphs are mainly based on Bollen/Lennox (1991, p. 305 et seqq.).

Reflective indicators (also named effect indicators) "reflect" a latent variable. The causality goes from the latent variable to its indicators. A main characteristic is that a change in the latent variables causes a change in all its reflective indicators simultaneously. Consequently the reflective indicators which operationalise one specific latent variable need to show high (positive) correlations. Basically, reflective indicators are interchangeable. A single reflective measurement model is

$$\mathbf{y} = \boldsymbol{\Lambda}\eta + \boldsymbol{\epsilon}. \tag{1.1}$$

The vector $\mathbf{y}$ consists of all indicators that operationalise the specific latent variable η. Consequently the parameter vector $\boldsymbol{\Lambda}$ and the disturbance term

[2] Wold (1982) uses the term "hierarchic structure" which implies a recursive model. Hui (1982) extended PLS to non-recursive models. But, the common PLS algorithm and standard software programs do not have this algorithm implemented and work only for recursive models (Barroso et al., 2010, 432).

[3] Another way to connect the indicators to a latent variable is the MIMIC way (multiple effect indicators for multiple causes), where a latent variable has both, cause and effect indicators (see further Tenenhaus et al., 2005, p. 161 et seqq.; Bollen, 1989, p. 331; and concerning applications see Woods et al., 2009; Winklhofer/Diamantopoulos, 2002; Stapleton, 1978).

vector $\boldsymbol{\epsilon}$, which describes the measurement errors, have the same length. An established example for a reflective operationalised construct is an ability, f.i. verbal or mathematical ability (Bollen/Lennox, 1991, p. 306; MacCallum/Browne, 1993, p. 533). The existing ability influences the performance on a test, i.e. influences the performance with respect to individual questions. Usually an endogenous latent variable (η) gets operationalised with a reflective measurement model (Cassel et al., 1999, p. 438; Vilares et al., 2010, p. 292). But this is not a principle. Indeed, there is a very long list of published studies using solely reflective measurement models for all exogenous and endogenous latent variables.[4] Referring to equation 1.1 η is then substituted by ξ.

Formative indicators (also named cause indicators) "form" a latent variable, in other words they cause it.[5] In this regard Rubin (1986, p. 962) stated the motto "no causation without manipulation". He meant that an indicator can only be regarded to be formative if the researcher has the ability to vary it exogenously. However, this motto is not strictly applicable in practice. Therefore, it was anew defined that physical manipulation is not required, "but rather that we be able, as observational analysts, to conceive of the conditions that would follow from a hypothetical (but perhaps physically impossible) intervention" (Morgan/Winship, 2007, p. 279).[6] A formative operationalised latent variable is composed of the indicators. Thus, in a formative measurement model all indicators that cause the respective latent variable must be included. Otherwise, with omitting an indicator a part of the formative measurement model would be missing and as a consequence the meaning of the latent variable would change (Bollen/Lennox, 1991, p. 308). Formative indicators do not need to show high correlations. Actually, a high correlation

[4]Examples are Birkinshaw et al. (1998), Hsu/Wang (2008) and Völckner et al. (2010).

[5]A hypothetical construct with only causal indicators is not a latent variable in the traditional sense. Because, traditionally a latent variable is a hypothetical construct operationalised only with multiple effect indicators (this arose from the literature of factor analysis and covariance structure modelling). But, in a formative measurement model the construct is a linear combination of its manifest indicators plus an error term and thus it is a "composite variable" (MacCallum/Browne, 1993, p.534).

[6]A good review on this is given by Bollen (2013, p. 17 et seq.).

can even be problematic because the separation of the individual indicator impacts becomes difficult (Bollen/Lennox, 1991, p. 307). This characteristic is opposed to reflective indicators.[7] A formative measurement model is

$$\xi = \boldsymbol{\pi}\mathbf{x} + \delta \tag{1.2}$$

(in the equation ξ can be substituted by η, see further below). ξ is a specific latent variable which is determined by several indicators. The latter are expressed by the vector $\mathbf{x}$, which has the same length as the corresponding coefficient vector $\boldsymbol{\pi}$. Besides, the construct consists of a disturbance term δ. The causal indicators $\mathbf{x}$ enter error free; they do not include an error term. Hence, only reflective indicators represent an error-afflicted measurement (MacCallum/Browne, 1993, p. 534; see equation 1.1). Diamantopoulos et al. (2007, p. 15) point out (referring to Jarvis et al., 2003, p. 202) that the error term δ "represents a surplus meaning of the construct which is not captured by the set of formative indicators included in the model specification". Formative measurement models often make sense for exogenous latent variables (Cassel et al., 1999, p. 438). But, since this is not a principle ξ could be substituted by η referring to equation 1.2. An established example for a formative operationalised construct is socio-economic status. Its indicators are education, income and occupational prestige. A job loss affects the socio-economic status in a negative way, but a decreased socio-economic status does not imply a job loss. Besides, the indicators do not necessarily have to be correlated (Chin, 1998a, p. ix).

There exist no unique overall rules regarding the way of operationalising a latent variable. Each construct needs to be analysed concerning its meaning. For example the construct "satisfaction" of hotel guests can be operationlised in a formative or reflective way depending on its meaning. If satisfaction and its components are regarded then the different components represent formative indicators (f.i. satisfaction with cleanliness). But, if the focus is on how satisfaction expresses itself then those expressions (f.i. the recommendation of

[7] There exist cases where indicators show (very) low correlations but still capture the same construct. An example for that phenomenon given from Fornell/Bookstein (1982, p. 442) is the marketing mix, which is a result of its indicators (plus a disturbance term).

the hotel) are reflective indicators (Albers/Hildebrandt, 2006, p. 11).[8]

In the literature a so-called total effect is mentioned repeatedly. It is the overall effect an exogenous variable has on an endogenous variable and is consequently defined as the sum of the direct and indirect effects. In the context of structural equation modelling the total effect often refers to the structural model (Bollen, 1987; Fornell, 1982; Sobel, 1987, among others). In figure 1.1 I illustrate an example for an inner model of a structural equation model, i.e. a structural model. According to the model there are several direct effects (ξ_1 on η_1, ξ_1 on η_2 and η_1 on η_2) and one indirect effect (ξ_1 on η_2 via η_1 which is γ_1 times γ_3). Hence, the total impact ξ_1 has on η_2 is $\gamma_2 + \gamma_1 \cdot \gamma_3$.

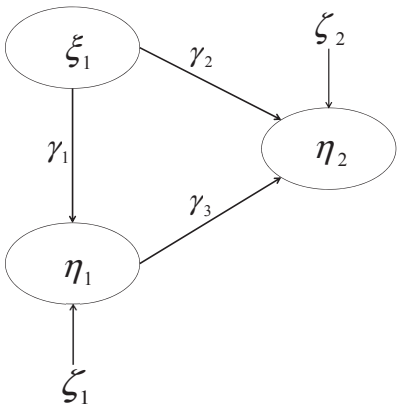

Figure 1.1: Example of a structural model.

In my study I apply total effects, but extend the perspective and include the measurement models. As I outlined before the impact a manifest driver variable has on a certain outcome may be of interest. Figure 1.2 shows the same structural model as figure 1.1, but is complemented by the indicators. ξ_1 is operationalised in a formative way and both η variables are operationalised in a reflective way. According to this model, the total effect x_1 has on y_4 is $\pi_1 \cdot \gamma_2 \cdot \lambda_4 + \pi_1 \cdot \gamma_1 \cdot \gamma_3 \cdot \lambda_4$.

[8]For further information regarding the operationalisation see among others Fornell/Bookstein (1982), Jarvis et al. (2003) and Diamantopoulos et al. (2007).

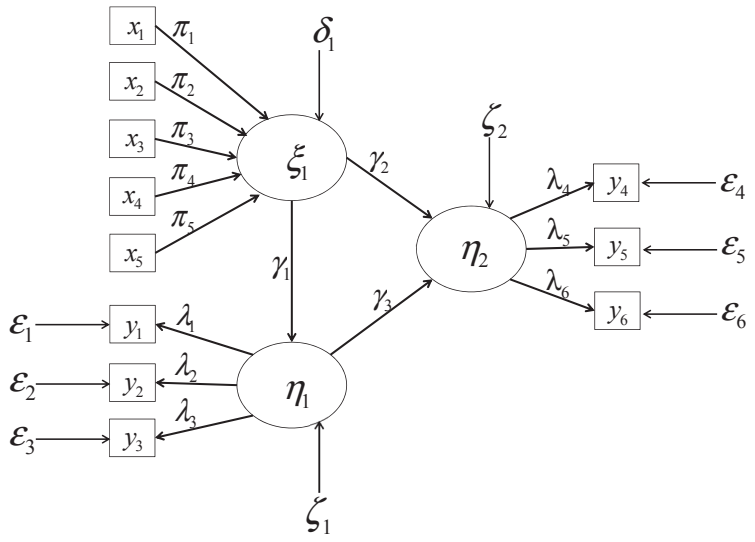

Figure 1.2: Example of a structural equation model.

1.2 Research Motivation

Researchers who start to get familiar with structural estimation modelling techniques are confronted with non-trivial estimation approaches. Further the literature reveals manifold inconsistencies, which can cause confusion. In the following I will give an overview over these inconsistencies and point out some sources.

In the PLS literature it is repeatedly stated that models which incorporate formative indicators cannot get estimated with ML, and consequently to estimate such models PLS needs to be favoured (Hsu et al., 2006, p. 369, among others). Further, the statement appears that PLS ought to be preferred over ML if the data is non-normally distributed (Fornell, 1982; Balzano/ Trinchera, 2011, p. 56, among others). The same statement appears with respect to small sample sizes, stating that "several hundreds of cases" are necessary to reason a ML application (Tenenhaus et al., 2005, p. 160). Moreover, PLS is described as powerful tool, good for an early research stage, good to handle a large number of variables, good in terms of statistical power and easy to apply since its convergence is almost sure (Gefen et al., 2000; Venaik et al., 2005, p. 665; Tenenhaus, 2008, p. 872; Henseler et al., 2009, p. 288 et seq.; Balzano/Trinchera, 2011, p. 56). Concerning the de-

tection of significant path coefficients and despite the fact of high power, it is stated that "PLS produces a conservative test of the substantive relationships" (Garnefeld et al., 2013, p. 26). In summary, ML is frequently described as very restricted approach, while in contrast PLS is frequently described as quite restriction-free. Hair et al. (2011, p. 139, referring to Diamantopoulos/Siguaw, 2000; Lohmöller, 1989; Reinartz et al., 2009; Ringle et al., 2009; and Wold, 1982) point this out as follows: "The CB-SEM model estimation requires a set of assumptions to be fulfilled, including the multivariate normality of data, minimum sample size, and so forth [...]. But if CB-SEM assumptions cannot be met, or the research objective is prediction rather than confirmation of structural relationships, then variance-based PLS-SEM is the preferred method" (CB-SEM stands for covariance-based structural equation modelling). Besides the stated PLS advantage of few restrictions, PLS is described as a match for ML in terms of estimation quality, such as by Götz et al. (2010, p. 691): "As an advantage, the PLS method demands significantly fewer requirements compared to that of covariance structure analyses, but nevertheless delivers consistent estimation results."

Other studies do not conform with these statements: Firstly, there are studies which apply the ML approach and whose specified model incorporates at least one formative measurement model, see f.i. Ringle et al. (2009). Consequently, the statement that a model which applies formative indicators cannot get estimated with ML is not (per se) correct. Secondly, according to Chou/Bentler (1995, p. 52 et seq.) and Dijkstra (2010, p. 24) among others, estimation accuracy of the coefficients is unaffected by non-normal data. In this regard Dijkstra (2010, p. 29) encapsulates: "It has been stated and is often repeated, seemingly thoughtlessly, that LISREL[9] is based on normality, in the sense that its use *requires* the data to be normally distributed. This is a prejudice that ought to be cancelled." Thirdly, Boomsma (1982, p. 156) f.i. suggests that with respect to accuracy the sample size shall not be smaller than 100 and Boomsma/Hoogland (2001, p. 2)[10] say that from 200

[9] "LISREL" is the name of a statistical software and is often used as a synonym for covariance-based structural equation modelling, see further the next section 2.1.1.

[10] The authors refer to the doctoral dissertation of Boomsma (1983), to which I did not gain access.

observations onwards hardly any convergence problems occur. These statements controvert the statement that "several hundreds" of observations are necessary. Fourthly, it is remarkable that the studies which ascertain high actual power for PLS did not investigate the test size, i.e. the frequency a type I error gets committed (Chin et al., 2003; Reinartz et al., 2009, among others). Consequently, not only the stated advantage of high PLS power becomes questionable,[11] but also the statement that PLS produces a conservative test can hardly be confirmed. The study of Goodhue et al. (2007, Appendix F) implies rather an exceeding of the respective significance level than a conservative test statistic, because in their study on the 5%-level PLS actual size lies between 5% and 7%. Fifthly, according to some studies (see f.i. Areskoug, 1982; Chou/Bentler, 1995) PLS estimators reveal systematic biases, while ML yields in general accurate estimates.

After all, some of the frequently stated ML and PLS requirements, pros and cons or implications appear to be incorrect. Nevertheless, they are to the present established in the literature. Therefore, there is a research need to contribute to the resolving of the appearing "prejudices" and confusions concerning ML and PLS performance and requirements.

Moreover, the studies which assessed ML and PLS performance show different limitations. Several studies assessed only one of the two approaches, i.e. solely the ML approach (Boomsma, 1982; Chou/Bentler, 1995, among others) or solely the PLS approach (Chin et al., 2003; Henseler, 2010, among others). Many ML studies or ML and PLS comparisons appear which applied solely reflective measurement models (f.i. Chin et al., 2003; Reinartz et al., 2009). Thus, there is a research need concerning ML and PLS comparisons applying a model which incorporates formative indicators. With respect to actual power and actual size I mentioned before, that most PLS studies assessed solely actual power without determining the frequency a type I error gets committed (Chin et al., 2003; Reinartz et al., 2009, among others). Monte Carlo simulations appear as powerful tool to assess estimator properties, but the number of iterations may not be too low to obtain reliable results. Nevertheless, studies appear which applied a low

[11] High power can be obtained by simply rejecting a formulated null hypothesis (too) often.

number of Monte Carlo iterations, such as 100 (f.i. Chou/Bentler, 1995 and Chin/Newsted, 1999), so that the results may be driven by simulation error.

This thesis contributes to the literature in the following ways:
Firstly, I will introduce in a comprehensible way the two estimation approaches ML and PLS. To contribute to the question how ML and PLS perform under different circumstances, I will summarise simulation study results, referring to estimator consistency, bias, as well as to other characteristics, such as convergence problems. Further, I will refer to the performance of the test for significance of the path coefficients, i.e. mainly actual power (only few results exist concerning the test size).

Secondly, to this non-trivial methods and complex research field I will contribute an approach, which is striking comprehensible. I introduce it as the so-called Ordinary Least Squares (OLS) approach, because it is exclusively based on OLS regressions and mathematical computations, emphasising its simplicity. To my best knowledge it does not yet get applied in structural equation modelling.

Thirdly, I will contribute a Monte Carlo study and thereby avoid the above described drawbacks. That is, my study is not restricted to a single approach, but constitutes a comparison of the ML, PLS and OLS approaches. My model will explicitly incorporate formative measurement models. Regarding the number of Monte Carlo iterations I will apply a very large number, i.e. 10,000 iterations per case, to gather reliable results. I will test the path coefficients on their significance and determine for all three approaches beside actual power explicitly the actual size of each test statistic. Concerning the "prejudices" and confusions, which I described above, I purpose to present systematic information with my Monte Carlo study. To do so, I will assess accuracy for all three approaches and cover many different cases: I will apply non-normal data, vary the proportions of unexplained variances incorporated in the model, vary the correlations between formative indicators as well as apply different sample sizes and number of indicators. My extensive Monte Carlo study is supposed to be transparent and replicable, including a systematic and reasonable presentation of the results.
To perform the simulation I will use the statistical software R (R Core Team,

2014). For the PLS estimation I will apply the *plspm* package (Sanchez et al., 2013) and for the ML estimation the *sem* package (Fox et al., 2013).

To accomplish the described purpose, the thesis is structured in the following way:
Firstly, I introduce the ML approach (section 2.1) and the PLS approach (section 2.2) and thereafter summarise available informations on both approaches mainly gained from simulation studies (section 2.3). In the subsequent section (2.4) I introduce the OLS approach. Concerning the presentation of the ML, PLS and OLS approach (in 2.1, 2.2 and 2.4), respectively, I firstly introduce the reader to the approach, secondly describe the estimation procedure, and thirdly elucidate the issue of identification. Although identification needs to be given for estimation I explain the estimation procedure prior to the identification, because I assume it is easier to comprehend the issue of identification when the estimation procedure is already known.
With respect to my Monte Carlo study (chapter 3) I describe in detail the simulation study set-up (section 3.1) and the analysis (section 3.2). Thereafter I present the results (section 3.3) by firstly describing them (sections 3.3.1 and 3.3.2) and subsequently drawing conclusions from them (section 3.3.3).
This thesis closes with a brief critical appraisal (chapter 4).

Chapter 2

Methodologies

2.1 Maximum Likelihood Approach

2.1.1 Introduction

The ML approach for the estimation of structural equation models is a so-called covariance-based methodology. Often "LISREL" (Linear Structural Relationships) is used as a synonym, though LISREL is the name of a very famous and widespread statistical software used in structural equation modelling. The first version of LISREL was presented by Karl Jöreskog in 1970 at a conference on Structural Equation Models in the Social Sciences (Madison, Wisconsin; Sörbom, 2001, p. 5). Today the software offers different estimation methods such as ML, GLS (Generalised Least Squares), WLS (Weighted Least Squares) and ULS (Unweighted Least Squares) among others (Mels, 2006). All those methods are covariance-based approaches. All covariance-based methods work with the sample variance-covariance matrix and all its information. Therefore, the ML approach is a so-called "full information approach" (Huber et al., 2007, p. 9). The individual observations do not directly get applied within the estimation procedure, but enter the estimation of the variance-covariance matrix. In this latter respect the sample size matters - it does not matter for the identification of a model.

The ML estimation results are model parameter estimations. With these parameter estimates fitted values for the latent variables can be computed. This proceeding is reverse to PLS, where so-called scores for the latent variables get

estimated first.

Traditionally, in the context of covariance-based structural equation modelling the equations are noted like the following (sources are mainly JÖRESKOG, 1982 and BOLLEN, 1989, p. 319 et seqq.; the notation is analogous to section 1.1). The inner model or structural model is

$$\boldsymbol{\eta} = \mathbf{B}\boldsymbol{\eta} + \boldsymbol{\Gamma}\boldsymbol{\xi} + \boldsymbol{\zeta}, \tag{2.1}$$

where $\boldsymbol{\eta}$ is a $m \times 1$ vector with all latent endogenous variables. The $m \times m$ matrix $\mathbf{B}$ consists of all coefficients between one latent endogenous variable and another one. Its main diagonal consists only of zeros. Furthermore, I regard only cases where $\mathbf{B}$ is a lower triangular matrix to ensure a recursive model, even if models with interdependencies can get estimated, too.[12] $\boldsymbol{\xi}$ is the latent exogenous variable vector with length n. The matrix $\boldsymbol{\Gamma}$ has the dimensions $m \times n$ and shows the coefficients for the effects of the latent exogenous on the latent endogenous variables. The disturbances vector $\boldsymbol{\zeta}$ has length m and consists of all influences that are not included in the equation. The expected value of each error term is zero ($E(\boldsymbol{\zeta}) = \mathbf{0}$). It is supposed to be uncorrelated with $\boldsymbol{\xi}$ ($\text{cov}(\xi_i, \zeta_i) = 0$).[13] To ensure a recursive model I expect the disturbances to be uncorrelated (RIGDON, 1995, p. 362). The (reflective) measurement models are

$$\mathbf{y} = \boldsymbol{\Lambda}_y\boldsymbol{\eta} + \boldsymbol{\epsilon} \tag{2.2}$$

and

$$\mathbf{x} = \boldsymbol{\Lambda}_x\boldsymbol{\xi} + \boldsymbol{\delta}. \tag{2.3}$$

The indicators, i.e. the observed variables, are the vectors $\mathbf{y}$ and $\mathbf{x}$ with length p and q, respectively.[14] The $\boldsymbol{\Lambda}$ matrices (with dimensions $p \times m$ or $q \times n$, respectively) show the coefficients for the relations between the respective latent

[12] As I mentioned before only recursive models can be estimated with PLS (WOLD, 1982, p. 40).

[13] In case this assumption is not satisfied, according to BOLLEN (2013, p. 3) the respective latent exogenous variable should be specified as an endogenous construct, because it is not exogenous.

[14] Only reflective indicators are given here. But the ML approach works as well with formative indicators. I will get to this in the next paragraph.

variables ($\boldsymbol{\eta}$ or $\boldsymbol{\xi}$) and the respective indicators ($\mathbf{y}$ or $\mathbf{x}$) according to the individual index. The error terms $\boldsymbol{\epsilon}$ ($p \times 1$) and $\boldsymbol{\delta}$ ($q \times 1$) are assumed to have expected values of zero ($E(\boldsymbol{\epsilon}) = \mathbf{0}$ and $E(\boldsymbol{\delta}) = \mathbf{0}$). In the context of covariance-based structural equation modelling the literature shows mainly specifications with only reflective measurement models, according to equation 2.2 and 2.3. However, formative measurement models can get applied, too. Bollen (1989, p. 321) modelled cause indicators as follows: Instead of specifying one formative measurement model he specified each indicator in a reflective way, each with a single latent variable. Then he restricted all individual coefficients to a value of one and set the error variances to zero. Hence, applying this "dodge" each of the respective indicators is set equal to one latent variable

$$\mathbf{x} = \boldsymbol{\xi}. \tag{2.4}$$

This enables the estimation and is further explained in section 2.1.2 (see figure 2.1 page 16). With $\boldsymbol{\eta}$ being still operationalised in a reflective way (equation 2.2) the inner model (previously equation 2.1) turns to

$$\boldsymbol{\eta} = \mathbf{B}\boldsymbol{\eta} + \boldsymbol{\Gamma}\boldsymbol{x} + \boldsymbol{\zeta} \tag{2.5}$$

(Bollen, 1989, p. 321). Also endogenous latent variables ($\boldsymbol{\eta}$) can be modelled in a formative way. But, it is not very common to operationalise endogenous constructs in a formative way (Cassel et al., 1999, p. 438).

Assuming a model is specified as equations 2.1, 2.2 and 2.3, the first four matrices a researcher needs to elaborate are $\mathbf{B}$, $\boldsymbol{\Gamma}$, $\boldsymbol{\Lambda}_y$ and $\boldsymbol{\Lambda}_x$. These matrices represent coefficient matrices. Besides, four variance-covariance matrices need to be patterned: $\boldsymbol{\Phi}$, $\boldsymbol{\Psi}$, $\boldsymbol{\Theta}_\epsilon$ and $\boldsymbol{\Theta}_\delta$. The first one, $\boldsymbol{\Phi}$, is the variance-covariance matrix of $\boldsymbol{\xi}$, the second one, $\boldsymbol{\Psi}$, is the variance-covariance matrix of $\boldsymbol{\zeta}$, and $\boldsymbol{\Theta}$ is the variance-covariance matrix of $\boldsymbol{\epsilon}$ or $\boldsymbol{\delta}$, respectively. It should be noted that the variance-covariance matrix of $\boldsymbol{\eta}$ can be derived from the other matrices (more precisely from $\mathbf{B}, \boldsymbol{\Gamma}, \boldsymbol{\Phi}, \boldsymbol{\Psi}$).[15]
The eight matrices ($\mathbf{B}, \boldsymbol{\Gamma}, \boldsymbol{\Lambda}_y, \boldsymbol{\Lambda}_x, \boldsymbol{\Phi}, \boldsymbol{\Psi}, \boldsymbol{\Theta}_\epsilon, \boldsymbol{\Theta}_\delta$) must be filled with as much information as available. That involves not only the paths between all variables and some coefficient restrictions, but also patterns regarding the variances

[15] $\mathrm{E}(\boldsymbol{\eta}\boldsymbol{\eta}') = (\mathbf{I} - \mathbf{B})^{-1}(\boldsymbol{\Gamma}\boldsymbol{\Phi}\boldsymbol{\Gamma}' + \boldsymbol{\Psi})[(\mathbf{I} - \mathbf{B})^{-1}]'$ (Bollen, 1989, p. 324).

and covariances of the error terms and of $\boldsymbol{\xi}$. In other words some unknown parameters might be fixed to a certain value or might equal at least one other parameter; all other unknown parameters which are not constrained are free. In practice this is a very difficult task for a researcher and probably there will remain uncertainties. At the same time this filling of the matrices allows great flexibility, e.g. reciprocal relationships as well as correlated error terms can be specified.[16] However, this flexibility enables also manipulation.
The described parameter restrictions must entail the scaling of the latent variables. The scale of each latent variable needs to be defined, because a latent variable does not have a unique, true scale. For this purpose either the latent variable variances get set equal to a value of one or some coefficients get restricted to a value of one. Both ways are possible and just one of them needs to be applied. In the ML approach it is common practice to set one coefficient in each measurement model to one. In doing so the latent variable adopts the scale of the respective indicator. That means that on average one unit shift of the exogenous variable leads to one unit shift in the endogenous variable.

2.1.2 Estimation

The matrix called $\boldsymbol{\Sigma}$ is the population covariance matrix of the observed variables $\mathbf{x}$ and $\mathbf{y}$. The most crucial assumption in covariance-based methodologies is that $\boldsymbol{\Sigma}$ can be written as a function of the unknown (i.e. free) model parameters $\boldsymbol{\theta}$. This relation is called the covariance structure hypothesis

$$\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\boldsymbol{\theta}) \tag{2.6}$$

(Bollen, 1989, p. 89, 333). In other words, the variance-covariance matrix of $\mathbf{x}$ and $\mathbf{y}$ can be defined using the model parameters. It is

$$\begin{aligned} \boldsymbol{\Sigma}(\boldsymbol{\theta}) &= \begin{bmatrix} \boldsymbol{\Sigma}_{yy}(\boldsymbol{\theta}) & \boldsymbol{\Sigma}_{yx}(\boldsymbol{\theta}) \\ \boldsymbol{\Sigma}_{xy}(\boldsymbol{\theta}) & \boldsymbol{\Sigma}_{xx}(\boldsymbol{\theta}) \end{bmatrix} \\ &= \begin{bmatrix} \boldsymbol{\Lambda}_y(\mathbf{I}-\mathbf{B})^{-1}(\boldsymbol{\Gamma}\boldsymbol{\Phi}\boldsymbol{\Gamma}' + \boldsymbol{\Psi})[(\mathbf{I}-\mathbf{B})^{-1}]'\Lambda_y' + \boldsymbol{\Theta}_\epsilon & \boldsymbol{\Lambda}_y(\mathbf{I}-\mathbf{B})^{-1}\boldsymbol{\Gamma}\boldsymbol{\Phi}\boldsymbol{\Lambda}_x' \\ \boldsymbol{\Lambda}_x\boldsymbol{\Phi}\boldsymbol{\Gamma}'[(\mathbf{I}-\mathbf{B})^{-1}]'\boldsymbol{\Lambda}_y' & \boldsymbol{\Lambda}_x\boldsymbol{\Phi}\boldsymbol{\Lambda}_x' + \boldsymbol{\Theta}_\delta \end{bmatrix} \end{aligned} \tag{2.7}$$

[16] Both cases entail non-recursive models (Rigdon, 1995, p. 362). I focus on recursive models.

for a model with solely reflective measurement models (Jöreskog, 1982, p. 85). The derivation is given in Appendix B. The implied variance-covariance matrix is applicable also with cause indicators, if Bollen's (1989, p. 321) "dodge" concerning the incorporation of formative indicators gets applied (equations 2.4 and 2.5 page 14). Otherwise, if formative indicators would get applied in the "normal manner", according to figure 2.1, the variance-covariance matrix cannot be derived as a function of the model parameters because the "magnitude of the indicator correlations is not explained by the model" (Bollen/Lennox, 1991, p. 307).

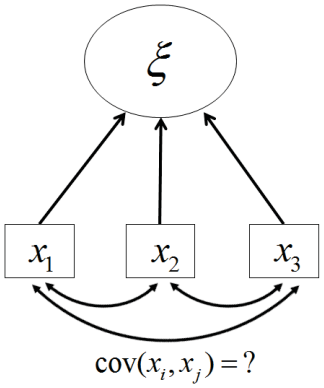

Figure 2.1: Covariances between formative indicators (according to Bollen/ Lennox, 1991, p. 306).

The sample variance-covariance matrix is $\mathbf{S}$. It is supposed to be a consistent, unbiased estimate of $\boldsymbol{\Sigma}$ which follows the specified model (Dijkstra, 2010, p. 27). The estimated matrix $\hat{\boldsymbol{\Sigma}}$ contains the variances and covariances as implied by the estimated parameters. The closer $\hat{\boldsymbol{\Sigma}}$ is to $\mathbf{S}$, the better the model fits the data.

The estimated parameters $\hat{\boldsymbol{\theta}}$ are obtained by maximising the Likelihood L that $\mathbf{S}$ is a sample drawn from a population with true variance-covariance matrix $\boldsymbol{\Sigma}(\boldsymbol{\theta})$. This procedure is analogous to minimising the discrepancy between $\mathbf{S}$ and $\hat{\boldsymbol{\Sigma}}$ or in other words minimising a so-called fitting function. The general fitting function is named

$$F(\mathbf{S}, \boldsymbol{\Sigma}(\boldsymbol{\theta}))$$

and is based on the sample variance-covariance matrix and the implied variance-covariance matrix (Kaplan, 2000, p. 27). As a matter of fact, a variance-

covariance matrix must be positive definite and the fitting function cannot take a variance-covariance matrix that is not positive definite (Yuan et al., 2011, p. 4). The fitting function has the property that it reaches the value zero only for $\mathbf{S} = \hat{\boldsymbol{\Sigma}}$ (Kaplan, 2000, p. 27).[17] The corresponding ML fitting function[18] to be minimised with respect to $\boldsymbol{\theta}$ is

$$F_{\mathrm{ML}} = \log|\boldsymbol{\Sigma}(\boldsymbol{\theta})| - \log(\mathbf{S}) + \mathrm{tr}[\mathbf{S}\boldsymbol{\Sigma}^{-1}(\boldsymbol{\theta})] - p - q \tag{2.8}$$

(Bollen, 1989, p. 334). The derivation - under the assumption that $\mathbf{x}$ and $\mathbf{y}$ are multinormally distributed - is shown by Bollen (p. 107, 131 et seqq.).[19] However, the equation can be understood intuitively. In the extreme case of perfect fit the first two summands cancel each other out. The third summand $\left(\mathrm{tr}[\mathbf{S}\boldsymbol{\Sigma}^{-1}(\boldsymbol{\theta})]\right)$ yields the trace of an identity matrix. Therefore, it equals the matrix size and the number is equivalent to $p + q$. Hence, the third summand and the last two cancel each other out in case of perfect fit. In conclusion F_{ML} is zero for the extreme case of perfect fit.
The iterative ML estimation procedure stops the minimisation of the residual covariances if a convergence criterion is fulfilled within a certain number of iterations, or if the maximum number of iterations is reached. The criterion is checked after each iteration and is fulfilled when "appropriate derivatives of the fit function are equal to zero" (Bentler/Chou, 1987, p. 100) and the difference between successive values is smaller than the convergence criterion (Jöreskog et al., 2000, p. 43). The convergence criterion can f.i. take the value 10^{-6} and the maximum number of iterations for instance 1,000.[20]

The standard errors of the estimated values can be estimated by taking the square root of the values on the main diagonal of the inverted information matrix (Bollen, 1989, p. 286). The information matrix is the matrix of

[17] The cited source refers to structural equation models with observed variables. But the characteristic is here true as well.

[18] Such functions exist for different methods, such as Unweighted Least Squares and Generalised Least Squares (Bollen, 1989, p. 106).

[19] However, multinormality is not required for consistency of the estimators (Dijkstra, 2010, p. 27). Simulation studies have shown that for non-normal data the estimates are still precise (Chou/Bentler, 1995), see further section 2.3 and chapter 3.

[20] In my following simulation study (chapter 3) I apply the `R` (R Core Team, 2014) package *sem* (Fox et al., 2013), which has the respective default settings.

second-order derivatives of the fitting function with respect to $\boldsymbol{\theta}$.[21]

At this point it is important to mention the issue of sample size. Given a large sample I can expect $\mathbf{S}$ to be an accurate estimate of $\boldsymbol{\Sigma}$. In that case large residuals (i.e. a large discrepancy between $\mathbf{S}$ and $\hat{\boldsymbol{\Sigma}}$) must be caused by a misspecified model. With a decreasing sample size residuals become more likely, even for a correctly specified model (Savalei/Bentler, 2006, p. 334).[22]

A problem which can arise during practical applications is the occurrence of non-convergence (Fornell/Bookstein, 1982; Boomsma, 1982). Some reasons for the occurrence of this problem refer to the population covariance matrix: Firstly, if the covariances get close to zero non-convergence becomes more likely. Secondly, the sign pattern of the covariances can matter. For example, if three indicators are attached to the same construct and one of them is positively correlated with the other two, but the other two show a negative correlation, then non-convergence is likely (Boomsma, 1985, p. 231 et seq.). Moreover, the sample sizes matters for the occurrence of non-convergence: the smaller the sample size, the more likely is non-convergence (Boomsma, 1982). As $\boldsymbol{\Sigma}(\boldsymbol{\theta})$ is composed of several "partial" variance-covariance matrices (see equation 2.7 page 15), the ML estimates "are obtained from different marginals" (Yuan et al., 2011, p. 4). The resulting variance-covariance matrix may not be positive definite when the sample size is small. In such case the involved logarithm in the fitting function (equation 2.8) cannot be calculated. Also a matrix which is only close to singular can entail non-convergence or "unstable parameter estimates" (Yuan et al., 2011, p. 4). One way to solve the problem of non-convergence can be the selection of appropriate starting values. The fit of the chosen starting values may influence the number of iterations until convergence is (possibly) reached. The better the chosen starting values the lower the number of iterations may be (Boomsma, 1985, p. 231, 239). Given a model that does not suffer from convergence problems, the choice of

[21] The information matrix can be noted as $plim \frac{\partial^2 F}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}'}$.

[22] To determine whether the model can be assumed to be correctly specified or not the hypothesis $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\theta)$ (which wants to be retained) can be tested with the test statistic $T = (N-1)F(\mathbf{S}, \hat{\boldsymbol{\Sigma}})$ which follows approximately a chi-square distribution (under certain assumptions), with the number of non-redundant elements of the covariance matrix (t) minus the number of free parameters as degrees of freedom (Savalei/Bentler, 2006, p. 334).

starting values does not influence the estimation results: either default, ideal or alternative starting values converge towards the same ultimate estimates (Boomsma, 1985, p. 239 et seq.).

Another problem which can arise during ML applications are improper solutions, like negative variances (Boomsma, 1985, p. 232 et seq.). This problem may occur even for correctly specified models. It becomes more likely the smaller the sample size is, but it can even occur with samples of 200 observations (Boomsma, 1985, p. 234). Moreover, the size of the population variances do matter again. The closer the variances get to zero the more likely are improper values (Boomsma, 1985, p. 233).
Concerning the characteristics and advices see further section 2.3 as well as chapter 3.

Now that I explained the ML estimation procedure and some of its characteristics I will talk about multinormality. In the literature (especially in the field of PLS applications) it is repeatedly stated that for estimation purposes multinormally distributed data is required (Mintu-Wimsatt/Graham, 2004; Huber et al., 2007, p. 10; Anderson/Swaminathan, 2011; or Balzano/Trinchera, 2011, among others). Concerning this issue I quote Dijkstra (2010, p. 27).[23]

> "More important perhaps is the fact that multinormality and the independence of the observational vectors is not required for consistency of LISREL-estimators, all that is needed is that the sample covariance matrix S is a consistent estimator for the theoretical covariance matrix Σ. [...] Also, asymptotic normality of the estimators is assured without the assumption of multinormality. All that is needed is asymptotic normality of S, and that is quite generally the case. Asymptotic optimality, and a proper interpretation of calculated standard errors as standard errors, as well as the correct use of test-statistics however does indeed impose heavy restrictions on the distribution [...]."

[23] The name LISREL is used as byword for the ML approach for structural equation models with latent variables (Dijkstra, 2010, p. 24).

Dijkstra's quoted statement makes clear that not the estimation quality of the estimators, but the reliability of the standard errors may be (particularly) the problem of non-multinormally distributed indicators. With $\mathbf{S}$ being asymptotically normally distributed, asymptotic normality of the estimators is assured (Dijkstra, 2010, p. 27). But, for inference purposes heavy distribution assumptions about the observed data are required. If these assumptions are not met the estimation of the standard errors applying the bootstrap technique represents one solution to obtain reliable standard errors (Djikstra, 1983; Yung/Bentler, 1998). A brief explanation of the bootstrap technique is given in Appendix C. But note, standard errors shall not simply always get bootstrapped, because if normality is given the ML estimates are accurate, while the bootstrap results can be severely biased, see further Nevitt/Hancock (2001). Another option is to apply robust standard errors (Satorra/Bentler, 1994), which "properly reflect additional variability in the estimates due to nonnormality" (Savalei/Bentler, 2006, p. 355). Especially if the non-normality is rather extreme they yield good estimates in terms of unbiasedness, see f.i. Chou/Bentler (1995, p. 52 et seq.).

With respect to other covariance-based methodologies I finally comment, that the ML approach performs generally better than GLS and ADF (Asymptotically Distribution-Free method) even in case the data is non-normal. This has been shown with simulations (Chou/Bentler, 1995, and Ringle et al., 2009, among others).

2.1.3 Identification

In general identification is given when each free parameter in $\boldsymbol{\theta}$ can be written as a function of at least one element of $\boldsymbol{\Sigma}$ (Bollen, 1989, p. 326). If only one of these parameters cannot be identified then the model is underidentified. Moreover, the solution needs to be unique. That is, the model is not identified if two different vectors $\boldsymbol{\theta}_1$ and $\boldsymbol{\theta}_2$ exist with $\boldsymbol{\Sigma}(\boldsymbol{\theta}_1) = \boldsymbol{\Sigma}(\boldsymbol{\theta}_2)$. Such a case implies arbitrary solutions.

One way to define identification is very simple, namely just verbally. ML estimations can often lead to improper solutions and factor indeterminacy.

Identification is given if the parameter estimations are in a proper and defined range (Bollen, 1989, p. 327). But, this definition is very superficial and does not help ex ante to assess identification.

To determine identification precisely there exist analytic procedures. In this section these procedures will be explained, but only for the later used recursive models. For models with reciprocal causations or feedback-loops different rules need to be applied.[24]

Some requirements hold in general for identification. One is the restriction of the diagonal elements of the matrix $\mathbf{B}$ to be zero (Bollen, 1989, p. 91). This is quite self-evident, because otherwise a variable would have a direct impact on itself, i.e. it would function as dependent and independent variable in one equation at the same time. Further, the scale of each latent variable must be defined. As I already mentioned in section 2.1.1 this is usually done by setting one coefficient in each measurement model to a value of one. Then the latent variables adopt the scale of the respective indicator. Moreover, $\boldsymbol{\zeta}$ needs to get a scale. This is usually done without noticing it explicitly. The (latent) error terms are scaled by setting their coefficient to one (Bollen, 1989, p. 91).

Another aspect which can get easily checked and which needs to be fulfilled for identification, refers to the number of reflective indicators per construct. In the case of a single reflective indicator (i.e. a latent variable is operationalised by only one indicator) the model is not identified, or more specifically the variance of the corresponding disturbance term is not identified. This problem can be fixed by specifying the variance to take on a concrete value.[25]

One way to determine identification is algebraically. In section 2.1.2 I showed that the variance-covariance matrix of the manifest variables ($\boldsymbol{\Sigma}$) can be written as a function of the model parameters ($\boldsymbol{\Sigma}(\boldsymbol{\theta})$). The number of available equations equals the number of non-redundant elements of the variance-covariance matrix. For a $l \,\mathrm{x}\, l$ variance-covariance matrix the number of non-redundant elements takes on the value $t = l \cdot (l + 1) \cdot \frac{1}{2}$. This number ($t$)

[24] For example the Rank or Order Condition is appropriate for such non-recursive models.

[25] The implementation of formative indicators according to equation 2.4 (page 14) includes error term variances equal to a value of zero.

represents the number of available equations. If each unknown (or unconstrained) parameter can be expressed as a function of one or more equations, the model is identified or overidentified (Bollen, 1989, p. 326).[26] Initially in each equation several unknown parameters may appear, but with a sufficient number of equations the parameters can be solved with algebraic manipulations. Consequently the identification of a structural equation model does not depend on the number of observations.

Overidentification implicates indeterminacies and therefore arbitrary solutions. MacCallum/Browne (1993, p. 537 et seq.) give in their paper a good example for a model with formative measurement models which incorporates indeterminacies. Applying algebraical manipulations of the structural equations they show how a structural model incorporates several indeterminacies (see an example in section 3.1.4, equations 3.4 and 3.5 page 65).

Underidentification can arise from insufficient equations, i.e. from insufficient information. Moreover, underidentification can arise when a covariance or a parameter equals a certain value. As the algebraic manipulations to solve the parameters include divisions, a denominator which equals a value of zero leads to an undefined solution (Bollen, 1989, p. 327).

For complex models, when the algebraic approach is not very convenient, rules exist to assess identification.

t-Rule

A necessary but not sufficient rule is the t-Rule (Bollen, 1989, p. 328). It is based again on the number of non-redundant elements the variance-covariance matrix has. The t-Rule says a model can only be identified if the number of available equations, i.e. the number of non-redundant elements of $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\boldsymbol{\theta})$ (equation 2.6 page 15), is greater or equal than the number of unknown parameters (t) of the structural equation model:

$$t \leq \left(\frac{1}{2}\right)(p+q)(p+q+1) \tag{2.9}$$

with p manifest y variables and q manifest x variables (Bollen, 1989, p. 328; Kaplan, 2000, p. 21).[27] If t equals $\frac{1}{2}(p+q)(p+q+1)$ then the model may

[26] In an overidentified model the parameters are still unique.

[27] Bollen (1989, p. 328) includes only the case t greater than the number of available equations. I include the case when t equals the number of available equations as f.i. Kaplan (2000, p. 21) does.

just be identified, if t is lower then the model may be overidentified (Kaplan, 2000, p. 21). If t is greater than the number of available equations the model cannot be identified.

Two-Step Rule

A sufficient but not necessary condition is the Two-Step Rule. If a model fulfils this rule then the model is for sure identified. If a model does not fulfil this condition it can even so be identified.[28] The Two-Step-Rule is relatively complex. As the name indicates it is composed of two steps.

First step of the Two-Step Rule

In the first step the model gets treated as a confirmatory factor analysis model and the measurement models get analysed regarding their identification. Subsequently the y variables will be named x and the η variables will be named ξ. The matrices $\mathbf{B}$, $\mathbf{\Gamma}$ and $\mathbf{\Psi}$ get ignored at this point. Regarding the relationships between latent variables only variances and covariances get taken into account. For clarification I present an example, see the model shown in figure 2.2. After the reformulation this model would look like figure 2.3. The identification of the reformulated model can be determined applying the following three rules (adapted from Bollen, 1989, p. 242 et seqq.):

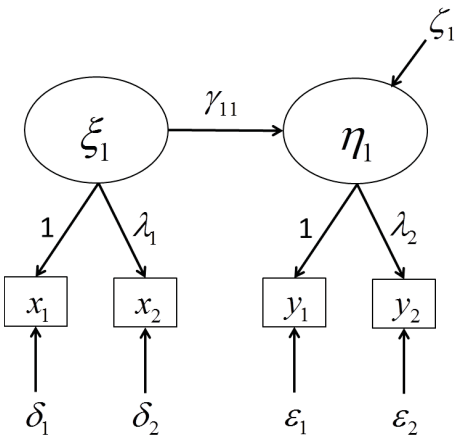

Figure 2.2: Example of a model according to Bollen (1989, p. 326).

The first rule is the *t-Rule*, equivalently to the t-Rule described above. That is, the number of non-redundant elements of the covariance matrix of $\mathbf{x}$ must

[28] Examples are given by Bollen (1989, p. 329 et seq.).

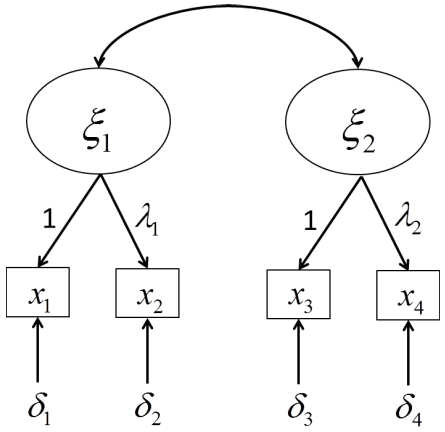

Figure 2.3: First step of the Two-Step Rule for the model shown in figure 2.2 (according to Bollen, 1989, p. 329).

be greater than or equal to the number of free parameters. The t-Rule is a necessary but not a sufficient condition. It is

$$t \leq \frac{1}{2}(q)(q+1)$$

with t representing the number of free parameters in $\boldsymbol{\theta}$ and q representing the number of manifest x variables (Bollen, 1989, p. 242 et seq.).

The second rule is the *Three-Indicator Rule*. If it is fulfilled, identification is given for sure, i.e. the condition is sufficient. According to this rule a one-factor model (only one ξ variable) with at least three indicators is identified when the error terms are uncorrelated ($\boldsymbol{\Theta_\delta}$ is diagonal). If there are several factors (ξ variables) the model is identified when each factor has at least three indicators, the coefficient matrix $\boldsymbol{\Lambda}_x$ has in each row exactly one non-zero element and the error term matrix $\boldsymbol{\Theta_\delta}$ is diagonal (Bollen, 1989, p. 244). The latter two assumptions imply that each indicator is related only to one latent variable and the error terms are uncorrelated. Further, each ξ_j must be scaled (one λ per latent variable is fixed to a value of one). With three indicators the variance-covariance matrix of the factors $\boldsymbol{\Phi}$ is unrestricted. In this regard the Three-Indicator Rule is distinct from the subsequently explained Two-Indicator Rule.

The third rule is the *Two-Indicator Rule*, which is as well sufficient (regarding the first step). It is an alternative to the Three-Indicator Rule for models with at least two ξ variables and at least two indicators per latent variable.

Analogous to before $\mathbf{\Lambda}_x$ must have only one non-zero coefficient per row and the error term matrix must be diagonal. Of course the factors need to be scaled. Therefore, one λ per factor must be set to a value of one. The variance-covariance matrix of the latent variables ($\mathbf{\Phi}$) must have only elements or at least one off-diagonal element per row which is non-zero.[29]
So far I explained the first step of the *Two-Step Rule*. The examination of the second step only makes sense if in the first step identification has been ascertained.

Second step of the Two-Step Rule

In the second step the inner model (i.e. the relationships between the latent variables) gets assessed regarding its identification, see figure 2.4. The latent variables get treated as if they were observed and perfectly measured. Under

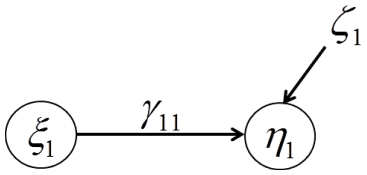

Figure 2.4: Second step of the Two-Step Rule for the model shown in figure 2.2 (according to Bollen, 1989, p. 329).

this assumption the identification of $\mathbf{B}$, $\mathbf{\Gamma}$ and $\mathbf{\Psi}$ needs to be determined. One requirement is that the diagonal elements of the matrix $\mathbf{B}$ need to be restricted to zero (Bollen, 1989, p. 91). Besides, $\boldsymbol{\zeta}$ needs to get a scale. Both requirements hold for identification in general (see above). Subsequently the identification can get examined algebraically. To assess identification in the context of only observable variables, as it is the case in the second step, I illustrate three rules which apply to recursive models.
Firstly, a necessary but not sufficient condition is again the *t-Rule*, which I explained above (see equation 2.9 page 22). Its use in this step is exactly analogous to before. The second rule is the so-called *Null B Rule*. It is a sufficient condition for identification, though not necessary. It says that a model is identified if $\mathbf{B} = \mathbf{0}$. This implies that the model has no paths between

[29] Bollen (1989, p. 245 et seq.) proves this for one specific model. For more detailed information concerning the identification in confirmatory factor analysis see Bollen (1989, p. 328 et seqq.).

one endogenous variable and another one. In such case "$\mathbf{\Phi}$, $\mathbf{\Gamma}$ and $\mathbf{\Psi}$ can be written as functions of the identified covariance matrix of the observed variables and are therefore identified" (Bollen, 1989, p. 95). The third rule is the so-called *Recursive Rule*, which is not necessary, but sufficient. It holds for recursive models, whose $\mathbf{B}$ matrix is a lower triangular matrix. Besides, $\mathbf{\Psi}$ must be diagonal (Bollen, 1989, p. 94 et seqq.).[30]
If identification can be ascertained in both, the first and the second step of the Two-Step Rule, the model is identified.

2.2 Partial Least Squares Approach

2.2.1 Introduction

Herman O. Wold introduced the PLS approach with its final formalisation in 1979 (Wold, 1979). The main references for PLS are Wold (1982) and Wold (1985a).

For notation of the PLS algorithm it is advantageous not to distinguish neither between exogenous and endogenous latent variables, nor between x and y. The notation specifics concerning this and the subsequent section (2.2.2) are inspired by Tenenhaus et al. (2005) and Ahrholdt (2010, p. 108 et seq.). In the model in figure 2.5 I apply the PLS notation.
The notation of the inner model becomes

$$\boldsymbol{\xi} = \mathbf{\Gamma}\boldsymbol{\xi} + \boldsymbol{\zeta}. \tag{2.10}$$

$\boldsymbol{\xi}$ and $\boldsymbol{\zeta}$ are vectors with length J. The coefficient matrix $\mathbf{\Gamma}$ is a lower triangular J x J matrix - otherwise a variable would cause itself or the model would not be recursive. The algebraic notation consists of at least one single and / or multiple regression (usually multiple regressions are the case).

In the following notations each measurement model j out of all J measurement models is regarded individually.

[30] For more detailed or further informations regarding the identification of structural equation models with observed variables (e.g. models with interdependencies) see Bollen (1989, p. 88 et seqq.).

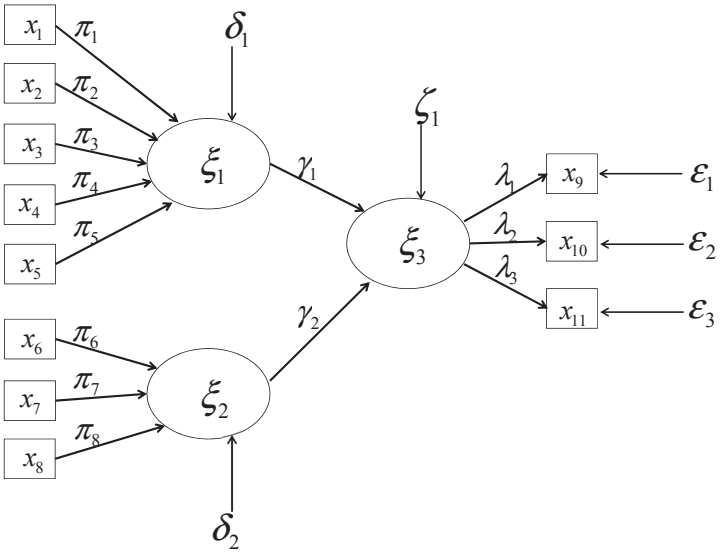

Figure 2.5: Model with variablenames as used for notation of the PLS algorithm.

A reflective measurement model j can be noted as

$$\mathbf{x}_j = \boldsymbol{\lambda}_j \xi_j + \boldsymbol{\epsilon}_j. \tag{2.11}$$

One specific latent variable ξ_j is operationalised by the set of manifest variables $\mathbf{x}_j$. Thereby, measurement model j is composed of H_j indicators. Consequently, the vectors $\boldsymbol{\lambda}_j$ and $\boldsymbol{\epsilon}_j$ have length H_j and the algebraic notation consists of H_j equation. Each equation corresponds with a simple linear regression. This way of operationalising a latent variable, referring to the causality between the indicators and the latent variable, is called "mode A".
A formative measurement model j can be noted as follows

$$\xi_j = \boldsymbol{\pi}_j' \mathbf{x}_j + \delta_j. \tag{2.12}$$

The algebraic notation consists of one equation, which corresponds with a multiple regression. Analogous to above one specific latent variable ξ_j is operationalised by H_j manifest variables $\mathbf{x}_j$. Consequently $\boldsymbol{\pi}_j$ is a vector with length H_j and δ_j represents the error term. This way of operationalising the latent variable, referring to the causality between the indicators and the latent variable, is called "mode B".

Regarding the inner model the latent variables need to be distinguished. Some latent variables are dependent and get explained by other independent

variables. A ξ_l variable that acts as dependent variable is named "follower" and the variables that are explaining ξ_l are named "predecessors". In the following the latter variables are labelled with a "P" in the exponent. One specific equation of the inner model is

$$\xi_l = \boldsymbol{\gamma}_l' \boldsymbol{\xi}_l^{(P)} + \zeta_l. \tag{2.13}$$

Its conditional expectation equals the systematic part of the linear regression.

$$\mathrm{E}(\xi_l | \boldsymbol{\xi}_l^{(P)}) = \boldsymbol{\gamma}_l' \boldsymbol{\xi}_l^{(P)}$$

With respect to linear regressions this assumption is well-known. In the PLS literature it is called the predictor specification condition. The assumption implies, that the residual mean equals a value of zero and that the correlation between the error term and each dependent variable is zero. With respect to equation 2.13 that means

$$\begin{aligned} \mathrm{E}(\zeta_l | \boldsymbol{\xi}_l^{(P)}) &= 0 && \forall\ l, \\ \mathrm{E}(\xi_l | \boldsymbol{\xi}_l^{(P)}) &= \boldsymbol{\gamma}_l' \boldsymbol{\xi}_l^{(P)} && \forall\ l. \end{aligned}$$

The predictor specification condition applies also to the regression equations concerning the measurement models. With respect to a reflective measurement model (equation 2.11) it implies

$$\begin{aligned} \mathrm{E}(\epsilon_{jh} | \xi_J) &= 0 && \forall\ h, j, \\ \mathrm{E}(x_{jh} | \xi_j) &= \lambda_{jh} \xi_j && \forall\ h, j. \end{aligned}$$

Referring to a formative measurement model (equation 2.12) the predictor specification implies

$$\begin{aligned} \mathrm{E}(\delta_j | \mathbf{x}_j) &= 0 && \forall\ j, \\ \mathrm{E}(\xi_j | \mathbf{x}_j) &= \boldsymbol{\pi}_j' \mathbf{x}_j && \forall\ j. \end{aligned}$$

2.2.2 Estimation

The core of the PLS approach is the estimation of scores for the specified latent variables. The underlying algorithm basically consists of OLS regressions. If the algorithm converges, estimated latent variable scores are available and

thereafter the latent variables get treated as if they were observed variables. In the literature the estimation of the scores is called stage one. Stage two is then the estimation of all coefficients, accomplished with OLS regressions again.
With respect to the core of the PLS approach, the literature reveals statements like "PLS-SEM maximizes the explained variance of the endogenous latent variables" (Hair et al., 2012b, p. 415) or PLS minimises error variances (e.g. Huber et al., 2007, p. 6) or PLS minimises the trace of the error variance-covariance matrix (Fornell/Bookstein, 1982, p. 449). Regarding this I point out that solely separate OLS regressions (i.e. no simultaneous equations) are incorporated within the PLS algorithm and that consequently the error variances get minimised separately.
As I mentioned in my introduction Wold (1982) and Wold (1985a) constitute the main sources and my notations are inspired by Tenenhaus et al. (2005) and Ahrholdt (2010).

The PLS algorithm is an iterative estimation technique. The procedure scheme is illustrated in figure 2.6. The estimation starts with an initialisation, named "step 0". After the initialisation the algorithm continues with the iteration of an inner and an outer estimation. In doing so the inner and outer model do not get estimated simultaneously. In both steps weights get estimated and with these weights latent variable scores get computed. Consequently there are inner and outer weights as well as inner and outer scores. The two parts get repeated until the outer weights fulfil a convergence criterion, see "step 1a" below. This criterion is checked every iteration. The procedure always ends with the computation of outer scores.
For the notation of the algorithm I add an index h (with $h = 1, ..., H_j$). The variable x_{jh} represents one indicator which belongs to the specific latent variable ξ_j, and ξ_j is operationalised by H_j indicators. Further, the weights and scores are labelled in the exponent with a "[2]" or "[1]", whether they result from the inner or outer estimation, respectively. In the following I will explain the scheme in detail.

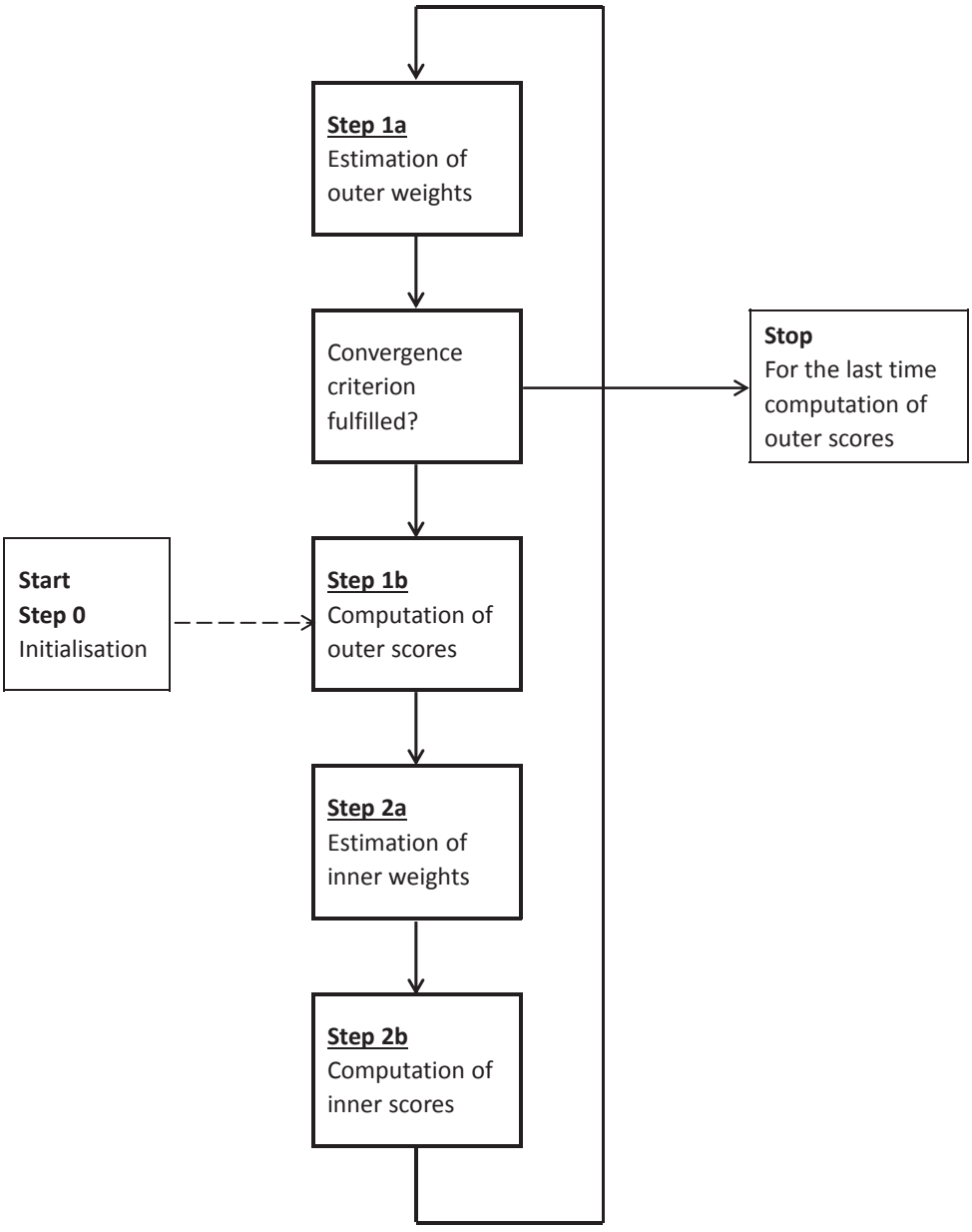

Figure 2.6: Scheme of the PLS algorithm.

Step 0: Initialisation

Observations are only available for the indicators. To obtain the first scores for the latent variables, outer weights are necessary. In the initialisation step the first set of outer weights takes arbitrary non-zero numbers:

$$\hat{w}_{jh}^{[0]} \neq 0 \qquad \forall\ j, h.$$

The "[0]" in the exponent indicates that this is an initialisation weight.[31] This step is performed just once. Subsequently step 1b gets performed. For the rest of the iterative estimation procedure the outer weights do get estimated according to step 1a, i.e. step 1a substitutes the initialisation step. Therefore, in the following I elucidate step 1a .

Step 1a: Estimation of outer weights

Within the iterative estimation procedure step 1a follows on step 2b (see below). In step 1a the outer weights get estimated applying the latent variable scores of step 2b ($\hat{\xi}_j^{[2]}$), which are available after the first iteration. The estimation depends on the mode of the measurement model. In mode A x_{jh} is explained by ξ_j. Its outer weight equals the regression coefficient of an OLS regression of x_{jh} on $\hat{\xi}_j^{[2]}$. In doing so the causality is taken into account. As step 2b includes a scaling of the $\hat{\xi}_j^{[2]}$ variances to a value of one, the outer weight estimation in mode A results in

$$\hat{w}_{jh}^{[1]} = \mathrm{cov}(x_{jh}, \hat{\xi}_j^{[2]}) \qquad \forall\ j, h \text{ in mode A.}$$

If the measurement model of ξ_j is mode B, the corresponding $\mathbf{x}_j$ "form" the latent variable. Taking the causality into account, the weights result from the multiple regression of $\hat{\xi}_j^{[2]}$ on the corresponding block of indicators:

$$\hat{\mathbf{w}}_\mathbf{j}^{[\mathbf{1}]} = (\mathbf{X}_\mathbf{j}'\mathbf{X}_\mathbf{j})^{-1}\mathbf{X}_\mathbf{j}'\hat{\boldsymbol{\xi}}_j^{[\mathbf{2}]} \qquad \forall\ j \text{ in mode B.}$$

After step 1a a convergence criterion gets checked. Convergence is reached when the sum of absolute changes between two successive outer weights of two successive iterations falls below the criterion, e.g. 10^{-5} (Wold, 1982, p. 14).[32]

[31] Often it is $\hat{w}_{jh}^{[0]} = \pm 1$. For the choice of the sign there exist some propositions, see further Tenenhaus et al. (2005, p. 171).

[32] An alternative is the sum of squared changes in weights.

In case of convergence the estimation procedure stops with computing the outer scores as explained in the following step 1b using the last estimated outer weights. If the convergence criterion is not fulfilled after an ex ante defined maximum number or iterations (e.g. 100) the procedure stops without having reached convergence.[33] Unless the convergence criterion is not fulfilled and the maximum number of iterations is not reached step 1 and 2 get reiterated.

Step 1b: Computation of outer latent variable scores

The outer scores of a latent variable ξ_j are just linear combinations of all x variables which belong to the j-th measurement model times their weights $\hat{\mathbf{w}}_\mathbf{j}$. The direction of causality is not taken into account. The equations are for mode A and B identical.

The computation of the scores is

$$\hat{\xi}_j^{[1]} = f_j^{[1]} \cdot \sum_{h=1}^{H_j} \hat{w}_{jh}^{[0]} x_{jh} \qquad \forall\ j \tag{2.14}$$

within the first iteration and otherwise

$$\hat{\xi}_j^{[1]} = f_j^{[1]} \cdot \sum_{h=1}^{H_j} \hat{w}_{jh}^{[1]} x_{jh} \qquad \forall\ j. \tag{2.15}$$

The equations differ regarding the $\hat{w}_{jh}$ depending on the preceding step. Since the initialisation pertains only to the first iteration, equation 2.14 is used only once. In the subsequent iterations equation 2.15 gets applied.

The "$f_j^{[1]}$" in both equations renders the variance of $\hat{\xi}_j^{[1]}$ to a value of one. Hence, it is the reciprocal of the standard deviation of the latent variable before its variance is adjusted

$$f_j^{[1]} = \frac{1}{\sqrt{\text{var}\left(\sum_{h=1}^{H_J} \hat{w}_{jh}^{[1]} x_{jh}\right)}} \qquad \forall\ j. \tag{2.16}$$

Step 2a: Estimation of inner weights

There are three different ways of estimating inner weights: the centroid, the factorial and the path weighting scheme.[34]

[33] A maximum of 100 iterations and a tolerance criterion of 10^{-5} are the default settings in the R (R Core Team, 2014) package *plspm* (Sanchez et al., 2013).

[34] The centroid scheme was the original one, implemented by Wold (1985a). The factorial and the path weighting scheme were implemented later by Lohmöller (1989, p. 40).

To determine the inner weights according to the centroid scheme adjacent latent variables get taken into account without considering the direction of the causality. The inner weight between two adjacent latent variables $\hat{\xi}_j^{[1]}$ and $\hat{\xi}_k^{[1]}$ $(j \neq k)$ equals the sign of the correlation ρ between those two variables, i.e. the inner weight attains either the value one or minus one. The strength of the correlation does not matter. For two ξ variables, which are not connected with a path, the weight is compulsory zero.

$$\hat{w}_{jk}^{[2]} = \begin{cases} sign\left(\rho\left(\hat{\xi}_j^{[1]}, \hat{\xi}_k^{[1]}\right)\right) & \text{if } \xi_j \text{ and } \xi_k \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases} \forall\ k, j$$

This scheme suffers from the disadvantage, that within the estimation procedure the inner weight can alternate between one and minus one. This is likely to occur if the corresponding correlation is very weak.

In the factorial scheme the exact correlation between two adjacent variables ξ_j and ξ_k is taken as weight. Therefore, this scheme does not suffer from the drawback of the centroid scheme. Both schemes do not take the causality into account.

$$\hat{w}_{jk}^{[2]} = \begin{cases} \rho\left(\hat{\xi}_j^{[1]}, \hat{\xi}_k^{[1]}\right) & \text{if } \xi_j \text{ and } \xi_k \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases} \forall\ k, j$$

In contrast to the previously described schemes, the path weighting scheme takes the causality into account. To do so the latent variables need to be distinguished between "followers" and "predecessors" as in the previous section 2.2.1. OLS regressions yield the inner weights: each follower l gets regressed on all its predecessors. The formula is

$$\hat{\mathbf{w}}_{\mathbf{l}}^{[\mathbf{2}]} = \left[\left(\hat{\boldsymbol{\xi}}_{\boldsymbol{l}}^{[\mathbf{1}]\boldsymbol{P}}\right)' \hat{\boldsymbol{\xi}}_{\boldsymbol{l}}^{[\mathbf{1}]\boldsymbol{P}}\right]^{-1} \left(\hat{\boldsymbol{\xi}}_{\boldsymbol{l}}^{[\mathbf{1}]\boldsymbol{P}}\right)' \hat{\boldsymbol{\xi}}_{\boldsymbol{l}}^{[\mathbf{1}]} \qquad \forall\ l.$$

According to Noonan/Wold (1982) and Ringle et al. (2009; among others) the PLS estimation results are robust towards the scheme, i.e. the results vary only slightly and no clear pattern can be derived.

Step 2b: Computation of inner latent variable scores

With respect to the computation of inner scores the causality is disregarded in any case. A specific latent variable ξ_j gets computed as a linear combination

of all its adjacent variables. With ξ_j having in number S_j adjacent latent variables its scores get computed as

$$\hat{\xi}_j^{[2]} = f_j^{[2]} \cdot \sum_{s=1}^{S_j} \hat{w}_{js}^{[2]} \hat{\xi}_s^{[1]} \qquad \text{for all } \hat{\xi}_s \text{ that are adjacent to } \hat{\xi}_j.$$

Such inner scores get computed for each latent variable. Analogous to before the "$f_j^{[2]}$" ensures the variance of the scores takes on the value one (see equation 2.16). Consequently it is

$$f_j^{[2]} = \frac{1}{\sqrt{\text{var}\left(\sum_{s=1}^{S_j} \hat{w}_{js}^{[2]} \hat{\xi}_s^{[1]}\right)}} \qquad \forall\ j.$$

After step 2b the procedure continues with step 1a (see above).

In case of convergence of the outer weights (step 1a) stage one gets accomplished by computing the final scores according to step 1b (equation 2.15). In stage two all path coefficients get estimated applying these scores. The estimates result from OLS regressions which get performed in all partial models according to the respective causality. In all reflective measurement models these OLS coefficients equal the respective correlation if the indicators are standardised. In all formative measurement models the OLS coefficients correspond with the outer weights which were estimated in the last realisation of step 1a. In the inner model a single (or multiple) regression is performed regressing each endogenous latent variable on (all) its predecessor(s).

A replicable numerical example of the algorithm, which can even be solved with a hand calculator, is given from Ahrholdt (2010, p. 112 et seq.).

In order to estimate standard errors of the estimated coefficients, resampling techniques should be applied, such as the bootstrap technique (Tenenhaus et al., 2005, p. 174).[35] In this regard I remark that in a formative measurement model the regression of a latent variable on its indicators necessarily

[35] Also the jackknife technique could be utilised. However, I do not illustrate this technique since it approximates the bootstrap (Efron/Tibshirani, 1993, p. 287) and bootstrapping is very established. The bootstrap technique is in general implemented in PLS and ML software as it is the case for the R (R Core Team, 2014) packages I utilise in my Monte Carlo simulation in chapter 3 (*plspm* by Sanchez et al., 2013, and *sem* by Fox et al., 2013).

yields standard deviations of the coefficient estimates that take on the value zero. This is tautological since the scores itself equal the weighted sum of its indicators.[36] I briefly explain how standard errors get bootstrapped in Appendix C.

After having illustrated the PLS algorithm I will further define the terms "composite variable" and "latent variable". In section 1.1 I distinguished these two expressions. As step 1b (page 32) of the algorithm reveals a reflective operationalised construct is not a latent variable in the traditional sense. In step 1b the outer scores get computed as linear combination of its indicators. Hence, when being very precise, both, formative and reflective operationalised constructs are composites (Rönkkö/Evermann, 2013, p. 426). However, for practical reasons I continue calling all not directly measurable constructs latent variables.

A characteristic of PLS is to avoid improper solutions (Fornell, 1982, p. 440). According to Henseler (2010, p. 108) this aspect goes hand in hand with the "belief" that PLS always converges.[37] Indeed, studies have shown that the PLS convergence rate is very high, but that convergence is not guaranteed (Henseler, 2010; see further section 2.3 as well as my Monte Carlo results in section 3.3).

Regarding the measurement scale or distribution of the indicators no assumptions are required, because PLS consists only of OLS regressions (Reinartz et al., 2009, p. 332 et seq.). As the OLS regressions get applied in parts of the structural equation model, PLS works as well with samples, which consist of less observations than the model consists of path coefficients (see further the identification issues in the subsequent section 2.2.3).

Another characteristic is that the PLS scores are inconsistent even when the model is correctly specified. Therefore, the resulting PLS estimates are inconsistent, too. But, the parameter estimates are "consistent at large". The

[36] In defiance of the literature Goodhue et al. (2007, Appendix F) applied the OLS standard errors to test the coefficients of the structural model on their significance. Their simulation study (applying a model which incorporates solely reflective measurement models) reveals an actual size about 35% on the 5%-level.

[37] A proof exists only for certain cases, see further Henseler (2010).

property "consistency at large" implies that the parameter estimates converge towards the population values as both, the number of indicators per latent variable and the sample size, increase (Hui/Wold, 1982, p. 123 et seq.; Wold, 1985b, p. 231; Schneeweiss, 1993, p. 309 et seqq.). According to Hui/Wold (1982, p. 122) the number of indicators must remain small in relation to the sample size.

2.2.3 Identification

With regard to PLS it is not extensive to determine whether a model is identified or not. The partial model which incorporates the largest number of independent variables (either in the inner model or in a measurement model) determines the minimal sample size. With an unsuppressed constant the minimum number of observations equals the respective number of independent variables plus one. According to this identification rule even models with less observations than variables can be identified. An example is given in section 3.1.2. How much sense an analysis with such a little sample size makes, is not discussed here.

2.3 Comparison of Maximum Likelihood and Partial Least Squares

In this section I will at first illustrate a general difference between the two approaches ML and PLS. In my introduction to ML and PLS (sections 2.1.1 and 2.2.1) I noted the measurement models and the structural model separately.[38] When looking at an entire model, such as the one in figure 2.7, an essential difference between ML and PLS appears. The difference necessarily pertains in one and the same model (figure 2.7) to the notation of η_1. The arrow relating δ_2 to η_1 is dashed, because it is only relevant for PLS.
In the ML world there is one equation with η_1 as endogenous variable (see e.g.

[38] See equation 2.1 page 13 for the ML structural model and equations 2.2 and 2.3 page 13 for the ML measurement models (and possibly equations 2.4 and 2.5 page 14). Referring to PLS see the structural model in equation 2.10 page 26 and the measurement models in equations 2.11 and 2.12 page 27.

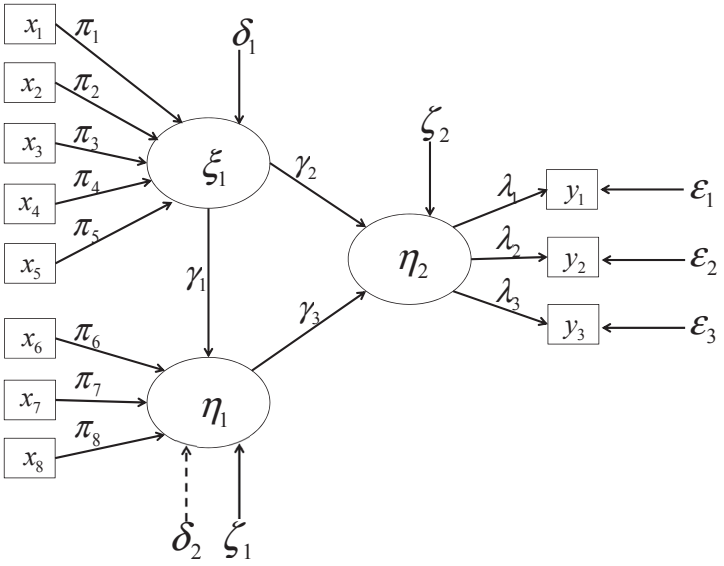

Figure 2.7: PLS vs. ML model.

MacCallum/Browne, 1993, p. 537). In the PLS world the measurement model and structural model get estimated separately, accordingly two separate equations appear. Using the variable names as in figure 2.7 the equations are the following:

$$\begin{aligned} \text{ML}: &\quad \eta_1 = \gamma_1\xi_1 + \pi_6 x_6 + \pi_7 x_7 + \pi_8 x_8 + \zeta_1 \\ \text{PLS}: &\quad \eta_1 = \pi_6 x_6 + \pi_7 x_7 + \pi_8 x_8 + \delta_2 \\ \text{PLS}: &\quad \eta_1 = \gamma_1\xi_1 + \zeta_1 \end{aligned} \tag{2.17}$$

This difference results from the different estimation procedures and cannot be prevented. It entails the following consequence: In the PLS world a change of a x variable which operationalises ξ_1 leads to a change in ξ_1. At the same time the measurement model of η_1 is not affected by the change of the respective x variable, thus η_1 is not affected. When looking at the structural model (equation 2.17) the change of ξ_1 enters completely the error term ζ_1 as η_1 does not change. This weakness does not occur in the ML world, as the model is not split into partial models.

With regard to practical applications the ML approach has a long tradition in all business disciplines (Hair et al., 2012b, p. 415). Only during the last years more and more studies have been published applying PLS. Hair

ET AL. (2012b) have investigated the "growth trend in PLS-SEM use" (p. 419). They listed all PLS applications that were published in the top 30 marketing journals[39] during 1981 and 2010. In their time series analysis they ascertained a growing number of PLS publications and an acceleration in growth of PLS publications (HAIR ET AL., 2012b, p. 419). The increase of PLS publications may have several reasons. HENSELER ET AL. (2009) and REINARTZ ET AL. (2009) investigated the individual reason(s) given in PLS application studies for their choice in favour of PLS (and against ML). I show a similar table in Appendix A, which shows some overlap with these two studies, but which (mainly) includes more recent studies. The reasons which are mentioned most often are a non-normal data distribution and a formative specification of at least one measurement model. Another recurring reason is that the sample size is absolutely small or relatively small to the number of indicators. Other reasons which appear are the model complexity, a prediction orientation[40] and an early research stage. Furthermore, the issue of identification (including convergence and admissible solutions) drives sometimes the decision. In a few studies PLS is preferred over ML because of assumed multicollinearity or misspecification. In some studies no reason is mentioned at all.

No matter what reasons are given in PLS application studies, the decision between either applying PLS or ML must be driven by the estimators properties such as consistency, bias and robustness considering the different research and data situation. RÖNKKÖ/EVERMANN (2013) state that the reasons which appear and imply that PLS is advantageous are rather "myths" than proven facts (see further in this section below and my Monte Carlo results in section 3.3). Only in case a model is not identified in terms of the ML approach or the sample consists only of a few observations the choice might be rather easy in favour of PLS. But, those cases may especially occur in the field of natural sciences such as in genetics or functional magnetic resonance imaging (REINARTZ ET AL., 2009, p. 336), where studies with low knowledge about the constructs, very large numbers of variables and small samples may occur.

To investigate consistency, bias and robustness of PLS and ML estimators

[39] According to HULT ET AL. (1997).

[40] Prediction orientation implies the prediction of concrete data points (HUBER ET AL., 2007, p. V).

simulation studies are a very powerful tool. With respect to the PLS algorithm Chin (1998b, p. 333) pointed out that for different model characteristics closed-form solutions are likely not available. He refers to McDonald's (1996, p. 240) statement: "The PLS methods are difficult to describe and extremely difficult to evaluate, partly because PLS constitutes a set of ad hoc algorithms that have generally not been formally analysed, or shown to possess any clear global optimising properties [...]". Hence, Monte Carlo based simulations can help.
Simulations have no limits regarding both, the model specification and the underlying assumptions, as long as no statistical assumption is violated: Firstly, a correlation matrix (needed for the data generation process) must be positive definite. Secondly, identification needs to be given to estimate the model (in terms of a specific estimation method). The estimators can then get assessed for example for different sample sizes, data distributions or appearing (imperfect) multicollineartiy. Besides, with the recent high computational power a large number of simulations can easily be run (e.g. 10,000 random samples), so that the results appear on average no more than marginally affected by random.

In the past many simulation studies have been performed. Hence, there exist many informations regarding consistency, accuracy and robustness of PLS and ML estimators. In Appendix D I describe briefly for a list of studies the study set-ups (i.e. model and data specifications, object of the study etc.) and the individual main findings. In the following I describe condensed Monte Carlo study findings without evaluating them:

The PLS estimators are inconsistent. In other words, PLS estimates do not become more accurate as sample size increases (Chin/Newsted, 1999; Cassel et al., 1999; Chin et al., 2003). In contrast ML estimates become more precise with increasing the sample size (Reinartz et al., 2009). PLS estimators are consistent at large, i.e. with increasing both, the sample size and the number of indicators per latent variable, the estimates become more accurate (Hui/Wold, 1982; Chin/Newsted, 1999).
Usually ML estimates are more accurate than PLS estimates (Areskoug, 1982; Reinartz et al., 2009; Ringle et al., 2009).[41] This is even the case

[41] But, ML may produce outliers (Ringle et al., 2009).

for non-normally distributed data. In general non-normality does not have an impact on estimator bias, neither for PLS nor for ML[42] (Chou/Bentler, 1995; Reinartz et al., 2009; Ringle et al., 2009).

In general adding indicators has a positive impact on accuracy for ML and PLS (which is even stronger as sample size increases), but for too little samples (e.g. 20 observations; Chin et al., 2003). In general eight (or even more) indicators lead to quite acceptable ML or PLS results (Areskoug, 1982; Chin/Newsted, 1999; Chin et al., 2003).

Strong correlations between formative indicators have no negative impact on PLS accuracy (Cassel et al., 1999). Positive correlations between formative indicators which operationalise the same construct can even increase PLS estimation accuracy (Cassel et al., 1999). Low (zero) correlations between some or all formative indicators appertaining to the same measurement model are problematic for ML estimates: the mean squared error increases because outliers appear (Ringle et al., 2009). In general a homogeneous correlation pattern between formative indicators increases accuracy for both methods (Ringle et al., 2009). Strong correlations between reflective indicators can lead to an increased mean squared error for ML (Ringle et al., 2009).

The convergence rate of the PLS algorithm is very high, but convergence is not guaranteed (Henseler, 2010, p. 113). However, convergence is much more a problem for ML than for PLS. The occurrence of improper solutions (such as negative variances) is a problem for ML. Both, ML non-convergence and improper solutions are likely to occur when the sample includes less than 200 observations (Boomsma/Hoogland, 2001 citing Hoogland, 1999; Reinartz et al., 2009).

Actual power is often higher for PLS than for ML: PLS is able to identify significant causalities (in the inner model) at least as often as ML, regardless the size of the respective coefficient, the sample size, the magnitude of the coefficients in the measurement model and the number of indicators. Under bad conditions (implying small coefficients in the measurement models and only two indicators per latent variable) the difference between ML and PLS actual power can be very large, f.i. 90% for PLS and 16% for ML referring to the same coefficient (Reinartz et al., 2009, p. 341). For example Reinartz

[42] I thereby refer to the path coefficients and not to the standard errors.

ET AL. (2009, p. 340) suggest that PLS is the method of choice "when the research focus lies on identifying relationships (i.e., prediction and theory development)".

For both approaches, but especially for ML, statistical power is positively affected by sample size (REINARTZ ET AL., 2009; GOODHUE ET AL., 2007). Furthermore, the number of indicators per latent variable has a positive impact on power (CHIN ET AL., 2003; REINARTZ ET AL., 2009). As intuitively conceivable the detection of a coefficient is more likely the larger a coefficient is. To some extent sample size can compensate for a small coefficient size (CHIN/NEWSTED, 1999; CHIN ET AL., 2003; REINARTZ ET AL., 2009).

GOODHUE ET AL. (2007, Appendix F) show PLS simulation results for the actual size of a test for significance of a coefficient in the structural model. Their results for the test size vary between 5% and 7% on the 5%-level. According to GOODHUE ET AL. (2007) this is acceptable. Also HENSELER ET AL. (2014, p. 195 et seqq.) investigated for PLS the respective test size referring to the inner model.[43] With respect to the "normal confidence intervals" it is not clear whether the deviations from the nominal size are due to random or not, as one ratio reaches f.i. 6.8% on the 5%-level. However, HENSELER ET AL. (2014, p. 196) interpret that the significance level of 5% is largely maintained. Further, their results hint at the relation between high power and a possible exceeding of the respective nominal size (HENSELER ET AL., 2014, p. 196). I did not find other PLS simulation studies in which explicitly the test size of a test for significance of the path coefficients got examined. This lack pertains also to studies which investigated the corresponding power, e.g. CHIN/NEWSTED (1999), CHIN ET AL. (2003) and REINARTZ ET AL. (2009).

With respect to the standard error estimation the data distribution can substantially affect the ML estimates, i.e. the standard deviations may be strongly biased for non-normally distributed data (CHOU/BENTLER, 1995, p. 46). Under such circumstances reliable ML standard error estimates can be obtained by estimating robust standard errors or by applying the bootstrap

[43] HENSELER ET AL. (2014) apply very simple models with two or four indicators, three indicators per latent variable, a sample size of 100 or 500 and perform 500 replications. The number of bootstrap replications is not given. To investigate the test size they apply four different bootstrap confidence intervals and refer in this regard to DICICCIO ET AL. (1996).

technique (Chou/Bentler, 1995; Nevitt/Hancock, 2001). For both approaches, but especially for the bootstrapping, accuracy of the estimates depends on the sample size. The bootstrap technique appears favourable if the sample consists of at least 200 observations while the data appears clearly non-normally distributed (Nevitt/Hancock, 2001, p. 371). With respect to the PLS approach the standard errors must get bootstrapped in any case (see section 2.2.2). The corresponding estimates decrease as sample size increases. In formative measurement models and in the structural model the estimates are negatively affected by skewness and correlations between the indicators (Cassel et al., 1999, p. 442 et seqq.). The application of the bootstrap technique requires the determination of a number of iterations. According to Nevitt/Hancock (2001, p. 371 et seq.) 250 iterations are sufficient for the ML approach (while 250 is the lowest number of replications the authors assessed). Concerning the PLS approach Hair et al. (2012a, p. 333) state that "using a small number of bootstrap samples, particularly when the original sample size is much larger, will considerably deflate standard errors", but do not suggest a specific number.

I conclude that in PLS application studies the appearing reasons for the application of PLS rather than ML do mostly not justify the choice of PLS over ML. In the following I explicate this conclusion more detailed.

In terms of accuracy ML generally outperforms PLS. The data distribution does not have an impact on estimation accuracy. Therefore, ML should be preferred even when the data is non-normally distributed.

The sample size affects estimator accuracy and power. As the ML estimators are consistent by all means ML shall be preferred over PLS if the sample consists of at least 250 observations. With samples smaller than 200 possibly ML non-convergence or inadmissible solutions arise. Incorporating information in the model specification might solve that problem. The PLS estimators are inconsistent, but consistent at large: to obtain fairly acceptable estimates the sample should consist of at least 150 observations and each latent variable should be operationalised by eight or more indicators. If a model incorporates measurement models that consist of only a few indicators, say two to four, the PLS results appear strongly biased. In general the PLS estimates appear biased, but the appearing biases remain somehow stable under varying circum-

stances. Therefore, the statement that PLS estimates appear "robust" towards small sample sizes even so implies biased estimates. Although admissible PLS estimates can usually be obtained with very small samples researchers must approach such estimates with caution.

ML identification might reach its limits faster than PLS, and ML identification problems cannot get solved by augmenting the sample size. One option to reach ML identification may be the incorporation of further information, i.e. the restriction of certain parameters. For ML identification the variance-covariance matrix of the indicators is crucial. The number of available equations to solve the model algebraically depends on the number of indicators, or more precise depends on the number of non-redundant elements of the variance-covariance matrix of the indicators. Concerning PLS additional path coefficients (i.e. model complexity increases) reduce the degrees of freedom.

In an early research stage the detection of significant causalities might matter when still theory needs to be developed. The fact that PLS shows higher actual power than ML might therefore motivate to apply PLS. To obtain good statistical power the PLS analysis should be based on at least 150 observations. The statements that PLS is favourable with respect to power must be regarded with caution because the PLS simulation studies which praise PLS power did not investigate the corresponding test size. In effect, good statistical power can be achieved by simply rejecting H_0 most of the times, and possibly doing that at the cost of an inflated actual size, i.e. rejecting H_0 erroneously too often. In my opinion the studies of Goodhue et al. (2007) and Henseler et al. (2014) do not rule out that the actual size systematically exceeds the respective α-level, although the authors find actual sizes between 5% and 7% on the 5%-level acceptable. I consider further and systematic investigations for PLS of the test size of a test for significance of the path coefficients necessary, f.i. including a larger number of Monte Carlo iterations and applying a model which incorporates formative indicators.

A model which incorporates formative indicators can get estimated with the ML approach. Specialised knowledge might be required because of its non-triviality, referring to the estimation procedure and model identification.

In summary the literature appears to some extent inconsistent as many statements are contradictory. Further, the increasing number of PLS studies

must be considered critically. In my opinion the reasons to apply the PLS approach cannot or only in seldom cases be justified in the field of business disciplines. On that account I will contribute an extensive Monte Carlo simulation (chapter 3). As I consider the investigation of the test size besides statistical power important (referring to the test for significance of path coefficients) and see in this regard a research need, I will explicitly investigate it. The model(s) I will apply will in particular incorporate formative measurement models, because ML and PLS have barely been compared under such circumstances. My simulation study will further incorporate a third estimation approach, namely the so-called OLS approach, which I present in the following section.

2.4 Ordinary Least Squares Approach

2.4.1 Introduction

The prior introduced methods ML and PLS get frequently applied in different fields of research. The ML approach has a long tradition and its properties are well known. The PLS approach has so to say become quite popular in marketing and management application studies. Both methods are not trivial but tools like user-friendly software make the application of both methods rather easy. In the following I will present another approach to estimate structural equation models with latent variables, which on contrast is very transparent and easy to understand. To my best knowledge this approach has not yet been applied to solve structural equation models. The approach is solely based on OLS regressions and mathematical computations. I will reveal that the presented approach underlies some limitations. I remark, that the presented OLS approach is distinct from the SEM regression approach, where values for the latent variables are simply computed as averages over equally weighted sums of the respective indicators (see hereto Gefen et al., 2000; Goodhue et al., 2007, among others).
In the subsequent section I demonstrate the estimation procedure for a structural model of low complexity.

2.4.2 Estimation

The procedure I will present comprises OLS regressions, the estimation of covariances, and assumptions concerning the latent variable variances and error covariances. I demonstrate the procedure for the model shown in figure 2.8. In this model the causality flows in one direction from the **x** indicators to the **y** indicators. Such a model serves to investigate the importance of success factors for some outcome variables. Compared to the models I introduced previously [44] this model is simplified, since the inner model incorporates solely direct effects and no error terms enter on the ξ variables. For the demonstration of the OLS estimation procedure this model is sufficient.

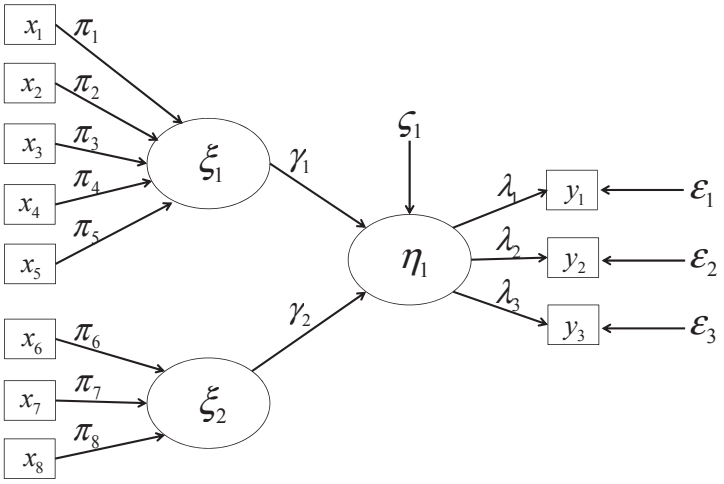

Figure 2.8: Model used to demonstrate the OLS estimation procedure.

The path coefficients of the applied model (figure 2.8) are labelled as follows:

- π_l with $l = 1, ..., L$ and here $L = 8$,
- γ_m with $m = 1, .., M$ and here $M = 2$, and
- λ_q with $q = 1, .., Q$ and here $Q = 3$.

[44] Referring to figure 2.5 page 27 and figure 2.7 page 37.

The corresponding equations are the following:

$$\begin{aligned}
\xi_1 &= \pi_1 x_1 + ... + \pi_5 x_5 \\
\xi_2 &= \pi_6 x_6 + ... + \pi_8 x_8 \\
\eta_1 &= \gamma_1 \xi_1 + \gamma_2 \xi_2 + \zeta_1 \\
&= \underbrace{\gamma_1 \pi_1}_{d_1^q} x_1 + ... + \underbrace{\gamma_2 \pi_8}_{d_8^q} x_8 + \zeta_1 \qquad (2.18) \\
y_q &= \lambda_q \eta_1 + \varepsilon_q \\
&= \underbrace{\lambda_q \gamma_1 \pi_1}_{e_1^q} x_1 + ... + \underbrace{\lambda_q \gamma_2 \pi_8}_{e_8^q} x_8 + \underbrace{\lambda_q \zeta_1 + \varepsilon_q}_{u_q} \qquad (2.19)
\end{aligned}$$

I introduce the parameters $\mathbf{d}^q$ and $\mathbf{e}^q$, which are composed of several parameters, according to the equations 2.18 and 2.19. In the latter equation I also introduce the error term u_q. According to the specified causality y_q can be regressed on $\mathbf{x}$. The index "q" indicates values which result from the regression of y_q on $\mathbf{x}$. The intercept in the regressions should be included, because it cannot cause less accurate parameter estimates. However, in the following I focus on the eight coefficients which belong to the eight x variables. The estimates $\hat{\mathbf{e}}^q$ are the OLS estimation coefficients

$$\hat{\mathbf{e}}^q = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}_q.$$

As the model consists of three y variables, three OLS regressions get performed. In one regression each of the eight OLS regression coefficients represents a total effect, which a single x_l variable has on the specific y_q. In the presented OLS approach I target the division of the estimated total effects into the single coefficients, i.e. into $\hat{\boldsymbol{\pi}}, \hat{\boldsymbol{\gamma}}$ and $\hat{\boldsymbol{\lambda}}$.

In the following I show the division for regression q:
At first fitted values get computed as

$$\hat{\eta}^{q*} = \hat{e}_1^q x_1 + ... + \hat{e}_8^q x_8.$$

In the equation $\hat{\eta}^{q*}$ equals the fitted values $\hat{y}_q$, but for didactic reasons I name these values $\hat{\eta}^{q*}$. It is crucial to note that the only difference between $\hat{\eta}^{q*}$ and

$\hat{\eta}_1$ is the factor $\hat{\lambda}_q$.[45] Therefore, the variance relation is

$$\text{var}(\hat{\eta}^{q*}) = \hat{\lambda}_q^2 \cdot \text{var}(\hat{\eta}_1).$$

$\hat{\eta}_1$ is unknown, but I specify the variance of $\hat{\eta}_1$ to take on the value one. As explained before, the scale of the latent variables needs to be defined (also PLS assumes latent variable variances of one). Accordingly, $\hat{\lambda}_q$ can be computed as

$$\text{var}(\hat{\eta}^{q*}) = \hat{\lambda}_q^2 \cdot \underbrace{\text{var}(\hat{\eta}_1)}_{\stackrel{!}{=}1} \tag{2.20}$$

$$\Rightarrow \qquad \hat{\lambda}_q = \sqrt{\text{var}(\hat{\eta}^{q*})}. \tag{2.21}$$

Applying the estimate $\hat{\lambda}_q$ I compute $\hat{\mathbf{d}}^q$ as follows:

$$\begin{aligned} \hat{\mathbf{e}}^q &= \hat{\boldsymbol{\lambda}}_q \hat{\boldsymbol{\gamma}}^q \hat{\boldsymbol{\pi}}^q \\ &= \hat{\boldsymbol{\lambda}}_q \hat{\mathbf{d}}^q \\ \Rightarrow \ \hat{\mathbf{d}}^q &= \hat{\boldsymbol{\gamma}}^q \hat{\boldsymbol{\pi}}^q = \frac{\hat{\mathbf{e}}^q}{\hat{\boldsymbol{\lambda}}_q} \end{aligned} \tag{2.22}$$

An example is $\hat{d}_1^q = \frac{\hat{e}_1^q}{\hat{\lambda}_q}$. With the vector $\hat{\mathbf{d}}^q$ new fitted values $\hat{\boldsymbol{\xi}}^{q*}$ can be computed as

$$\begin{aligned} \hat{\xi}_1^{q*} &= \hat{d}_1^q x_1 + ... + \hat{d}_5^q x_5, \\ \hat{\xi}_2^{q*} &= \hat{d}_6^q x_6 + ... + \hat{d}_8^q x_8. \end{aligned}$$

The only difference between $\hat{\xi}_g^*$ and $\hat{\xi}_g$ (for $g = 1, 2$) constitutes the factor $\hat{\gamma}_m$. Analogous to before I specify the variance of each latent variable to take on the value one. The variance relation implies (for $g = m$)

$$\text{var}(\hat{\xi}_g^{q*}) = (\hat{\gamma}_m^q)^2 \cdot \underbrace{\text{var}(\hat{\xi}_g^q)}_{\stackrel{!}{=}1} \tag{2.23}$$

$$\Rightarrow \qquad \hat{\gamma}_m^q = \sqrt{\text{var}(\hat{\xi}_g^{q*})}.$$

Using the estimates $\hat{\lambda}_q$, $\hat{\gamma}_1^q$ and $\hat{\gamma}_2^q$ subsequently $\hat{\boldsymbol{\pi}}^q$ can get estimated

$$\hat{\boldsymbol{\pi}}^{\boldsymbol{q}} = \frac{\hat{\mathbf{e}}^q}{\hat{\boldsymbol{\lambda}}\hat{\boldsymbol{\gamma}}^{\boldsymbol{q}}}. \tag{2.24}$$

[45] $\hat{\eta}^{q*} = \hat{e}_1^q x_1 + ... + \hat{e}_8^q x_8 = \hat{\lambda}_q \hat{\gamma}_1 \hat{\pi}_1 x_1 + ... + \hat{\lambda}_q \hat{\gamma}_8 \hat{\pi}_8 x_8 = \hat{\lambda}_q (\hat{\gamma}_1 \hat{\pi}_1 x_1 + ... + \hat{\gamma}_8 \hat{\pi}_8 x_8) = \hat{\lambda}_q \hat{\eta}_1$ (according to equation 2.18) with $\hat{\eta}_1 = \hat{\gamma}_1 \hat{\pi}_1 x_1 + ... + \hat{\gamma}_8 \hat{\pi}_8 x_8$.

For example the estimate $\hat{\pi}_1$ is

$$\hat{\pi}_1^1 = \frac{\hat{e}_1^1}{\hat{\lambda}_1 \hat{\gamma}_1^1} \tag{2.25}$$

based on the regression y_1 on $\mathbf{x}$.

This procedure needs to be done for each y variable. In my model there are eight total effect coefficients for each y_q. The result is one estimate $\hat{\lambda}_q$ and Q estimates for each $\hat{\gamma}$ and $\hat{\pi}$ (the model consists of $Q = 3$ y variables). Thus, $\hat{\pi}_1$ can be estimated according to equation 2.25 as well as according to the equations:

$$\hat{\pi}_1^2 = \frac{\hat{e}_1^2}{\hat{\lambda}_2 \hat{\gamma}_1^2}, \tag{2.26}$$

$$\hat{\pi}_1^3 = \frac{\hat{e}_1^3}{\hat{\lambda}_3 \hat{\gamma}_1^3}. \tag{2.27}$$

The model contains more information than has been used so far. This information is revealed by the covariances between the three y variables. In the equation

$$\text{cov}(\hat{y}_k, \hat{y}_s) = \text{cov}(\hat{\lambda}_k \hat{\eta}_1,\ \hat{\lambda}_s \hat{\eta}_1) \tag{2.28}$$

the indices k and s label two different y variables ($k \neq s$), which belong to the same latent variable η_1 (the error terms are uncorrelated). Applying the covariances between the fitted values of the y variables the $\hat{\lambda}_q$ can get estimated as follows:

$$\begin{aligned}
\text{cov}(\hat{y}_1, \hat{y}_2) &= \text{cov}(\hat{\lambda}_1 \hat{\eta}_1,\ \hat{\lambda}_2 \hat{\eta}_1) \\
&= \hat{\lambda}_1 \hat{\lambda}_2 \underbrace{\text{var}(\hat{\eta}_1)}_{\stackrel{!}{=}1} \\
\hat{\lambda}_2 &= \frac{\text{cov}(\hat{y}_1, \hat{y}_2)}{\hat{\lambda}_1} \\
\text{cov}(\hat{y}_1, \hat{y}_3) &= \text{cov}(\hat{\lambda}_1 \hat{\eta}_1,\ \hat{\lambda}_3 \hat{\eta}_1) \\
&= \hat{\lambda}_1 \hat{\lambda}_3 \underbrace{\text{var}(\hat{\eta}_1)}_{\stackrel{!}{=}1} \\
\hat{\lambda}_3 &= \frac{\text{cov}(\hat{y}_1, \hat{y}_3)}{\hat{\lambda}_1}
\end{aligned} \tag{2.29}$$

$$\begin{aligned}
\operatorname{cov}(\hat{y}_2, \hat{y}_3) &= \operatorname{cov}(\hat{\lambda}_2\hat{\eta}_1,\ \hat{\lambda}_3\hat{\eta}_1) \\
&= \hat{\lambda}_2\hat{\lambda}_3 \underbrace{\operatorname{var}(\hat{\eta}_1)}_{\overset{!}{=}1} \\
&= \frac{\operatorname{cov}(\hat{y}_1, \hat{y}_2)}{\hat{\lambda}_1} \cdot \frac{\operatorname{cov}(\hat{y}_1, \hat{y}_3)}{\hat{\lambda}_1} \\
\implies \hat{\lambda}_1 &= \sqrt{\frac{\operatorname{cov}(\hat{y}_1, \hat{y}_2) \cdot \operatorname{cov}(\hat{y}_1, \hat{y}_3)}{\operatorname{cov}(\hat{y}_2, \hat{y}_3)}}
\end{aligned} \tag{2.30}$$

The variance of the latent variable is consistently specified to take on the value one. With the estimate $\hat{\lambda}_1$ the two other parameters $\hat{\lambda}_2$ and $\hat{\lambda}_3$ can be estimated according to the system of equations. As this example demonstrates a reflective specified latent variable needs at least three indicators for this kind of estimation procedure. The application of equation 2.30 becomes particularly important for models which incorporate solely reflective indicators, see at the end of this section and figure 2.9 page 52.

According to equation 2.30 the fraction below the square root must take on a non-negative number. Moreover, the denominator may not be zero. The latter condition is true for all fractions, i.e. for the equations 2.22 and 2.24. Even values close to zero can be problematic because the respective fraction becomes irregular large and can thereby distort the results. This fact constitutes a "limitation" to which I referred in section 2.4.1.

The procedure has several starting points. Instead of solving $\hat{\lambda}_1$ first alternatively $\hat{\lambda}_2$ or $\hat{\lambda}_3$ can get solved first. If a latent variable has more than three indicators, it does make a difference which parameter gets estimated first. The number of possible starting points corresponds with a combination without repetition, because $\operatorname{cov}(\hat{y}_k, \hat{y}_s)$ equals $\operatorname{cov}(\hat{y}_s, \hat{y}_k)$. In case a latent variable is operationalised by five reflective indicators there are

$$\binom{5}{2} = 10$$

starting points, because two indicators get picked out of five (i.e. $\hat{y}_k$ and $\hat{y}_s$) to examine $\operatorname{cov}(\hat{y}_k, \hat{y}_s)$. Further, each starting point can be varied three times $(= 5 - 2)$. As an example I show the three variations for one starting point $\operatorname{cov}(\hat{y}_1, \hat{y}_2) = \hat{\lambda}_1\hat{\lambda}_2$ (see equation 2.29):

$$
\begin{aligned}
1. \quad \hat{\lambda}_1 &= \frac{\mathrm{cov}(\hat{y}_1, \hat{y}_3)}{\hat{\lambda}_3} \\
\hat{\lambda}_2 &= \frac{\mathrm{cov}(\hat{y}_2, \hat{y}_3)}{\hat{\lambda}_3} \\
\Rightarrow \hat{\lambda}_3 &= \sqrt{\frac{\mathrm{cov}(\hat{y}_1, \hat{y}_3) \cdot \mathrm{cov}(\hat{y}_2, \hat{y}_3)}{\mathrm{cov}(\hat{y}_1, \hat{y}_2)}} \\
2. \quad \hat{\lambda}_1 &= \frac{\mathrm{cov}(\hat{y}_1, \hat{y}_4)}{\hat{\lambda}_4} \\
\hat{\lambda}_2 &= \frac{\mathrm{cov}(\hat{y}_2, \hat{y}_4)}{\hat{\lambda}_4} \\
\Rightarrow \hat{\lambda}_4 &= \sqrt{\frac{\mathrm{cov}(\hat{y}_1, \hat{y}_4) \cdot \mathrm{cov}(\hat{y}_2, \hat{y}_4)}{\mathrm{cov}(\hat{y}_1, \hat{y}_2)}} \\
3. \quad \hat{\lambda}_1 &= \frac{\mathrm{cov}(\hat{y}_1, \hat{y}_5)}{\hat{\lambda}_5} \\
\hat{\lambda}_2 &= \frac{\mathrm{cov}(\hat{y}_2, \hat{y}_5)}{\hat{\lambda}_5} \\
\Rightarrow \hat{\lambda}_5 &= \sqrt{\frac{\mathrm{cov}(\hat{y}_1, \hat{y}_5) \cdot \mathrm{cov}(\hat{y}_2, \hat{y}_5)}{\mathrm{cov}(\hat{y}_1, \hat{y}_2)}}
\end{aligned}
$$

On the basis of the covariances between the fitted y values 30 ($= 10 \cdot 3$) equations appear to estimate five λ coefficients, i.e. six equations appear for each λ_q.

Further, I illustrate how estimates for the error variances can be obtained, referring to figure 2.8 (page 45). A result of an OLS regression q are the errors $\hat{u}_q$. The covariance between two errors $\hat{u}_k$ and $\hat{u}_s$ ($k \neq s$) provides information, because the covariance ascribes to the common error ζ_1, see equation 2.19 (page 46). The latter equation reveals that the residuals u_q are composed of $\lambda_q\zeta_1 + \varepsilon_q$. For uncorrelated errors the variance relation is

$$\mathrm{var}(u_q) = \lambda_q^2 \cdot \mathrm{var}(\zeta_1) + \mathrm{var}(\varepsilon_q). \tag{2.31}$$

Assuming uncorrelated error terms and using the estimated values, the covariance between two different errors is:

$$
\begin{aligned}
\mathrm{cov}(\hat{u}_k, \hat{u}_s) &= \mathrm{cov}(\hat{\lambda}_k\hat{\zeta}_1 + \hat{\varepsilon}_k,\ \hat{\lambda}_s\hat{\zeta}_1 + \hat{\varepsilon}_s) \\
&= \hat{\lambda}_k \cdot \hat{\lambda}_s \cdot \mathrm{var}(\hat{\zeta}_1)
\end{aligned}
$$

In doing so $\binom{Q}{2} = \binom{3}{2} = 3$ estimates $\text{var}(\hat{\zeta}_1)$ can be obtained.
According to equation 2.31 the variances of the other error terms ε equal

$$\text{var}(\hat{\varepsilon}_q) = \text{var}(\hat{u}_q) - \hat{\lambda}_q^2 \cdot \text{var}(\hat{\zeta}_1).$$

According to the presented approach several estimates for one and the same parameter exist. Although estimates can be obtained in different ways, the estimates cannot take on two different values such as $\hat{\lambda}_q$ and $\hat{\lambda}_q + c$ for any constant c. Possible differences are only marginal. Hence, the estimates are non-arbitrary and determined. By estimating the parameters in different ways I incorporate all information the model contains. At this point I refer to my simulation study in chapter 3 and briefly anticipate that my study ascertains consistent and accurate estimates, so that the proceeding seems appropriate to receive the best estimate.

So far I concentrated on the estimation of the π, γ and λ coefficients and of the variances $\text{var}(\zeta)$ and $\text{var}(\varepsilon)$. The variances of the coefficient estimates can get estimated as follows:

The variances of the regression coefficients $\hat{\mathbf{e}}^q$ (representing the total effects) result as well known OLS standard deviations:

$$\text{var}\left(\hat{\mathbf{e}}^q\right) = \left(\sigma^q\right)^2 \left(\mathbf{X}'\mathbf{X}\right)^{-1}$$

The variances belonging to $\hat{\boldsymbol{\pi}}$, $\hat{\boldsymbol{\gamma}}$ and $\hat{\boldsymbol{\lambda}}$ can be estimated by applying the bootstrap technique. Initially, the $\hat{\mathbf{e}}^q$ get bootstrapped (for each q). These estimates get divided into the individual coefficients. The variances of these estimates (the number of bootstrap replications determines the number of available estimates) represent the estimated (bootstrapped) variances. For an introduction to the bootstrap technique see Appendix C.

Finally, I want to call attention to another model specification. In the literature many studies can be found using exclusively reflective measurement models, see e.g. figure 2.9.[46] The OLS approach works as well for such specifications. In Appendix E I present the estimation procedure, referring to figure 2.9. The model does not comprise the error terms $\boldsymbol{\delta}$ and ζ, but to present the procedure this simplified model is sufficient.

[46] In practical applications measurement models may be incorrectly specified in a reflective way, see hereto Jarvis et al. (2003).

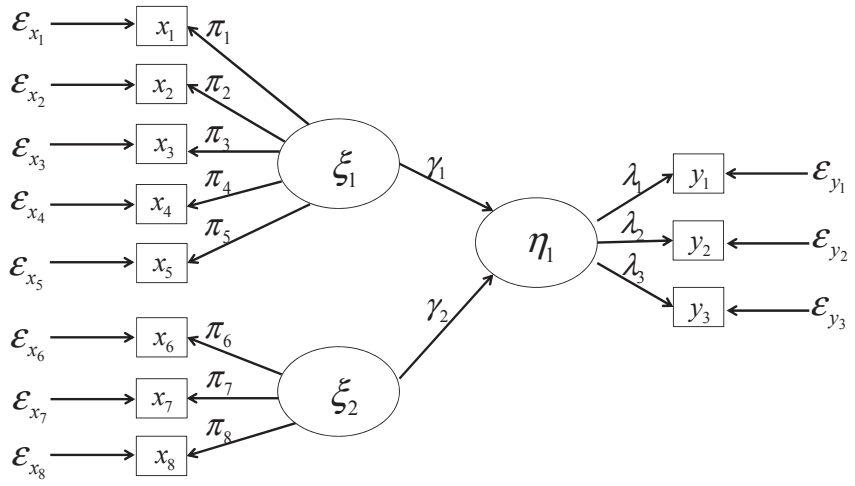

Figure 2.9: Model with solely reflective indicators.

2.4.3 Identification

With respect to the OLS approach the identification of a structural equation model requires a sufficient sample size and all parameters need to be determined.

Referring to sample size OLS identification is partially analogous to the identification of a multivariate regression. The sample needs to obtain at the very least as many observations as the model contains regressors (plus one for the intercept), i.e. degrees of freedom ≥ 0. In a model where all exogenous latent variables are operationalised in a formative way and all endogenous latent variables in a reflective way, the required minimal sample size equals the number of formative indicators (i.e. x variables) plus one for the intercept. For example in the model shown in figure 2.8 (page 45) the minimum sample size is nine, if an intercept is included.

In Appendix E I show the estimation procedure for a model which incorporates solely reflective indicators. To estimate such models each latent variables needs to be operationalised by at least three indicators (according to equation 2.30).

Another restriction for identification is analogous to the identification in the ML world. A model might incorporate indeterminacies which in general imply somehow missing information and arbitrary results. The incorporation of information, i.e. imposing restrictions can solve the indeterminacies, for example to specify an error variance to take on the value zero. Concerning this I refer again (as in section 2.1.3) to MacCallum/Browne (1993, p. 537 et seq.) and to section 3.1.4 (equations 3.4 and 3.5 page 65 et seq.), in which I give an example for exactly this kind of indeterminacy. For this very reason in the model 2.8 shown in figure I specified $\boldsymbol{\xi}$ error free.

Usually, when we talk about a model, which does not have unique solutions for parameters, we imply arbitrary results. In the OLS approach determined results may not be unique in the traditional sense. Parameters can sometimes be solved in different manners, but still without being arbitrary. I even argue that by solving parameters in different manners more given information gets incorporated in the resulting estimates.
My simulation study will ascertain that the average over all available estimates for one and the same parameter yields a very accurate estimate (see the results in section 3.3.1).

Chapter 3

Simulation Study

3.1 Set-up

3.1.1 Study Design

I purpose to investigate and compare estimation qualities for the three presented approaches ML, PLS and OLS. To do so a Monte Carlo simulation is appropriate, as it represents a powerful tool to assess estimator behaviour, for example estimator robustness towards multicollinearity or different error term distributions. In my study I specify many different cases and assess them by performing 10,000 (K) iterations per case. All estimations get performed with the software `R` (R Core Team, 2014), including in particular the contributed packages *plspm* (Sanchez et al., 2013) and *sem* (Fox et al., 2013).

The specified model, see figure 3.1, has three latent variables incorporated. Two of them are operationalised in a formative way and one in a reflective way. Looking at the indicators the model shows a straightforward causality going from the $\mathbf{x}$ to the $\mathbf{y}$ variables. This case is quite important since the object of a study is often to investigate the role of drivers / success factors on a particular outcome, e.g. financial performance. The model design is quite simple. I choose this model on purpose since it corresponds with the model I used for the introduction of the OLS approach (section 2.4). Therefore, my work becomes replicable and transparent.

I determine the number of variables, the paths between them and the error terms according to figure 3.1. Additionally, the following aspects need to be

determined:

- The variance-covariance matrix $\mathbf{V}$ of $\mathbf{x}$,
- the distribution of the $\mathbf{x}$ variables,
- the eight $\boldsymbol{\pi}$ coefficients ($L = 8$),
- the two $\boldsymbol{\gamma}$ coefficients ($M = 2$),
- the three $\boldsymbol{\lambda}$ coefficients ($Q = 3$),
- the distribution of the error terms,
- the determination coefficients (R^2) and
- the sample size (n).

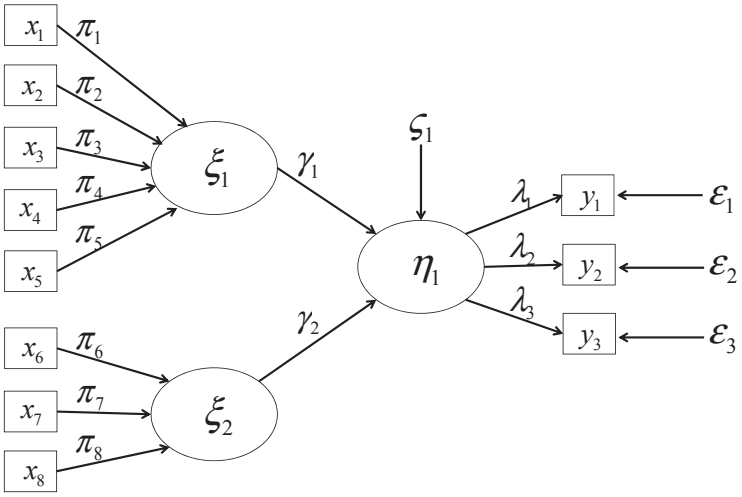

Figure 3.1: Specified model for simulation study.

Furthermore, the different assumptions of the three investigated approaches need to be taken into account. The ML approach restricts some coefficients to take on the value one (see section 2.1.1). The PLS algorithm ensures that the variances of the latent variable scores equal a value of one, respectively (see section 2.2.2). The OLS approach assumes that the variances of the fitted values of the latent variables take on the value one, respectively (see

section 2.4.2). Any of these assumptions determines the scale of the latent variables and constitutes a criterion for identification. Before starting the data generation process the different suppositions of the methods ought to be considered. In this study the model gets specified in order to obtain latent variable variances equal to a value of one, referring only to the explained sum of squares (ESS). This can be realised by choosing appropriate coefficients (see section 3.1.3). To compare all estimates with the population parameters, the estimates must rely on the same scaling as the true model. Therefore, all estimates, which rely on a different scaling, must get rescaled.
The data generation characteristic ESS=1 is in line with the OLS assumption. Consequently, the OLS results can be compared with the the population parameters without scaling them.
Although both, the PLS and the OLS approach suppose both latent variable variances equal to a value of one, the assumptions do somehow differ. Only when looking at a formative measurement model the PLS estimates do not need to get rescaled to compare them with the population parameters. The underlying supposition is in line with ESS=1 (referring to ξ_1 and ξ_2) as the PLS approach computes in general scores as weighted sum of the indicators and in formative measurement model regresses thereafter these scores on its indicators. Consequently, in formative measurement models each performed linear regression results in perfect fit, or to put it in other words the error term is zero and the variance of the scores (here ξ_1 and ξ_2) is only composed of ESS (i.e. ESS=TSS, total sum of squares). Concerning the rest of the model the PLS estimates need to get rescaled. As a part of the algorithm the variance of the scores of η_1 is scaled to a value of one, while the true variance of the latent variable η_1 is different from one, because the true variance of η_1 is composed of ESS (which I set one) and the variance of ζ_1 (RSS, residual sum of squares). Consequently, with respect to the structural model and the reflective measurement model the PLS estimates need to get another scale.
The ML estimates need to get rescaled concerning the entire model, because its latent variable scaling does not correspond with the population parameters.

The data generation process, which ensures that ESS of all latent variables takes on the value one, is delineated in section 3.1.3. The scaling procedures are elucidated in section 3.2.1.

In the following section I designate all specifications I investigate.

3.1.2 Specifications

The starting point constitutes the model shown in figure 3.1 (page 55). For this model I determine the specification and name the setting "basic model". Later on I perform variations based on this basic model.

The design determinants of the basic model look in detail like the following: The variance-covariance matrix of $\mathbf{x}$, $\mathbf{V}^{\mathrm{I}}$, has on the main diagonal only values of one.[47] The correlations (covariances and correlations are identical) between the formative measurement blocks range between 0.01 and 0.2 and within the measurement blocks they range between 0.15 and 0.35.

$$\mathrm{E}(\mathbf{x}\mathbf{x}') = \mathbf{V}^{\mathrm{I}} = \begin{pmatrix} 1 & 0.25 & 0.30 & 0.35 & 0.20 & 0.05 & 0.01 & 0.05 \\ 0.25 & 1 & 0.30 & 0.20 & 0.15 & 0.15 & 0.05 & 0.15 \\ 0.30 & 0.30 & 1 & 0.35 & 0.20 & 0.01 & 0.04 & 0.02 \\ 0.35 & 0.20 & 0.35 & 1 & 0.25 & 0.05 & 0.01 & 0.02 \\ 0.20 & 0.15 & 0.20 & 0.25 & 1 & 0.10 & 0.15 & 0.20 \\ 0.05 & 0.15 & 0.01 & 0.05 & 0.10 & 1 & 0.25 & 0.30 \\ 0.01 & 0.05 & 0.04 & 0.01 & 0.15 & 0.25 & 1 & 0.20 \\ 0.05 & 0.15 & 0.02 & 0.02 & 0.20 & 0.30 & 0.20 & 1 \end{pmatrix}$$

In order to represent a correlation matrix $\mathbf{V}^{\mathrm{I}}$ is positive definite.

Settings of the specification are

- normally distributed $\mathbf{x}$ variables with $\boldsymbol{\mu} = \mathbf{0}$ and $\boldsymbol{\sigma}^{\mathbf{2}} = \mathbf{1}$,
- $\boldsymbol{\pi}' = (0.8,\ 0.5,\ 0.8,\ 0.6,\ 0.4,\ 0.6,\ 0.4,\ 0.5)$,
- $\boldsymbol{\gamma}' = (0.9,\ 0.9)$,
- $\boldsymbol{\lambda}' = (1,\ 0.7,\ 0.9)$,[48]

[47] The index "I" (in $\mathbf{V}^{\mathrm{I}}$) indicates that this matrix is the first one out of several specified variance-covariance matrices.

[48] The coefficients $\boldsymbol{\pi}$, $\boldsymbol{\gamma}$ and $\boldsymbol{\lambda}$ are preliminary, because they do not lead to latent variable variances that equal a value of one, respectively. The coefficient adjustment is illustrated in section 3.1.3.

- $(R^2)^{\text{fMM}} = 1$ (determination coefficient in the formative measurement model),[49]
- $(R^2)^{\text{SM}} = 0.5$ (determination coefficient in the structural model),
- $(R^2)^{\text{rMM}} = 0.5$ (determination coefficient in the reflective measurement model),
- normally distributed error terms with $\boldsymbol{\mu} = \mathbf{0}$, the variances depend i.a. on the determined R^2 (see section 3.1.3) and
- a sample size of $n = 300$.

To compare estimation qualities for different cases I systematically vary the specification of the basic model by changing one specific aspect at a time:
I incorporate a lower amount of explained variance, since such cases can be considered to play a role in practical applications. The same is true for appearing non-normality, so that I incorporate non-normally distributed error terms. With regard to sample size I assess different cases, ranging from very small to very large sample sizes. Further, the PLS property "consistency at large" is of interest and how the three approaches differ from each other in terms of accuracy, when the sample size is large and each latent variable gets operationalised by a relatively large number of indicators. Moreover, I vary the variance-covariance matrix of $\mathbf{x}$: To understand the behaviour of the estimators I apply an identity matrix (although this case may not occur in practical applications) and a matrix which features (imperfect) multicollinearity. Furthermore, I simulate a case where the exogenous indicators are discrete such that they can represent questionnaire data. I specify a model which includes coefficients which take on the value zero. This model serves to investigate the test size and statistical power of a test for significance of the path coefficients.

I specify the following cases:

A The determination coefficient R^2 is 0.2 in both, the reflective measurement model and the structural model. In the formative measurement model it is kept 1.

[49] $(R^2)^{\text{fMM}} = 1$ implies that the formative measurement model incorporates no error term, as it is depicted in figure 3.1. I reason this specific aspect in section 3.1.4.

B The error terms follow a non-central chi-squared distribution (B1) or a continuous uniform distribution (B2), respectively, see for details Appendix F.

C The sample size is 15 (C1), 50 (C2), or 1,000 (C3).

D The number of indicators increases together with the sample size: The number of indicators remains as specified above (11) and the sample size is 50 (D1), the number of indicators per latent variable doubles (22) while n is 300 (D2), and the number of indicators quadruples (44) while n is 1,000 (D3). As the cases differ in the number of x variables, the variance-covariance matrices of $\mathbf{x}$ necessarily differ. To make the cases perfectly matchable, I apply for all three cases an identity matrix as variance-covariance matrix of $\mathbf{x}$.[50] The coefficient values correspond with those specified above, i.e. the respective π and λ coefficients double or quadruple.

E As variance-covariance matrix of $\mathbf{x}$ I apply an identity matrix

$$\mathbf{V}^{\mathrm{II}} = \mathbf{I} \quad \text{(E1)}$$

and a matrix which features (imperfect) multicollinearity[51]:

$$\mathbf{V}^{\mathrm{III}} = \begin{pmatrix} 1 & 0.9 & 0.8 & 0.9 & 0.85 & 0.45 & 0.4 & 0.5 \\ 0.9 & 1 & 0.8 & 0.8 & 0.85 & 0.45 & 0.4 & 0.4 \\ 0.8 & 0.8 & 1 & 0.9 & 0.95 & 0.4 & 0.4 & 0.4 \\ 0.9 & 0.8 & 0.9 & 1 & 0.85 & 0.4 & 0.4 & 0.45 \\ 0.85 & 0.85 & 0.95 & 0.85 & 1 & 0.45 & 0.4 & 0.45 \\ 0.45 & 0.45 & 0.4 & 0.4 & 0.45 & 1 & 0.9 & 0.95 \\ 0.4 & 0.4 & 0.4 & 0.4 & 0.4 & 0.9 & 1 & 0.9 \\ 0.5 & 0.4 & 0.4 & 0.45 & 0.45 & 0.95 & 0.9 & 1 \end{pmatrix} \quad \text{(E2)}$$

[50] The case D1 differs from B2, as in D1 an identity matrix and in B2 the matrix $\mathbf{V}^{\mathrm{I}}$ constitutes the variance-covariance matrix of $\mathbf{x}$.

[51] 10,000 $\mathbf{x}$ samples ($n = 300$) yielded on average the following adjusted determination coefficients: $\overline{R}^2 = 0.958249$ for x_1 regressed on x_2 to x_8; $\overline{R}^2 = 0.9396271$ for x_1 regressed on x_2 to x_5; $\overline{R}^2 = 0.9124331$ for x_6 regressed on x_7 and x_8.

The matrices $\mathbf{V}^{\mathrm{II}}$ and $\mathbf{V}^{\mathrm{III}}$ are positive definite, too.[52] The variance-covariance matrix impacts the variances of the endogenous variables, but I ensure that the proportion between explained and unexplained variance of the endogenous variables explicitly remains unchanged, respectively.

F The exogenous indicators $\mathbf{x}$ are discrete. I first sample the x variables from a multivariate normal distribution according to the basic model and thereafter aggregate them to 7 values.

G I augment each measurement model by one extra regressor whose true influence is zero, see figure 3.2. The dashed lines in the figure indicate that these coefficients take on the value zero. As all other coefficients correspond with those specified above, the coefficients are the following: $\boldsymbol{\pi}' = (0.8,\ 0.5,\ 0.8,\ 0.6,\ 0.4,\ 0,\ 0.4,\ 0.6,\ 0.5,\ 0)$, $\boldsymbol{\gamma}' = (0.9,\ 0.9)$ and $\boldsymbol{\lambda}' = (1,\ 0.7,\ 0.9,\ 0)$.[53] The variance-covariance matrix is defined as

$$\mathbf{V}^{\mathrm{G}} = \begin{pmatrix} 1 & 0.25 & 0.30 & 0.35 & 0.20 & 0.20 & 0.05 & 0.01 & 0.05 & 0.05 \\ 0.25 & 1 & 0.30 & 0.20 & 0.15 & 0.20 & 0.15 & 0.05 & 0.15 & 0.15 \\ 0.30 & 0.30 & 1 & 0.35 & 0.20 & 0.20 & 0.01 & 0.04 & 0.02 & 0.01 \\ 0.35 & 0.20 & 0.35 & 1 & 0.25 & 0.20 & 0.05 & 0.01 & 0.02 & 0.05 \\ 0.20 & 0.15 & 0.20 & 0.25 & 1 & 0.20 & 0.10 & 0.15 & 0.20 & 0.10 \\ 0.20 & 0.20 & 0.20 & 0.20 & 0.20 & 1 & 0.05 & 0.01 & 0.05 & 0.05 \\ 0.05 & 0.15 & 0.01 & 0.05 & 0.10 & 0.05 & 1 & 0.25 & 0.30 & 0.20 \\ 0.01 & 0.05 & 0.04 & 0.01 & 0.15 & 0.01 & 0.25 & 1 & 0.20 & 0.20 \\ 0.05 & 0.15 & 0.02 & 0.02 & 0.20 & 0.05 & 0.30 & 0.20 & 1 & 0.20 \\ 0.05 & 0.15 & 0.01 & 0.05 & 0.10 & 0.05 & 0.20 & 0.20 & 0.20 & 1 \end{pmatrix}$$

and is based on $\mathbf{V}^{\mathrm{I}}$.

The specified cases A to G differ from the basic model only in the defined specification aspect. To simulate an extreme case of non-normality I combine

[52] The variance-covariance matrix of $\mathbf{x}$ constitutes an identity matrix in variation E1 as well as in all D cases. Although the cases include different number of x variables, implying different dimensions of their variance-covariance matrix, I will label all identity matrices $\mathbf{V}^{\mathrm{II}}$.

[53] Analogous to before this coefficients do not yield ESS=1 referring to the latent variables. Thus, the coefficients still need to get adjusted according to the subsequent section 3.1.3.

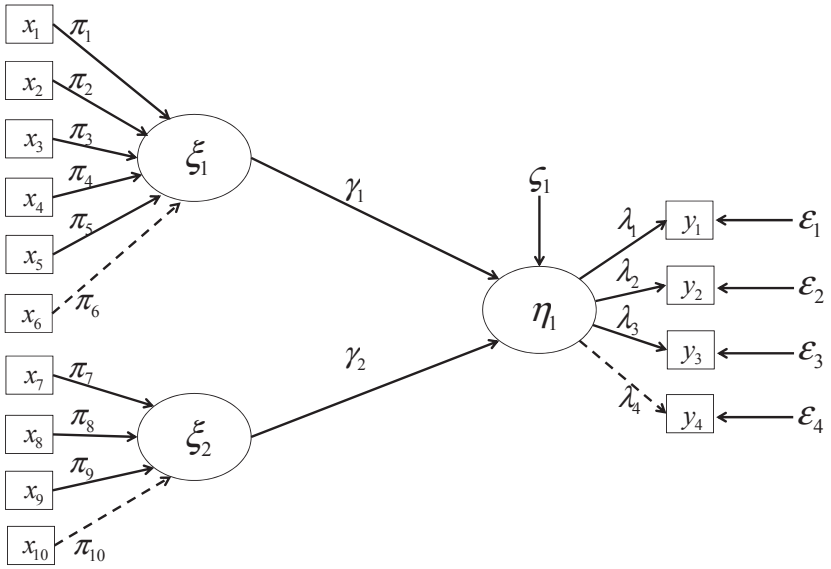

Figure 3.2: Model for case G.

variation A and the two B cases, named AB1 and AB2. These cases involve non-normally distributed errors and the variation due to error makes 80% referring to η_1 and each y_q, respectively.

I investigate estimation accuracy (section 3.3.1) for all cases, but for variation G. Additionally I investigate accuracy of the PLS estimates applying the different PLS inner schemes:[54] the centroid, factorial and path weighting scheme, in this respect see further section 3.1.4.

On the basis of variation G I investigate size and power of the test for significance of the path coefficients (section 3.3.2). The PLS standard errors need to get bootstrapped to determine significance. I specify the number of bootstrap replications to 100 (K_B), which is the default number of bootstrap replications in the *plspm* package (Sanchez et al., 2013) in R (R Core Team, 2014). Additionally I perform two extra simulations including 300 or 1,000 PLS bootstrap replications, because a too low number of bootstrap replications may lead to deflated standard deviations (Hair et al., 2012a, p. 333). In the ML world bootstrapping is not always the best choice. If the assumption of multinormality is met bootstrapping is not necessary or

[54] See step 2a in section 2.2.2.

should even be avoided (NEVITT/HANCOCK, 2001, p. 369 et seqq.). Since case G is correctly specified[55] and incorporates solely normally distributed data I consequently use the standard deviations which result from the ML estimation. Nevertheless, I estimate also the bootstrapped standard errors (with $K_B = 300$), but consider this as an additional check. Further, I investigate whether the PLS inner schemes have an impact on test size and power.
I will present my simulation results in section 3.3 and prior to this tabulate all specified cases, see table 3.1 page 76 et seq.

3.1.3 Data Generation

The data generation process is supposed to produce latent variable variances equal to a value of one referring only to the explained variation (see section 3.1.1). To do so the specified coefficients need to get adjusted. Referring to the basic model the adjustment works as follows:

The variance-covariance matrix of $\boldsymbol{\xi}$ depends on the specified variance-covariance matrix of $\mathbf{x}$ and on the theoretical values $\boldsymbol{\pi}$. It is

$$\mathrm{E}(\boldsymbol{\xi}\boldsymbol{\xi}') = \boldsymbol{\pi}'\mathbf{V}^{\mathrm{I}}\boldsymbol{\pi} \tag{3.1}$$

with $\boldsymbol{\pi}$ representing a 8×2 matrix

$$\boldsymbol{\pi}' = \begin{pmatrix} 0.8 & 0.5 & 0.8 & 0.6 & 0.4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.6 & 0.4 & 0.5 \end{pmatrix}$$

according to the basic specification. To render the variances of ξ_1 and ξ_2 equal to a value of one, the coefficients need to get divided by the respective variances (the values on the main diagonal of $\mathrm{E}(\xi\xi')$).

$$\pi_l^{\text{true}} = \frac{\pi_l}{\sqrt{\text{var}(\xi_1)}} \qquad \text{for } l = 1, ..., 5$$

$$\pi_l^{\text{true}} = \frac{\pi_l}{\sqrt{\text{var}(\xi_2)}} \qquad \text{for } l = 6, ..., 8$$

With respect to η_1 the value ESS_{η_1} is supposed to take on the value one. The procedure is analogous to before. The preliminary variance of η_1 gets computed

[55] A correct model specification is required to obtain unbiased estimates of the standard errors (KAPLAN, 1989, p. 44).

as $\text{var}(\eta_1) = \mathbf{d'V^I d}$. The vector $\mathbf{d}$ has length eight. Its first five elements take on the values $\gamma_1 \cdot \pi_l^{\text{true}}$ with $l = 1, ..., 5$ and the last three take on the values $\gamma_2 \cdot \pi_l^{\text{true}}$ with $l = 6, ..., 8$. With

$$\boldsymbol{\gamma}^{\text{true}} = \frac{\boldsymbol{\gamma}}{\sqrt{\text{var}(\eta_1)}}$$

my purpose is accomplished: $\text{ESS}_{\xi_1} = \text{ESS}_{\xi_2} = \text{ESS}_{\eta_1} = 1$, while for both ξ variables this values corresponds with TSS_{ξ_g} $(g = 1, 2)$. The variances of the y variables do not need to get a certain scale.

Finally, the coefficients take on the following values:

- $(\boldsymbol{\pi}^{\text{true}})' = (0.55874,\ 0.34921,\ 0.55874,\ 0.41906,\ 0.27937,\ 0.45584,\ 0.68376,\ 0.56980)$,
- $(\boldsymbol{\gamma}^{\text{true}})' = (0.70711,\ 0.70711)$,
- $\boldsymbol{\lambda}' = (1,\ 0.7,\ 0.9)$.

In the following procedure I exclusively apply these coefficients (referring to the basic model).

Further, the variances of the error terms need to be determined. The variance of ζ_1 is

$$\text{var}(\zeta_1) = \text{RSS}_{\eta_1} = \text{ESS}_{\eta_1} \cdot \left(\frac{1}{(R^2)^{\text{SM}}} - 1 \right). \tag{3.2}$$

As in the basic model $(R^2)^{\text{SM}} = 0.5$ the variance of ζ_1 takes on the value 1.00. Subsequently, the variance of each error term ϵ_q can be determined:

$$\begin{aligned} \text{var}(\epsilon_q) &= \text{ESS}_{y_q} \cdot \left(\frac{1}{(R^2)^{\text{rMM}}} - 1 \right) \\ &= \lambda_q^2 \cdot \text{var}(\eta_1) \cdot \left(\frac{1}{(R^2)^{\text{rMM}}} - 1 \right), \end{aligned} \tag{3.3}$$

with $\text{var}(\eta_1) = \text{ESS}_{\eta_1} + \text{RSS}_{\eta_1}$. For the basic model the variances of the respective error terms take on the values $\boldsymbol{\epsilon}' = (2.00,\ 0.98,\ 1.28)$.
To generate the data sets no more values are required.

The data generation process looks like the following. Initially, $\mathbf{x}$ gets sampled from a multivariate normal distribution with sample size n. For this purpose I use the R (R Core Team, 2014) package *simFrame* (Alfons, 2014). With the $\mathbf{x}$ sample the $\boldsymbol{\xi}$ variables can be computed as

$$\xi_1 = \sum_{l=1}^{5} \pi_l^{\text{true}} \cdot \mathbf{x},$$
$$\xi_2 = \sum_{l=6}^{8} \pi_l^{\text{true}} \cdot \mathbf{x}.$$

To compute η_1 the error term ζ_1 must get sampled from a certain distribution with certain population parameters (see section 3.1.2). For normally distributed error terms I sample ζ_1 from a normal distribution with mean zero and $\text{var}(\zeta_1)$ according to equation 3.2. Then η_1 can be computed as

$$\eta_1 = \gamma_1^{\text{true}} \cdot \xi_1 + \gamma_2^{\text{true}} \cdot \xi_2 + \zeta_1.$$

Further, η_1 serves the generation of the three y variables. The required error terms ε_q get sampled from the same population as ζ_1. The respective distribution is characterised by mean zero and a variance which corresponds with equation 3.3. With three different samples of ε_q all y variables can get computed:

$$\mathbf{y} = \boldsymbol{\lambda}\eta_1 + \boldsymbol{\epsilon}.$$

For the cases in which the error terms are non-normally distributed see further Appendix F.

The variance-covariance matrix of $\mathbf{y}$ is not required for the data generation process, but is a result from the prior specifications. For the basic model it is

$$\text{E}(\mathbf{y}\mathbf{y}') = \begin{pmatrix} 4.00 & 1.40 & 1.80 \\ 1.40 & 1.96 & 1.26 \\ 1.80 & 1.26 & 3.24 \end{pmatrix}$$

since the error terms are completely uncorrelated.[56]

[56]This matrix arises independent from the applied variance-covariance matrix of $\mathbf{x}$, f.i. it is $\text{cov}(y_1, y_2) = \text{cov}(\lambda_1\eta_1 + \varepsilon_1,\ \lambda_2\eta_1 + \varepsilon_2) = \lambda_1\lambda_2\text{var}(\eta_1)$. Since $\text{var}(\eta_1)$ is constantly 2 (because $\text{ESS}_{\eta_1} = 1$ and $(R^2)^{\text{SM}} = 0.5$) the variances and covariances can only be influenced by adjusting the λ coefficients.

3.1.4 Comments on Model Identification and Estimation

A model needs to fulfil certain requirements in order to be identified in terms of a certain estimation approach.

The presented approaches scale the latent variables in different manners. Within the OLS and PLS approach the variances of the latent variable get fixed to a value of one. In the ML world the respective variances get their scale by fixing some coefficients.

My specified model (figure 3.1 page 55) is in terms of PLS identified when the sample consists of at least 6 observations. Concerning ML and OLS the identification is somehow more extensive. In the following I elucidate these identification issues.

For ML identification I restrict three coefficients since my specified model incorporates three latent variables. Precisely I fix one coefficient per measurement model to a value of one, see figure 3.3. In doing so ξ_1 adopts the scale of x_1, ξ_2 adopts the scale of x_6 and η_1 adopts the scale of y_1. Since the assumption that ESS of each latent variable equals a value of one is not met, the resulting estimates need to get rescaled such that the results can be compared with the population parameters, see section 3.2.1.

Further, some restrictions concerning the error terms are required in respect of both, OLS and ML identification. If the variances of the errors, which enter ξ_1, ξ_2 and η_1, would be specified "free" the following indeterminacy would appear: Substituting $\xi_1 = \pi_1 x_1 + ... + \pi_5 x_5 + \delta_1$ and $\xi_2 = \pi_6 + ... + \pi_8 x_8 + \delta_2$ into $\eta_1 = \gamma_1 \xi_1 + \gamma_2 \xi_2 + \zeta_1$ leads to a total error $u_{\eta_1} = \gamma_1 \delta_1 + \gamma_2 \delta_2 + \zeta_1$. As the errors are assumed to be uncorrelated (with each other and with the respective independent variables) the total error variance is

$$\text{var}(u_{\eta_1}) = \gamma_1^2 \cdot \text{var}(\delta_1) + \gamma_2^2 \cdot \text{var}(\delta_2) + \text{var}(\zeta_1). \tag{3.4}$$

Adding arbitrarily chosen constants in the following manner reveals the inde-

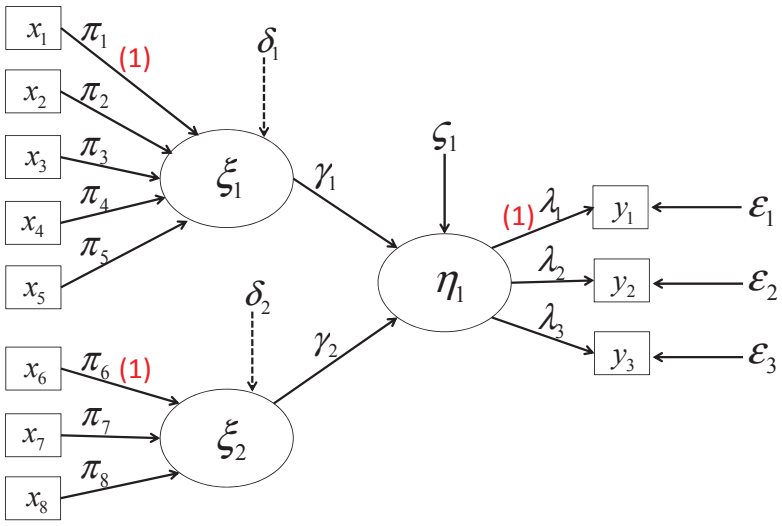

Figure 3.3: Model to explain identification (referring to figure 3.1).

terminacies:[57]

$$\begin{aligned}
\text{var}(\delta_1)^\star &= \text{var}(\delta_1) + c_1 \\
\text{var}(\delta_2)^\star &= \text{var}(\delta_2) + c_2 \\
\text{var}(\zeta_1)^\star &= \text{var}(\zeta_1) - \gamma_1^2 \cdot c_1 - \gamma_2^2 \cdot c_2 \\
\text{var}(u_{\eta_1})^\star &= \gamma_1^2 \cdot \text{var}(\delta_1)^\star + \gamma_2^2 \cdot \text{var}(\delta_2)^\star + \text{var}(\zeta_1)^\star \\
&= \gamma_1^2 \cdot \text{var}(\delta_1) + \gamma_1^2 \cdot c_1 + \gamma_2^2 \cdot \text{var}(\delta_2) + \gamma_2^2 \cdot c_2 \\
&\quad + \text{var}(\zeta_1) - \gamma_1^2 \cdot c_1 - \gamma_2^2 \cdot c_2 \\
&= \text{var}(u_{\eta_1}) \qquad (3.5)
\end{aligned}$$

Hence, an infinite number of solutions for the error variances exists which fulfil equation 3.4. Consequently, it is not an option to specify $\text{var}(\delta_1)$, $\text{var}(\delta_2)$ and $\text{var}(\zeta_1)$ as free parameters. However, imposing some restrictions solves the problem. I choose the restriction

$$\text{var}(\delta_1) = \text{var}(\delta_2) = 0 \qquad (3.6)$$

and let $\text{var}(\zeta_1)$ free.[58]

Restriction 3.6 ensures identification for ML and OLS and is in terms of PLS

[57] See also MacCallum/Browne (1993) to whom I referred earlier in section 2.1.3.

[58] Alternatively identification could be reached by setting $\text{var}(\delta_1) = \text{var}(\delta_2) = \text{var}(\zeta_1)$.

favourable. Due to a characteristic of the PLS algorithm equation 3.6 is as well met in PLS without explicitly imposing this restriction. PLS scores for a latent variable result as linear combination of its respective indicators (see section 2.2.2). Thereafter the scores get regressed on the respective indicators (e.g. $\hat{\xi}_1^{\text{PLSscores}}$ on x_1 to x_5). Consequently, such multiple regression yields a determination coefficient which takes on the value one, i.e. the error variance takes on the value zero. This is the case for ξ_1 and ξ_2.

The OLS specification is equivalent to the ML specification, but instead of fixing the red coloured coefficients (see figure 3.3 page 66) the latent variable variances are fixed to a value of one. The OLS regressions get performed including intercepts. As I elucidated earlier for some parameters several OLS estimates might be obtained depending on the model specification. In this model this is the case for $\boldsymbol{\pi}$, $\boldsymbol{\gamma}$ and $\boldsymbol{\lambda}$ as well as for $\text{var}(\zeta_1)$. For each parameter the average over all available estimates yields the parameter estimate, which gets assessed regarding its accuracy.

Concerning the ML approach I set ex ante starting values. For some cases ML may converge and yield an inconspicuous estimate of the variance-covariance matrix but show some implausible estimates of some coefficients and their standard deviations. This may be the case if the likelihood maximisation does not have a unique solution and several maxima exist. Given a single case a conscientious researcher would reject these results. Including starting values (or changing them) may possibly yield the appropriate ML maximum. Also appearing non-convergence may get solved by applying good starting values. Within my Monte Carlo simulation I set in advance starting values (instead of varying them for each case and assessing the results individually). I do this solely for the π coefficients which are specified free. To get the highest chance to get appropriate estimates I use the true values.

With respect to PLS three options exist to estimate the inner weights: the centroid, the factorial and the path weighting scheme (see section 2.2.2). For

all specified cases I apply the centroid scheme. In addition to that I apply the factorial and the path weighting scheme for the basic model and for variation G (see section 3.1.2) to compare parameter accuracy as well as test size and power of a test for significance of the path coefficients.[59]

Regarding variation G there is one more thing to add. As the model includes coefficients which take on the value zero, some total effects take on the value zero. Therefore, an accurate OLS estimate of such total effect results in a value close to zero. A value of zero as well as a value close to zero cannot be divided accurately. In the equations 2.22 and 2.24 page 47 a small value in the denominator, yields inflated estimates, respectively. Moreover, the covariance between y_4 and another y_q variable is zero and an accurate estimate will yield a value close to zero. Consequently, the estimation of the λ coefficients according to equation 2.30 page 49 becomes problematic, too. Therefore, with respect to variation G I analyse the total effect coefficients in terms of the OLS approach. As these coefficients equal the OLS estimates also the corresponding standard errors serve to investigate parameter significance and it is not necessary to apply the bootstrap technique.

3.2 Analysis

3.2.1 Scaling of the ML and PLS Results

The population parameters and the estimates must match concerning their underlying scaling, i.e. ESS of each latent variable takes on the value one. A scaling is necessary for the ML and the PLS approach. The scaled coefficients can then get compared with the theoretical values and are labelled with “final”.

I begin with the scaling of the ML estimates according to the deployed model, see figure 3.3 page 66.

[59] According to Noonan/Wold (1982) and Ringle et al. (2009) the weighting scheme has only a marginal (and unsteady) impact on the estimation results and the centroid scheme may get applied. On the contrary Hair et al. (2012a, p. 333) state “[...]researchers have to consider that the schemes are not universally applicable to all kinds of model set-ups. For instance, the centroid scheme must not be used when estimating higher order models”. Therefore, I compare the results for all weighting schemes.

In order to imply a variance of $\hat{\boldsymbol{\xi}}^{\mathrm{ML}}$ equal to a value of one, the ML estimates $\hat{\boldsymbol{\pi}}^{\mathrm{ML}}$ get scaled as follows:[60]

$$\hat{\pi}_l^{\mathrm{MLfinal}} = \frac{\hat{\pi}_l^{\mathrm{ML}}}{\sqrt{\mathrm{var}\left(\hat{\xi}_1^{\mathrm{ML}}\right)}} \qquad \text{for } l = 1, ..., 5 \tag{3.7}$$

and

$$\hat{\pi}_l^{\mathrm{MLfinal}} = \frac{\hat{\pi}_l^{\mathrm{ML}}}{\sqrt{\mathrm{var}\left(\hat{\xi}_2^{\mathrm{ML}}\right)}} \qquad \text{for } l = 6, ..., 8. \tag{3.8}$$

The scaled $\hat{\boldsymbol{\pi}}^{\mathrm{MLfinal}}$ coefficients imply a variance of each exogenous latent variable equal to a value of one: $\mathrm{var}(\hat{\xi}_1^{\mathrm{MLfinal}}) = \mathrm{var}(\hat{\xi}_2^{\mathrm{MLfinal}}) = 1$. This scaling affects the $\hat{\boldsymbol{\gamma}}^{\mathrm{ML}}$ coefficients in the inner model, where the $\hat{\boldsymbol{\xi}}^{\mathrm{ML}}$ variables enter as independent variables. The corresponding adjustment of $\hat{\boldsymbol{\gamma}}^{\mathrm{ML}}$ is done in two steps. At first it is

$$\hat{\gamma}_1^{\mathrm{MLprel}} = \hat{\gamma}_1^{\mathrm{ML}} \cdot \sqrt{\mathrm{var}\left(\hat{\xi}_1^{\mathrm{ML}}\right)},$$
$$\hat{\gamma}_2^{\mathrm{MLprel}} = \hat{\gamma}_2^{\mathrm{ML}} \cdot \sqrt{\mathrm{var}\left(\hat{\xi}_2^{\mathrm{ML}}\right)},$$

with "prel" meaning "preliminary". The coefficients are not yet final, because up to here the variance of $\hat{\eta}_1^{\mathrm{ML}}$ has not been adjusted. To do so, I compute the $\hat{\boldsymbol{\xi}}^{\mathrm{MLfinal}}$ fitted values with the scaled $\hat{\boldsymbol{\pi}}^{\mathrm{MLfinal}}$ coefficients. In the next step final $\boldsymbol{\gamma}$ coefficients get computed such that they lead to $\mathrm{var}(\hat{\eta}_1^{\mathrm{MLfinal}}) = 1$. With

$$\hat{\eta}_1^{\mathrm{MLprel}} = \hat{\gamma}_1^{\mathrm{MLprel}} \hat{\xi}_1^{\mathrm{MLfinal}} + \hat{\gamma}_2^{\mathrm{MLprel}} \hat{\xi}_2^{\mathrm{MLfinal}}$$

the final $\boldsymbol{\gamma}$ coefficients result as

$$\hat{\boldsymbol{\gamma}}^{\mathrm{MLfinal}} = \frac{\hat{\boldsymbol{\gamma}}^{\mathrm{MLprel}}}{\sqrt{\mathrm{var}\left(\hat{\eta}_1^{\mathrm{MLprel}}\right)}}. \tag{3.9}$$

The latter adjustment according to equation 3.9 has not only consequences for the inner model, where η is the dependent variable, but as well for the reflective measurement model where η is the independent variable. Therefore, the λ coefficients need to be rescaled, too:

$$\hat{\boldsymbol{\lambda}}^{\mathrm{MLfinal}} = \hat{\boldsymbol{\lambda}}^{\mathrm{ML}} \cdot \sqrt{\mathrm{var}\left(\hat{\eta}_1^{\mathrm{MLprel}}\right)}. \tag{3.10}$$

After all, the scaling process does not change the variance of each y_q.

[60] The variances of $\hat{\boldsymbol{\xi}}^{\mathrm{ML}}$ can be computed analogous to equation 3.1 page 62.

With respect to variation G I investigate the significance of the parameters. The previously performed scaling of the coefficients entails also a scaling of the respective standard deviations, which I need to determine significance. However, a parameter scaling does not have an impact on parameter significance, i.e. on the value of the test statistic. Consequently, to determine significance the unscaled parameter estimate and the unscaled standard deviation (whether bootstrapped or not is irrelevant) can be applied to compute the test statistic. Nevertheless, I briefly illustrate how the estimated ML standard errors get scaled, according to the upper described coefficient scaling. Instead of deploying the square root of the respective variance as scaling factor (equations 3.7, 3.8, 3.9 and 3.10) the variance must be deployed:

$$\begin{aligned}
\operatorname{var}\left(\hat{\pi}_l^{\mathrm{MLfinal}}\right) &= \frac{\operatorname{var}\left(\hat{\pi}_l^{\mathrm{ML}}\right)}{\operatorname{var}\left(\hat{\xi}_1^{\mathrm{ML}}\right)} && \text{for } l = 2, ..., 6 \\
\operatorname{var}\left(\hat{\pi}_l^{\mathrm{MLfinal}}\right) &= \frac{\operatorname{var}\left(\hat{\pi}_l^{\mathrm{ML}}\right)}{\operatorname{var}\left(\hat{\xi}_2^{\mathrm{ML}}\right)} && \text{for } l = 8, ..., 10 \\
\hat{\gamma}_m^{\mathrm{MLfinal}} &= \frac{\hat{\gamma}_m^{\mathrm{MLprel}}}{\operatorname{var}\left(\hat{\eta}_1^{\mathrm{MLprel}}\right)} && \text{for } m = 1, 2 \\
\operatorname{var}\left(\hat{\lambda}_q^{\mathrm{MLfinal}}\right) &= \operatorname{var}\left(\hat{\lambda}_q^{\mathrm{ML}}\right) \cdot \operatorname{var}\left(\hat{\eta}_1^{\mathrm{MLprel}}\right) && \text{for } q = 2,\ 3
\end{aligned}$$

For the ML fixed parameters (π_1, π_7 and λ_1, see figure 3.2 page 61) no standard errors get estimated as the parameters themselves do not get estimated.

The scaling of the PLS estimates is more compact. The PLS estimates of the latent variables ξ_g do not need to get scaled as the PLS assumptions fits the assumption of the data generation (see section 3.1). Consequently, the scaling confines to the scores of η_1. As I elucidated above its true variance and the PLS assumption do not match. PLS fixes the latent variable variance to a value of one, while the true variance of η_1 is larger than one (according to the data generation it is $\mathrm{TSS}_{\eta_1} = \frac{1}{(R^2)^{\mathrm{SM}}}$ with $\mathrm{ESS}_{\eta_1} = 1$). Thus, the relation is

$$\operatorname{var}\left(\hat{\eta}_1^{\mathrm{PLSfinal}}\right) = \overbrace{\operatorname{var}\left(\hat{\eta}_1^{\mathrm{PLSscores}}\right)}^{=1} \cdot \frac{1}{(R^2)^{\mathrm{SM}}}$$

and the scaled η_1 scores result as

$$\hat{\eta}_1^{\mathrm{PLSfinal}} = \hat{\eta}_1^{\mathrm{PLSscores}} \cdot \sqrt{\frac{1}{(R^2)^{\mathrm{SM}}}}\,.$$

The new scale of the η_1 scores implies scaled γ and λ coefficients. For the partial models where the latent variable η_1 enters, a new performance of OLS regressions (second stage of the PLS algorithm, see section 2.2.2) applying the $\hat{\eta}^{\text{PLSfinal}}$ values yields the final / scaled PLS γ and λ coefficients.[61]
As mentioned before the test decision, whether a path coefficient is significantly different from zero or not, is unaffected by the scaling. Thus, the original PLS estimates and the PLS bootstrapped standard deviations serve to determine significance of the path coefficients.

In the following all so-called final values serve for the comparison with the theoretical coefficients.

3.2.2 Evaluation of the Estimation Results

I evaluate the estimated coefficients $\boldsymbol{\pi}$, $\boldsymbol{\gamma}$ and $\boldsymbol{\lambda}$ by comparing them with the population parameters. The estimation procedures for the ML, PLS and OLS approaches were illustrated in chapter 2. Regarding ML and partially PLS rescaled estimates enter the comparison (see section 3.2.1). Regarding the OLS approach and the PLS π coefficients the unscaled estimated coefficients enter the comparison. Moreover, I investigate the total effects. With respect to the OLS approach the regression coefficients represent the total effects. In the ML and PLS approach the total effects (TE) need to get computed:

$$\mathbf{TE_{xy}} = \boldsymbol{\pi}^{\text{true}}\boldsymbol{\gamma}^{\text{true}}\boldsymbol{\lambda}'.^{62}$$

For example, the total effect of x_1 on y_3 is $TE_{x_1y_3} = \pi_1^{\text{true}} \cdot \gamma_1^{\text{true}} \cdot \lambda_3$. To investigate the bias and variability of both, the individual coefficients and the total effects, I apply the following measures of accuracy:

In the following a "β" coefficient stands for any individual coefficient, i.e. for a π_l in a formative measurement model, a γ_m in the inner model, a λ_q in

[61] The variance of the indicators must be considered, too, i.e. whether they enter standardised or not. In my case I apply unstandardised indicators.

[62] The factors are $(\boldsymbol{\pi}^{\text{true}})' = \begin{pmatrix} \pi_1^{\text{true}} & \pi_2^{\text{true}} & \pi_3^{\text{true}} & \pi_4^{\text{true}} & \pi_5^{\text{true}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \pi_6^{\text{true}} & \pi_7^{\text{true}} & \pi_8^{\text{true}} \end{pmatrix}$, $(\boldsymbol{\gamma}^{\text{true}})' = (\gamma_1^{\text{true}} \quad \gamma_2^{\text{true}})$ and $\boldsymbol{\lambda}' = (\lambda_1 \quad \lambda_2 \quad \lambda_3)$. Consequently, $\mathbf{TE_{xy}}$ is a 8 x 3 matrix. In Appendix G I show the values for the basic model.

the reflective model, or a total effect coefficient. A distinction is not necessary. If $\hat{\beta}$ has an index i then it reflects a single estimation result out of the $K = 10,000$ iterations. Sometimes no estimation results can be obtained due to non-convergence of the algorithm (referring to ML and PLS). Therefore, I compute in general an average over k estimates which are de facto available (with $k \leq K$). A theoretical coefficient which enters the data generation process is called β^{true}.

The *mean* of the k estimated coefficients is

$$\overline{\hat{\beta}} = \frac{1}{k} \sum_{i=1}^{k} \hat{\beta}_i.$$

The mean deviation measures the bias. An estimator is unbiased if the mean over all samples approaches the true value with increasing the number of samples. The mean deviation *md* is

$$md(\hat{\beta}) = \overline{\hat{\beta}} - \beta^{\text{true}}.$$

The mean squared error *mse* measures the robustness of an estimator because large errors are valued strong. It is crucial to investigate the *md* and the *mse* in order to make precise distinctions between unbiasedness and small variance of an estimator. An unbiased estimator with large variab ility may be less favourable compared to an estimator which shows some bias but small variability. This is because the individual results of an estimator with large variability behave erratically since their deviation from the population parameter is often large. In this study I use the root mean squared error *rmse*, which is simply the square root of the *mse*:

$$rmse(\hat{\beta}) = \sqrt{\frac{1}{k} \sum_{i=1}^{k} (\hat{\beta}_i - \beta^{\text{true}})^2}.$$

In order to give a condensed overview I aggregate the results: I compute *md* and *rmse* mean values per partial model, i.e. for each measurement model and for the inner model. Furthermore, I compute such mean values for the total effect coefficients per y_q. Regarding the basic model that implies 3 values, whereas the model has $8 \cdot 3 = 24$ total effects. With respect to the *md* means I do not want a negative *md* value to neutralise a positive one and therefore take the respective absolute values (while $rmse \geq 0$ anyhow).

Moreover, I investigate the prediction quality. According to my specified model (see figure 3.1 page 55) each endogenous outcome variable y_q can be predicted by $\mathbf{x}$. Adequate measures are again the *md* and the *rmse*:

$$md(\hat{y}_q) = \frac{1}{k}\sum_{i=1}^{k}\frac{1}{n}\sum_{j=1}^{n}(\hat{y}_{qij} - y_{qij}^{\text{true}}), \tag{3.11}$$

$$rmse(\hat{y}_q) = \sqrt{\frac{1}{k}\sum_{i=1}^{k}\frac{1}{n}\sum_{j=1}^{n}(\hat{y}_{qij} - y_{qij}^{\text{true}})^2}. \tag{3.12}$$

As a characteristic of OLS each $md(\hat{y}_q)$ takes on the value zero. I condense the results again by taking the mean over the respective values.

Another issue I focus on is the investigation of the test size and statistical power referring to a test for significance of the coefficients. With variation G I contribute a specification which is suitable to determine both rates (see figure 3.2 page 61). With respect to ML and PLS I assess significance of the individual coefficients $\boldsymbol{\pi}$, $\boldsymbol{\gamma}$ and $\boldsymbol{\lambda}$, excluding for ML the coefficients which get ex ante fixed. With respect to the OLS approach I observe actual size and actual power for the total effects $\hat{\mathbf{e}}$ (see section 3.1.4).
To determine the actual size and the actual power the question is whether a parameter (β_j) is significantly different from zero or not ($H_0 : \beta_j = 0$, $H_1 : \beta_j \neq 0$). This can be tested with

$$T = \frac{\hat{\beta}_j}{\sqrt{\widehat{\text{var}}\left(\hat{\beta}_j\right)}}.$$

Referring to ML the upper test statistic T is approximately standard normally distributed, because the estimator approximates a normal distribution as the sample size increases (Schermelleh-Engel et al., 2003, p. 26). As in variation G ($n = 300$) multinormality and a correctly specified model is given it is rational to apply the standard deviations that result from the ML estimation. Additionally I check the respective bootstrapped values (with $K_B = 300$). Referring to the PLS and OLS approaches the test statistic (T) is t-distributed with $n - m - 1$ degrees of freedom (m represents the number of regressors). Concerning PLS the standard deviations always get bootstrapped. In general I perform 100 bootstrap replications, but alternatively specify K_B to 300 and

1,000. Since I analyse for OLS the total effects, which are represented by the OLS parameter estimates, I apply the corresponding standard errors.[63]

I assess parameter significance on the 1%-, 5%- and 10%-level, respectively. I exemplify the precise critical values for the 1%-level, although the t-distribution approximates the z-distribution for increasing n. For ML the critical value is $z[0.995] = 2.57583$. For PLS there are three critical values, because the number of parameters that get estimated within each partial model is relevant. The values differ only marginally because n is large: $t[0.995,\ 300-6-1] = 2.59271$ for the first formative measurement model, $t[0.995,\ 300-4-1] = 2.59260$ for the second formative measurement model and $t[0.995,\ 300-1-1] = 2.59243$ for each single regression within the reflective measurement model. With respect to the significance of a OLS total effect coefficient the critical value is $t[0.995,\ 300-8-1] = 2.59295$.

The actual size is the number of erroneously rejected true null hypothesis divided by k and consequently refers to coefficients which truly equal zero. Actual power is the number of correctly rejected null hypothesis divided by k and consequently refers to coefficients which truly are different from zero.

Regarding variation E I narrow down the presented results and tabulate only actual size and actual power. With respect to accuracy the results of variation E can be expected to not differ much from the basic model, since the only difference between both models constitute the coefficients which truly take on the value zero: π_6, π_{10} and λ_4.[64]

[63] In section 2.4.2 I proposed to bootstrap the standard deviations of the individual coefficient estimates.

[64] In Appendix H I show the corresponding results with respect to accuracy.

3.3 Results

3.3.1 Estimator accuracy: bias and variability

Before I start presenting the Monte Carlo simulation study results I find it helpful to recap all specifications and what I respectively assess, see table 3.1.[65] The table comprises also variation G and its associated cases, whose results I show in the subsequent section 3.3.2.

In this section I reveal the results concerning accuracy for the basic model and the variations A to F. I tabulate the results for each case, such as in table 3.2 page 78 for the basic model. Each table shows the number of missing values, whereby the number referring to OLS is put in brackets. It indicates the number of missing OLS $\hat{\lambda}$ estimates. The OLS approach may lead to covariances between $\hat{y}_k$ and $\hat{y}_s$ $(k \neq s)$ such that a negative value appears under the root in equation 2.30 page 49. An OLS estimate for each λ coefficient is available in any case because the solution via equation 2.21 page 47 is always possible. Further, each table shows the averages of the measures of accuracy, which are calculated according to section 3.2.2. Concerning these measures each lowest number is printed in bold.

The individual results per coefficient are shown in Appendix H. Table H.1 to H.16 refer to the basic model and the variations A to F. Table H.17 and H.18 refer to variation G[66].

In this section, as well as in section 3.3.2, I restrict myself to the description of the results, the conclusions follow in section 3.3.3.

[65] With respect to table 3.1 I introduce the following abbreviations: *distrib.* stands for distribution, *inner est.* for inner estimation (referring to the PLS schemes), *sd* for standard deviation, *miss. res.* for missing results, *cent.* for the PLS centroid scheme, *fact.* for the PLS factorial scheme, *path* for the PLS path weighting scheme, *cont. unif.* for the continuous uniform distribution, *signif.* for significance, and *boot.* for bootstrapped.

[66] In section 3.3.2 I show the results for variation G, which are related to the significance of the path coefficients. In Appendix H I show the results concerning accuracy.

	Applied method(s)	(Mainly) Assessed	Specification						Estimation			
			$\mathrm{E}(\mathbf{xx}')$	error term distrib.	n	$(R^2)^{\mathrm{SM}} = (R^2)^{\mathrm{rMM}}$	no. of indicators	$\mathbf{x}$ aggregated	PLS inner est.	PLS sd	ML sd	K_B
Basic	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{I}}$	normal	300	0.5	11	no	cent.	-	-	-
extra to Basic	PLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{I}}$	normal	300	0.5	11	no	cent., fact., path	-	-	-
A	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{I}}$	normal	300	0.2	11	no	cent.	-	-	-
B1	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{I}}$	chi-squared	300	0.5	11	no	cent.	-	-	-
B2	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{I}}$	cont. unif.	300	0.5	11	no	cent.	-	-	-
AB1	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{I}}$	chi-squared	300	0.2	11	no	cent.	-	-	-
AB2	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{I}}$	cont. unif.	300	0.2	11	no	cent.	-	-	-
C1	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{I}}$	normal	15	0.5	11	no	cent.	-	-	-
C2	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{I}}$	normal	50	0.5	11	no	cent.	-	-	-
C3	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{I}}$	normal	1,000	0.5	11	no	cent.	-	-	-
D1	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{II}}$	normal	50	0.5	11	no	cent.	-	-	-

Table 3.1 continues on the next page.

			Specification						Estimation			
	Applied method(s)	(Mainly) Assessed	$\mathrm{E}(\mathbf{xx}')$	error term distrib.	n	$(R^2)^{\mathrm{SM}} = (R^2)^{\mathrm{rMM}}$	no. of indicators	$\mathbf{x}$ aggregated	PLS inner est.	PLS sd	ML sd	K_B
D2	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{II}}$	normal	300	0.5	22	no	cent.	-	-	-
D3	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{II}}$	normal	1,000	0.5	44	no	cent.	-	-	-
E1	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{II}}$	normal	300	0.5	11	no	cent.	-	-	-
E2	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{III}}$	normal	300	0.5	11	no	cent.	-	-	-
F	ML, PLS, OLS	miss.res., $\hat{\boldsymbol{\beta}}, \hat{\mathbf{y}}$	$\mathbf{V}^{\mathrm{I}}$	normal	300	0.5	11	yes	cent.	-	-	-
G	ML, PLS, OLS	signif.	$\mathbf{V}^{\mathrm{G}}$	normal	300	0.5	14	no	cent.	boot.	original	100
extra to G	PLS	signif.	$\mathbf{V}^{\mathrm{G}}$	normal	300	0.5	14	no	cent., fact., path	boot.	-	100
extra to G	PLS	sd	$\mathbf{V}^{\mathrm{G}}$	normal	300	0.5	14	no	cent.	boot.	-	100
extra to G	PLS	sd	$\mathbf{V}^{\mathrm{G}}$	normal	300	0.5	14	no	cent.	boot.	-	300
extra to G	PLS	sd	$\mathbf{V}^{\mathrm{G}}$	normal	300	0.5	14	no	cent.	boot.	-	1,000
extra to G	ML	sd	$\mathbf{V}^{\mathrm{G}}$	normal	300	0.5	14	no	-	-	boot.	300

Table 3.1: Simulation study cases (from page 76 on).

In my basic specification, see table 3.2, the non-convergence rate is negligible low for ML and exactly zero for PLS. Concerning the OLS approach each λ_{qi} (for $i = 1, ..., 10,000$ and q=1,...,3) got estimated applying the covariances of the fitted values.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0.00120	0	(0)			
$\pi_1 - \pi_5$	**0.00673**	0.09322	0.01284	0.12017	0.15083	**0.11810**
$\pi_6 - \pi_8$	**0.00461**	0.01678	0.00951	0.11109	0.11088	**0.11027**
γ_1, γ_2	**0.00319**	0.10248	0.00637	0.06179	0.11954	**0.06025**
$\lambda_1 - \lambda_3$	**0.01598**	0.13180	0.02014	0.09062	0.14678	**0.08645**
TE per y_1	**0.00068**	0.04097	0.00097	**0.08449**	0.09852	0.11100
TE per y_2	0.00046	0.04011	**0.00046**	**0.05916**	0.06495	0.07776
TE per y_3	0.00060	0.03994	**0.00056**	**0.07618**	0.08518	0.10044
prediction of $y_1 - y_3$	0.00034	0.00029	**0**	1.48885	1.49572	**1.47802**

Table 3.2: Simulation study results for the basic model.

With respect to the individual coefficients the ML estimates appear on average the least biased. The ML bias averages are only slightly lower than those of OLS, the difference amounts to the third decimal place. Concerning the variability of the estimates, OLS shows on average the lowest values, whereas the measures appear only slightly lower than the respective ML values. In summary, for ML and OLS the individual estimates of each coefficient appear on average similar accurate, referring to md and $rmse$. On contrast the PLS estimates show larger biases: the individual PLS biases (see Appendix H table H.1 page 148) lie between circa the 2.5 times (π_6) and 42.5 times (γ_2) the respective ML bias. Further, table H.1 reveals that large differences between the individual md values appear for PLS: $md(\hat{\lambda}_1^{\text{PLS}}) = 0.228$ and $md(\hat{\lambda}_2^{\text{PLS}}) = 0.026$. The same appears with respect to $rmse$, i.e. PLS shows noticeably larger values than ML and OLS (excluding the second formative measurement model) and large differences appear for the values within one partial model, e.g. in the reflective measurement model: $rmse(\hat{\lambda}_1^{\text{PLS}}) = 0.240$ and $rmse(\hat{\lambda}_2^{\text{PLS}}) = 0.061$.

Some readers may be interested in the signs of the mean deviations, which are not identifiable in table 3.2, since the aggregated results base on absolute values. Appearing (systematic) over- or underestimation can be identified in Appendix H (e.g. table H.1 for the basic model). Concerning PLS the

parameters systematically get overestimated in the structural model as well as in the reflective measurement model. In the respective formative measurement models the signs alternate: some coefficients are on average overestimated whilst others are underestimated. For ML and OLS the respective signs appear strictly negative in the formative measurement models and strictly positive in the reflective measurement model. Concerning the structural model no clear sign pattern appears.

The mean biases of the total effect coefficients appear low for ML and OLS. With respect to PLS the respective biases appear larger. Apparently PLS over- and underestimation of the individual coefficients do not cancel each other out. In terms of *rmse* all three approaches vary in the same range, while ML shows the lowest values.

The predicted values appear for OLS unbiased, which is a characteristic of OLS. ML and PLS show low biases. Regarding the *rmse* averages the values lie in the same range for all three approaches, while OLS reveals the lowest value.

At this point I additionally bring up a result regarding prediction accuracy of the latent variables. For the basic model I assessed for ML, PLS and OLS the fitted values of all latent variables as well as the PLS scores of η_1. In a formative measurement model PLS scores and fitted values are identical. The fitted values of all latent variables depend directly or indirectly on $\mathbf{x}$, according to the specified model. The PLS scores $\hat{\eta}_1^{\text{PLSscores}}$ rely on the corresponding indicators, i.e. on $\mathbf{y}$, irrespective of the causality in the model.

I briefly summarise my results: With respect to the fitted values the measures of accuracy take on similar values for all three approaches, while the largest values appear in general for PLS. The PLS scores $\hat{\eta}_1^{\text{PLSscores}}$ appear more precise in terms of *rmse* than all fitted values.[67] However, whether fitted values or scores result more precise depends on the model causalities and on the determination coefficients. In the basic model the PLS scores of η_1 result directly as weighted sum of $\mathbf{y}$. In contrast, the fitted values of η_1 rely indirectly on $\mathbf{x}$. Depending on $(R^2)^{\text{rMM}}$ and $(R^2)^{\text{SM}}$ either the fitted values of η_1 or the the scores of η_1 result more accurate. In case $(R^2)^{\text{rMM}}$ is relatively small compared

[67] Although my summary is very condensed I mention some values: $rmse(\hat{\eta}_1^{\text{ML}}) = 0.99812$, $rmse(\hat{\eta}_1^{\text{OLS}}) = 0.99704$, $rmse(\hat{\eta}_1^{\text{PLSfits}}) = 1.01480$ and $rmse(\hat{\eta}_1^{\text{PLSscores}}) = 0.76002$.

to $(R^2)^{\mathrm{SM}}$ the scores of η_1 result less accurate than the respective fitted values. I assessed this for the basic model by changing the determination coefficients to $(R^2)^{\mathrm{SM}} = 0.8$ and $(R^2)^{\mathrm{rMM}} = 0.1$. In effect, the PLS scores appear then less precise than the PLS fitted values. Even more precise appear the ML and OLS fitted values.[68]

As mentioned before the presented PLS results base on the centroid scheme. For the basic model I additionally applied the factorial and the path weighting scheme. The differences in accuracy appear vanishingly low for the different schemes. Therefore I show the results in Appendix H, see table H.2 page 149.[69]

So far all presented results are related to the basic model. The extra results were either presented additionally (concerning the latent variable prediction) or arose from a change concerning the PLS estimation procedure (with respect to the PLS inner schemes). In the following I present the results for the variations A to F.

In model A, see table 3.3, the determination coefficients are specified lower than in the basic model ($(R^2)^{\mathrm{SM}} = (R^2)^{\mathrm{rMM}} = 0.2$). Comparing the results with those of the basic model (table 3.2) I can summarise the following: The ML non-convergence rate appears in the A model higher than in the basic model: 15.7% of the 10,000 samples did not converge. PLS did only a few times not converge, namely in 2 out of 10,000 cases. The OLS estimation of the λ coefficients applying the covariances between the fitted value was in a few cases not possible.

The coefficient estimates show clearly larger *md* averages for all three approaches compared to the basic model. For PLS the values are low for the measurement model of ξ_2. In the structural model PLS biases are very large and in the reflective measurement model they are extremely large. In summary, the ML estimates appear the least biased. Regarding variability all three approaches yield similar values for the formative measurement models. For the

[68] The respective values are $rmse(\hat{\eta}_1^{\mathrm{ML}}) = 0.61461$, $rmse(\hat{\eta}_1^{\mathrm{OLS}}) = 0.57798$, $rmse(\hat{\eta}_1^{\mathrm{PLSfits}}) = 0.73434$ and $rmse(\hat{\eta}_1^{\mathrm{PLSscores}}) = 1.13333$.

[69] For variation G I apply the different PLS schemes and investigate test size and statistical power of a test for significance of the path coefficients, see section 3.3.2 page 97 tables 3.22 and 3.23.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0.15740	0.00020	(0.00870)			
$\pi_1 - \pi_5$	**0.04815**	0.09923	0.08393	0.26724	0.27149	**0.24866**
$\pi_6 - \pi_8$	0.03746	**0.03243**	0.08387	0.26260	**0.25082**	0.26125
γ_1, γ_2	**0.02300**	0.19194	0.03958	0.12729	0.22329	**0.10792**
$\lambda_1 - \lambda_3$	**0.10975**	0.43570	0.14090	**0.25888**	0.43319	0.29830
TE per y_1	0.01450	0.04830	**0.00300**	**0.21431**	0.23390	0.31457
TE per y_2	0.01016	0.05092	**0.00125**	0.15064	**0.11849**	0.22007
TE per y_3	0.01308	0.03833	**0.00165**	0.19385	**0.18410**	0.28430
prediction $y_1 - y_3$	0.00082	0.00094	**0**	4.21718	4.22121	**4.18088**

Table 3.3: Simulation study results for variation A.

structural model and the reflective measurement model the *rmse* values appear much higher for PLS. Finally, two facts stand out referring to the individual coefficients estimates: Firstly, ML and OLS yield for the structural models very good estimators. Secondly, the PLS estimators concerning the reflective measurement model are outstanding bad and very bad for the structural model.

For PLS the *md* values of the total effect coefficients appear on average similar to those of the basic model. For the other two approaches the respective values appear higher compared to the basic model. Nevertheless they deviate on average less from the true parameters than PLS does. OLS reveals on average the highest accuracy, i.e. the lowest *md* value. On the other hand, the OLS estimators vary the most. In terms of *rmse* the PLS and ML estimates appear similar precise.

The predicted values of the y variables must deviate sometimes strongly from the true values as the very large *rmse* values indicate. All values lie in the same range, while OLS shows slightly lower values than ML and PLS.

The B models, see tables 3.4 and 3.5, incorporate non-normally distributed error terms (following a chi-squared distribution in B1 and following a continuous uniform distribution in B2). The non-convergence rate of PLS is zero and for ML close to zero. Concerning OLS all λ estimates were available in all cases. The ratios are similar to those in the basic model (table 3.2 page 78). In general the differences between the measures of the B cases and those of

the basic model are only marginal. Thus, regarding accuracy of the individual estimates ML shows on average the smallest biases, while the OLS estimations vary the least. The ML and OLS values appear again similar. With respect to the total effect coefficients ML reveals consistently the highest accuracy. Due to the similarity to the basic model it seems appropriate to proceed to the cases AB1 and AB2.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0.00130	0	(0)			
$\pi_1 - \pi_5$	**0.00675**	0.09258	0.01277	0.11968	0.15031	**0.11797**
$\pi_6 - \pi_8$	**0.00460**	0.01608	0.00954	0.11083	0.11118	**0.11020**
γ_1, γ_2	**0.00477**	0.10240	0.00787	0.06244	0.12054	**0.06092**
$\lambda_1 - \lambda_3$	**0.01542**	0.13145	0.01950	0.09129	0.15045	**0.08720**
TE per y_1	**0.00069**	0.04054	0.00082	**0.08449**	0.09881	0.11096
TE per y_2	**0.00053**	0.04021	0.00092	**0.05908**	0.06517	0.07768
TE per y_3	**0.00068**	0.03991	0.00086	**0.07604**	0.08540	0.10002
prediction $y_1 - y_3$	0.00098	0.00107	**0**	1.48907	1.49609	**1.47832**

Table 3.4: Simulation study results for variation B1.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0.00190	0	(0)			
$\pi_1 - \pi_5$	**0.00649**	0.09368	0.01260	0.11901	0.15055	**0.11708**
$\pi_6 - \pi_8$	**0.00449**	0.01673	0.00946	0.10934	0.11000	**0.10832**
γ_1, γ_2	**0.00353**	0.10368	0.00673	0.06310	0.12086	**0.06145**
$\lambda_1 - \lambda_3$	**0.01417**	0.13125	0.01821	0.09027	0.14601	**0.08672**
TE per y_1	**0.00069**	0.04124	0.00092	**0.08360**	0.09807	0.11035
TE per y_2	**0.00052**	0.04052	0.00073	**0.05856**	0.06490	0.07730
TE per y_3	**0.00063**	0.04034	0.00077	**0.07539**	0.08488	0.09981
prediction $y_1 - y_3$	0.00064	0.00066	**0**	1.48929	1.49613	**1.47855**

Table 3.5: Simulation study results for variation B2.

The models AB1 and AB2 constitute a combination of variation A with variation B1 or B2, respectively, see tables 3.6 and 3.7. Therefore, the errors constitute a larger proportion of the variation of the endogenous variables and the errors are non-normally distributed. The results do quite correspond with

those of the previously described model A. The following summary holds for both models (AB1 and AB2) since the results of both models appear very similar. The non-convergence rates resemble with model A: it is almost zero for PLS and about 15% for ML. In a few cases the OLS λ coefficients could not be estimated applying the covariances between the fitted values.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0.15730	0.00010	(0.01020)			
$\pi_1 - \pi_5$	**0.04579**	0.09797	0.08265	0.26428	0.27026	**0.24783**
$\pi_6 - \pi_8$	0.03688	**0.03249**	0.08457	0.26012	**0.25098**	0.26130
γ_1, γ_2	**0.02582**	0.19271	0.04189	0.13082	0.22574	**0.11067**
$\lambda_1 - \lambda_3$	**0.10700**	0.43492	0.13867	**0.25909**	0.43967	0.26756
TE per y_1	0.01391	0.04568	**0.00239**	**0.21291**	0.23422	0.31340
TE per y_2	0.01001	0.05098	**0.00235**	0.14896	**0.11888**	0.21948
TE per y_3	0.01256	0.03744	**0.00228**	0.19177	**0.18519**	0.28243
prediction $y_1 - y_3$	0.00261	0.00258	**0**	4.21619	4.22127	**4.18102**

Table 3.6: Simulation study results for variation AB1.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0.15690	0	(0.00870)			
$\pi_1 - \pi_5$	**0.04789**	0.10032	0.08350	0.26576	0.27066	**0.24741**
$\pi_6 - \pi_8$	0.03724	**0.03203**	0.08546	0.26074	**0.24843**	0.25848
γ_1, γ_2	**0.02411**	0.19497	0.04101	0.13239	0.22697	**0.11075**
$\lambda_1 - \lambda_3$	**0.10411**	0.43505	0.13438	0.25751	0.43246	**0.24845**
TE per y_1	0.01491	0.04754	**0.00292**	**0.21262**	0.23131	0.31257
TE per y_2	0.01046	0.05175	**0.00210**	0.14894	**0.11783**	0.21892
TE per y_3	0.01320	0.03869	**0.00230**	0.19166	**0.18265**	0.28250
prediction $y_1 - y_3$	0.00138	0.00182	**0**	4.21927	4.22219	**4.18215**

Table 3.7: Simulation study results for variation AB2.

Referring to the coefficient estimates, much higher *md* and *rmse* averages appear compared to the basic model. ML and OLS yield quite good estimates for the structural model. The PLS *md* averages appear particularly high for the reflective measurement model. The corresponding values vary again strongly, between 0.101 and 0.738. The *rmse* averages referring to the γ coefficients appear low for ML and OLS. For the rest of the model all *rmse* appear relatively

high for all approaches.

Also when referring to the total effect estimates the pattern is identical to case A. For PLS the biases (referring to *md*) of the total effect coefficients appear lower than those of the individual coefficients. Yet, ML and OLS yield lower biases. Referring to *rmse* the lowest values appear for PLS. The corresponding values appear for OLS noticeably higher.

With respect to the predicted values large *rmse* averages reveal that much larger deviations appear compared to the basic model. The measures appear again similar to variation A.

The C models vary in sample size. The results of the three specifications are shown in table 3.8, 3.9 and 3.10, respectively.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0.59530	0.00230	(0.06870)			
$\pi_1 - \pi_5$	0.17341	**0.10440**	0.16189	0.55027	0.54668	**0.47377**
$\pi_6 - \pi_8$	0.19746	**0.09069**	0.22308	0.56246	0.54521	**0.52763**
γ_1, γ_2	**0.05077**	0.10450	0.15601	0.42592	0.40852	**0.25632**
$\lambda_1 - \lambda_3$	0.22182	**0.07930**	0.36402	0.53637	**0.35513**	0.54017
TE per y_1	0.10959	0.06326	**0.00746**	0.62285	**0.47308**	0.84412
TE per y_2	0.07677	0.05593	**0.00474**	0.43677	**0.28221**	0.59003
TE per y_3	0.09439	0.06349	**0.00809**	0.56184	**0.39899**	0.75847
prediction $y_1 - y_3$	0.00196	0.00338	**0**	1.33322	1.36384	**0.95094**

Table 3.8: Simulation study results for variation C1.

C1 ($n = 15$) reveals a high non-convergence rate for ML, i.e. almost 60% of all cases did not converge. The non-convergence rate of PLS remains low, as only 23 cases out of 10,000 did not converge. The number in brackets referring to OLS appears larger compared to the basic model.

OLS yields on average the largest coefficient biases, which appear much higher than in the basic model. Also the ML biases increased compared to the basic model. But, the ML estimates of γ are clearly the least biased. For PLS the *md* averages appear not larger compared to the basic model. But, the values referring to both formative measurement models and the structural model lie now in the same range. Regarding the reflective measurement model the bias appears even lower compared to the basic model. Concerning the

measurement models PLS yields on average the lowest biases. The individual results in Appendix H (table H.8 page 152) reveal that for each approach the individual *md* values vary strongly. The *rmse* averages appear mainly the lowest for OLS, while the γ estimates vary the least. Only for the reflective measurement model the respective PLS value appears lower. Finally, all *rmse* values appear very high.

The total effect coefficients appear for all approaches less accurate compared to the basic model (referring to *md*). The OLS estimates appear on average most accurate. The largest biases reveals on average the ML approach. The variability of the estimated values appears high for all approaches (referring to *rmse*). The largest variability appears for OLS and the lowest variability for PLS.

With respect to prediction the *rmse* averages appear lower for all approaches compared to the basic model. In summary, OLS yields the best prediction. Perhaps it appears confusing to some readers that the coefficient estimates appear less precise, but the prediction more precise. The reason for this is the following: as n increases large differences between the fitted values and the observed values appear in number more often. Since the differences enter quadratic the *mse* or *rmse* increase remarkably.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0.18470	0	(0.00090)			
$\pi_1 - \pi_5$	**0.04905**	0.09840	0.06845	0.28634	0.30063	**0.27219**
$\pi_6 - \pi_8$	0.03172	**0.02912**	0.06712	0.28622	0.28492	**0.28386**
γ_1, γ_2	**0.02572**	0.07425	0.03685	0.14649	0.17202	**0.12615**
$\lambda_1 - \lambda_3$	**0.09100**	0.11519	0.11019	0.24529	**0.20661**	0.21778
TE per y_1	0.01714	0.04249	**0.00264**	0.22518	**0.22310**	0.29843
TE per y_2	0.01206	0.04409	**0.00145**	0.15710	**0.13658**	0.20918
TE per y_3	0.01551	0.04531	**0.00243**	0.20185	**0.19068**	0.26983
prediction $y_1 - y_3$	0.00185	0.00137	**0**	1.42965	1.44670	**1.35893**

Table 3.9: Simulation study results for variation C2.

In the C2 model ($n = 50$) the ML approach did not converge in 18% of all cases, whereas PLS did always converge. For 9 out of 10,000 cases the λ coefficients could not get estimated with the OLS approach applying the

covariances between the fitted values.

Compared to C1 the coefficient biases appear in C2 on average much lower, but larger compared to the basic model. The *md* averages appear mostly the lowest for ML. Only for the second formative measurement model PLS yields a lower value. The respective value appeared also in the basic model relatively low for PLS. Likewise to the basic model ML and OLS yield the lowest mean biases within the structural model. With respect to variability the lowest *rmse* values appear for OLS. An exception constitutes the *rmse* measure referring to the reflective measurement model, where PLS yields a slightly lower value than OLS.

The *md* and *rmse* averages referring to the total effect coefficients appear throughout larger compared to the basic model. Compared to variation C1 the values appear lower. In terms of *md* OLS reveals the best results, whereas the *rmse* averages appear the largest for OLS. On that latter score PLS reveals the lowest values.

The prediction of all y variables appears most accurate for OLS (in terms of *md* and *rmse*). For all approaches the *rmse* averages appear larger compared to C1 and marginally lower than in the basic model.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0	0	(0)			
$\pi_1 - \pi_5$	**0.00204**	0.09267	0.00389	0.06538	0.11402	**0.06504**
$\pi_6 - \pi_8$	**0.00141**	0.01632	0.00285	0.06011	0.06215	**0.05990**
γ_1, γ_2	**0.00130**	0.10742	0.00228	0.03472	0.11277	**0.03445**
$\lambda_1 - \lambda_3$	**0.00487**	0.13395	0.00609	0.04913	0.13616	**0.04750**
TE per y_1	**0.00028**	0.04120	0.00050	**0.04568**	0.06685	0.06008
TE per y_2	**0.00019**	0.03990	0.00027	**0.03199**	0.04888	0.04207
TE per y_3	**0.00024**	0.03973	0.00036	**0.04114**	0.05899	0.05427
prediction $y_1 - y_3$	0.00084	0.00087	**0**	1.49770	1.50336	**1.49453**

Table 3.10: Simulation study results for variation C3.

In variation C3 ($n = 1,000$) ML and PLS converged for all samples. With respect to OLS the λ coefficients got estimated in all possible manners.

Compared to the basic model ML and OLS show lower *md* values for the individual coefficients as well as for the total effect coefficients. Table H.10 (Appendix H page 153) reveals that for each parameter the *md* appears lower. For PLS the *md* values appear similar to those of the basic model. For the reflective measurement model and the structural model the respective values appear even slightly larger. ML yields the smallest coefficient biases. Referring to the *rmse* averages ML and OLS reveal lower values compared to the basic model. The OLS estimates show the lowest variability. Like in the basic model the measures of accuracy appear very close for ML and OLS. The variability of the PLS estimates appears lower than in the basic model, but still larger compared to ML and OLS.

For all approaches the *rmse* averages of the predicted y variables appear slightly larger compared to C2. OLS yields the best prediction.

The D models, see tables 3.11, 3.12 and 3.13, are specified such that both, sample size and the number of indicators, increase. The absolute number of indicators increases from 11 (D1) to 22 (D2) to 44 (D3) together with the sample size which increases from 50 (D1) to 300 (D2) to 1,000 (D3). In all D models an identity matrix gets applied as variance-covariance matrix of $\mathbf{x}$.

Referring to D1 the non-convergence rate is zero for PLS and less than 5% for ML. Compared to variation C2 the ML non-convergence rate appears much lower here (D1 and C2 differ only with respect to the variance-covariance matrix of $\mathbf{x}$). Concerning OLS no missing results appeared during the simulation.

In D1 ML shows consequently the lowest *md* averages. The variability is mainly the lowest for OLS. Only for the reflective measurement model PLS yields a slightly lower *md* average than OLS. A comparison of D1 with C2 reveals, that the estimates are on average similar accurate, just the *md* average of the second formative measurement model is now the lowest for ML, too.

The total effect coefficients are on average most accurately estimated by OLS in terms of *md*. The lowest variation (referring to *rmse*) is on average twice revealed by ML and once by PLS.

The lowest measures of accuracy concerning the prediction of the y variables appear for OLS.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0.04890	0	(0)			
$\pi_1 - \pi_5$	**0.04991**	0.06346	0.08620	0.24804	0.27650	**0.23968**
$\pi_6 - \pi_8$	**0.03397**	0.04350	0.06923	0.24959	0.27225	**0.24303**
γ_1, γ_2	**0.02563**	0.09071	0.03489	0.13917	0.19632	**0.12135**
$\lambda_1 - \lambda_3$	**0.08703**	0.11498	0.11023	0.24370	**0.21020**	0.21734
TE per y_1	0.00375	0.01627	**0.00241**	**0.21553**	0.22642	0.27390
TE per y_2	0.00254	0.04782	**0.00142**	0.15044	**0.14363**	0.19202
TE per y_3	0.00319	0.03227	**0.00247**	**0.19338**	0.19524	0.24747
prediction $y_1 - y_3$	0.00122	0.00143	**0**	1.42969	1.45061	**1.35893**

Table 3.11: Simulation study results for variation D1.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0.00160	0	(0)			
$\pi_1 - \pi_{10}$	**0.01088**	0.01501	0.03604	0.09107	0.10522	**0.09081**
$\pi_{11} - \pi_{16}$	**0.00760**	0.01072	0.03823	**0.08983**	0.10334	0.09166
γ_1, γ_2	**0.00609**	0.05545	0.03641	**0.05427**	0.07996	0.06688
$\lambda_1 - \lambda_6$	**0.02667**	0.06640	0.04110	**0.08798**	0.09721	0.10051
TE per y_1	**0.00053**	0.00205	0.00078	**0.07054**	0.07986	0.10338
TE per y_2	**0.00033**	0.01713	0.00055	**0.04934**	0.05390	0.07210
TE per y_3	**0.00046**	0.00941	0.00049	**0.06344**	0.07014	0.09266
TE per y_4	**0.00052**	0.00229	0.00070	**0.07041**	0.07975	0.10288
TE per y_5	**0.00035**	0.01697	0.00055	**0.04935**	0.05386	0.07221
TE per y_6	**0.00044**	0.00976	0.00064	**0.06328**	0.07003	0.09276
prediction $y_1 - y_6$	0.00092	0.00087	**0**	1.48177	1.48790	**1.45738**

Table 3.12: Simulation study results for variation D2.

Regarding variation D2 the non-convergence rate is zero for PLS and less than 2% for ML. Referring to OLS the estimation of the λ coefficients was throughout possible.

Compared to D1 the PLS estimates appear more accurate in terms of *md* and *rmse*. However, this is also the case for the ML and OLS approach. The lowest *md* averages for the individual coefficient estimates as well as for the total effect estimates are consequently revealed by the ML approach. Moreover, the ML estimates show the lowest *rmse* averages. Only the value referring to the first measurement model is slightly lower for OLS. The best prediction is

revealed by OLS.

In variation D3 no missing estimates appear for all three approaches. Comparing all three D models, the results of all approaches become better as both, sample size and number of indicators, increase. For D3 all presented measures of accuracy, either for the coefficient estimates or for the total effect estimates, appear best for ML. In the previously described variations the PLS averages of the measures of accuracy concerning the structural model and the reflective measurement models often appeared remarkably large. In D3 the respective values are still the largest for PLS, but the differences to ML and OLS are not any more striking. The total effect coefficients appear in general for all approaches on average more accurate in terms of *md* and *rmse*.

OLS yields the most accurate prediction of $\mathbf{y}$ in terms of *md* and *rmse*.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0	0	(0)			
$\pi_1 - \pi_{20}$	**0.00456**	0.00647	0.01127	**0.04759**	0.05631	0.04728
$\pi_{21} - \pi_{32}$	**0.00346**	0.00490	0.00901	**0.04726**	0.05573	0.04706
γ_1, γ_2	**0.00274**	0.03193	0.00705	**0.02839**	0.04413	0.02777
$\lambda_1 - \lambda_{12}$	**0.01516**	0.03485	0.02630	**0.04720**	0.05133	0.05716
TE per y_1	**0.00028**	0.00194	0.00037	**0.03525**	0.04110	0.05569
TE per y_2	**0.00020**	0.00718	0.00031	**0.02470**	0.02833	0.03900
TE per y_3	**0.00025**	0.00452	0.00048	**0.03174**	0.03659	0.05023
TE per y_4	**0.00028**	0.00188	0.00043	**0.03527**	0.04112	0.05572
TE per y_5	**0.00019**	0.00724	0.00033	**0.02470**	0.02834	0.03913
TE per y_6	**0.00026**	0.00442	0.00037	**0.03178**	0.03661	0.05023
TE per y_7	**0.00028**	0.00185	0.00052	**0.03528**	0.04112	0.05568
TE per y_8	**0.00020**	0.00721	0.00034	**0.02470**	0.02834	0.03899
TE per y_9	**0.00025**	0.00445	0.00040	**0.03174**	0.03658	0.05023
TE per y_{10}	**0.00028**	0.00178	0.00056	**0.03528**	0.04113	0.05584
TE per y_{11}	**0.00020**	0.00724	0.00025	**0.02471**	0.02835	0.03896
TE per y_{12}	**0.00025**	0.00449	0.00041	**0.03176**	0.03660	0.05018
prediction $y_1 - y_{12}$	0.00029	0.00030	**0**	1.49147	1.49525	**1.47612**

Table 3.13: Simulation study results for variation D3.

The E models, see tables 3.14 and 3.15, incorporate different variance-covariance matrices of $\mathbf{x}$: $\mathbf{V}^{\mathrm{II}}$ shows no correlations at all (E1) and $\mathbf{V}^{\mathrm{III}}$ implies

some degree of multicollinearity (E2). The matrix $\mathbf{V}^{\mathrm{I}}$, which I applied in the basic model, shows moderate correlations within the blocks of indicators and weak correlations between the blocks of indicators.

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0	0	(0)			
$\pi_1 - \pi_5$	**0.00802**	0.01107	0.01555	0.09742	0.11081	**0.09642**
$\pi_6 - \pi_8$	**0.00468**	0.00672	0.00987	0.09141	0.10347	**0.09096**
γ_1, γ_2	**0.00291**	0.09739	0.00588	0.05869	0.11415	**0.05735**
$\lambda_1 - \lambda_3$	**0.01604**	0.13182	0.02022	0.09054	0.14397	**0.08541**
TE per y_1	**0.00058**	0.01319	0.00086	**0.07882**	0.09070	0.10156
TE per y_2	**0.00038**	0.02944	0.00051	**0.05521**	0.06189	0.07119
TE per y_3	0.00051	0.00670	**0.00050**	**0.07120**	0.07711	0.09201
prediction $y_1 - y_3$	0.00031	0.00029	**0**	1.48883	1.49248	**1.47802**

Table 3.14: Simulation study results for variation E1.

With respect to variation E1 no missing values appear for all three approaches.

A comparison of the measures of accuracy of E1 with those of the basic model reveals that ML and OLS yield slightly larger values in the formative measurement models. On the contrary the values appear lower in the structural model and effectively equal in the reflective measurement model. For both approaches the corresponding *rmse* averages appear lower compared to the basic model. With respect to PLS the mean biases appear clearly lower in the formative measurement models and slightly lower in the structural model. For the reflective measurement model the respective value appears effectively equal. The *rmse* values appear lower for all approaches compared to the basic model. As in the basic model the PLS *md* averages appear much larger for the structural model and especially larger for the reflective measurement model.

All approaches yield more accurate estimates of the total effects compared to the basic model. The largest *md* values appears for PLS and the largest *rmse* values for OLS. ML and OLS yield similarly low *md* averages. The ML estimates vary the least as ML yields the lowest *rmse* values.

The predicted y variables deviate the less from the observed values for OLS.

Referring to variation E2 PLS converged for all cases while ML shows a

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0.44320	0	(0)			
$\pi_1 - \pi_5$	0.21263	0.12034	**0.01574**	0.54763	**0.41127**	0.55418
$\pi_6 - \pi_8$	0.23731	0.11031	**0.01673**	0.51589	**0.31554**	0.52011
γ_1, γ_2	**0.01044**	0.07950	0.01934	0.07470	0.10593	**0.07449**
$\lambda_1 - \lambda_3$	**0.01637**	0.13177	0.02002	0.09058	0.14231	**0.08947**
TE per y_1	0.13172	0.06873	**0.00254**	0.32476	**0.23431**	0.45140
TE per y_2	0.09258	0.04524	**0.00119**	0.22780	**0.13981**	0.31649
TE per y_3	0.11864	0.06053	**0.00289**	0.29250	**0.19908**	0.40908
prediction $y_1 - y_3$	0.00103	0.00029	**0**	1.48900	1.49341	**1.47802**

Table 3.15: Simulation study results for variation E2.

non-convergence rate of approximately 45%. OLS was always able to estimate the λ coefficients in all manners.

Compared to model E1 and to the basic model the results change remarkably referring to the formative measurement models. For ML and OLS the *md* and *rmse* measures appear much larger. For PLS the *rmse* measure appears much larger. For PLS the *md* value of the second formative measurement model lies now in the same range as the value of the first measurement model. With respect to the other partial models the PLS results appear slightly more accurate. Nevertheless, PLS yields less accurate results referring to the structural model and the reflective measurement model .

Regarding the total effect estimates very large *rmse* averages appear for all three approaches, while the PLS estimates vary the least. ML shows the largest *md* averages. OLS shows on the one hand the lowest *md* values and on the other hand the largest *rmse* values.

Concerning prediction the measures appear similar to those of the basic model. OLS yields the highest accuracy.

In table 3.16 I show the results for variation F, in which I classified $\mathbf{x}$ to seven discrete values. The numbers of missing results appear nearly identical to those of the basic model, i.e. they are zero for PLS and OLS, and close to zero for ML.

Referring to the individual coefficients the *md* averages appear very similar to those of the basic model: the ML and OLS measures appear similar, while

	md			***rmse***		
	ML	PLS	OLS	ML	PLS	OLS
missing results	0.00130	0	(0)			
$\pi_1 - \pi_5$	**0.01196**	0.08590	0.01773	0.11241	0.14039	**0.11093**
$\pi_6 - \pi_8$	**0.01593**	0.01911	0.02042	0.10428	0.10500	**0.10415**
γ_1, γ_2	**0.00219**	0.09279	0.00397	0.06048	0.11097	**0.05894**
$\lambda_1 - \lambda_3$	**0.03301**	0.13933	0.03706	0.09576	0.14840	**0.09017**
TE per y_1	**0.00061**	0.03702	0.00088	**0.08058**	0.09376	0.10562
TE per y_2	**0.00043**	0.03750	0.00053	**0.05642**	0.06203	0.07414
TE per y_3	0.00053	0.03642	**0.00043**	**0.07265**	0.08104	0.09561
prediction $y_1 - y_3$	0.00915	0.36484	**0**	1.62075	1.67672	**1.47795**

Table 3.16: Simulation study results for variation F.

ML yields the lowest *md* values and OLS the lowest *rmse* values. As in the basic model PLS shows in general the largest biases and the largest variabilities.

The similarity to the basic model appears also with respect to the accuracy of the total effect coefficients: PLS shows in general the largest *md* values and OLS the largest *rmse* values.

The prediction of the y variables appears most accurate for OLS.

3.3.2 Significance test of coefficients: actual size and actual power

In this section I present the results concerning the significance of the path coefficients. All results refer to variation G.[70] As in the previous section I restrict myself to the description of the results. The conclusion follows in the subsequent section 3.3.3. I start with the description of the results for variation G, the results concerning the extra cases are shown below. I show the ratios of rejected null hypothesis (i.e. actual power and actual size) for the 1%-, 5%- and 10%-significance level. The ML and PLS results are tabulated together (see tables 3.17 and 3.19), because for these two approaches I refer to the individual coefficient estimates. The OLS results are tabulated separately (see tables 3.18 and 3.20), because the corresponding values refer to the total effect estimates.

[70]The specification characteristics of variation G and the extra cases I investigate are summarised in table 3.1 page 77.

The non-convergence rate for variation G is 0.001 for ML and 0 for PLS. As I did not estimate the OLS individual coefficients no number of missing λ coefficients appears.

With respect to ML and PLS actual power see table 3.17. The ratios appear for ML clearly lower in the formative measurement models, whereby ML reveals values close to zero, e.g. for π_2 on the 1%-level actual power is 0.02 for ML versus 0.69 for PLS. For both approaches actual power is much lower in the first measurement model than in the second formative measurement model. In the structural model and in the reflective measurement model PLS detects the paths, which are truly different from zero, as good as certain. Concerning the structural model the difference between ML and PLS lessens and for the reflective measurement model it disappears.

	$\alpha = 0.01$		$\alpha = 0.05$		$\alpha = 0.1$	
	ML	PLS	ML	PLS	ML	PLS
π_1	-	0.61370	-	0.79870	-	0.87200
π_2	0.02262	0.69290	0.20180	0.85860	0.39279	0.91540
π_3	0.10691	0.48530	0.49199	0.69610	0.72062	0.78890
π_4	0.01682	0.28950	0.20440	0.49240	0.43654	0.60620
π_5	0.01512	0.67420	0.14174	0.83720	0.29289	0.90380
π_7	-	0.97180	-	0.99330	-	0.99670
π_8	0.31241	0.66860	0.74374	0.84260	0.87748	0.90440
π_9	0.49800	0.92670	0.88639	0.97620	0.96306	0.98930
γ_1	0.71411	1.00000	0.88008	1.00000	0.93353	1.00000
γ_2	0.97317	0.99990	0.99469	1.00000	0.99770	1.00000
λ_1	-	1.00000	-	1.00000	-	1.00000
λ_2	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
λ_3	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000

Table 3.17: Actual power for ML and PLS (variation G).

The OLS results concerning actual power are shown in table 3.18. The ratios appear quite similar when comparing the values per column. In other words, the non-zero effects a certain x variable has on y_1, y_2 or y_3 are detected similarly often. Between the different x variables (referring to the rows) the ratios vary quite strong. When comparing the ratios with the magnitude of the population coefficients (see the calculated population values in Appendix G), they appear to be related: on each significance level the two largest coefficients ($TE_{x_7 y_q}$

	OLS, $\alpha = 0.01$			OLS, $\alpha = 0.05$		
	y_1	y_2	y_3	y_1	y_2	y_3
x_1	0.3871	0.3885	0.4002	0.6330	0.6368	0.6465
x_2	0.1362	0.1397	0.1356	0.3156	0.3125	0.3164
x_3	0.3877	0.3828	0.3823	0.6341	0.6209	0.6264
x_4	0.1907	0.1895	0.1923	0.3989	0.3983	0.4005
x_5	0.0827	0.0830	0.0844	0.2202	0.2152	0.2221
x_7	0.7758	0.7804	0.7839	0.9162	0.9175	0.9202
x_8	0.3895	0.3827	0.3841	0.6368	0.6256	0.6302
x_9	0.5838	0.5907	0.5770	0.7962	0.7983	0.7941

	OLS, $\alpha = 0.1$		
	y_1	y_2	y_3
x_1	0.7454	0.7455	0.7515
x_2	0.4349	0.4342	0.4399
x_3	0.7446	0.7374	0.7423
x_4	0.5214	0.5222	0.5245
x_5	0.3302	0.3260	0.3212
x_7	0.9553	0.9544	0.9541
x_8	0.7464	0.7391	0.7429
x_9	0.8680	0.8766	0.8737

Table 3.18: Actual power for OLS (variation G).

and $TE_{x_9y_q}\ \forall\ q$) are detected most often and the two smallest coefficients the least frequent ($TE_{x_5y_q}$ and $TE_{x_2y_q}\ \forall\ q$).

In table 3.19 I display how often ML and PLS committed a type I error (relative to k). For ML in the formative measurement models , referring to π_6 and π_{10}, the actual size is clearly lower than the respective nominal size (α). Concerning the reflective measurement model (λ_4) for ML the actual size fairly equals the respective α-level. On the contrary, for PLS the actual sizes throughout exceed the respective nominal sizes. The exceeding is not very large for λ_4, compared with the exceeding concerning π_6 and π_{10}. Especially for the latter coefficient the actual size is clearly larger than the respective nominal size.

For OLS the actual sizes of the hypothesis test are tabulated in table 3.20. All values appear in the range of the respective nominal size, in other words the empirical rates fairly coincide the respective α-level.

	$\alpha = 0.01$		$\alpha = 0.05$		$\alpha = 0.1$	
	ML	PLS	ML	PLS	ML	PLS
π_6	0.00140	0.01390	0.01772	0.06280	0.05736	0.11290
π_{10}	0.00420	0.02790	0.03714	0.08950	0.08679	0.14930
λ_4	0.00921	0.01090	0.05025	0.05350	0.10150	0.10500

Table 3.19: Actual size for ML and PLS (variation G).

	OLS, $\alpha = 0.01$				OLS, $\alpha = 0.05$			
	y_1	y_2	y_3	y_4	y_1	y_2	y_3	y_4
x_1	-	-	-	0.0098	-	-	-	0.0524
x_2	-	-	-	0.0121	-	-	-	0.0508
x_3	-	-	-	0.0094	-	-	-	0.0482
x_4	-	-	-	0.0104	-	-	-	0.0504
x_5	-	-	-	0.0102	-	-	-	0.0516
x_6	0.0106	0.0094	0.0100	0.0112	0.0495	0.0531	0.0492	0.0510
x_7	-	-	-	0.0084	-	-	-	0.0450
x_8	-	-	-	0.0089	-	-	-	0.0471
x_9	-	-	-	0.0096	-	-	-	0.0520
x_{10}	0.0103	0.0103	0.0124	0.0113	0.0518	0.0525	0.0549	0.0538

	OLS, $\alpha = 0.1$			
	y_1	y_2	y_3	y_4
x_1	-	-	-	0.1026
x_2	-	-	-	0.1000
x_3	-	-	-	0.1008
x_4	-	-	-	0.1020
x_5	-	-	-	0.1050
x_6	0.0995	0.1036	0.0968	0.1036
x_7	-	-	-	0.0961
x_8	-	-	-	0.0921
x_9	-	-	-	0.1009
x_{10}	0.0985	0.1019	0.1023	0.1075

Table 3.20: Actual size for OLS (variation G).

In the following I present the PLS bootstrapped standard deviations based on 100, 300 or 1,000 bootstrap replications.[71] In table 3.21 I show for each

[71]The previously presented PLS results base on standard deviations, which were bootstrapped applying 100 bootstrap replications.

coefficient the mean of the bootstrapped standard deviations[72] for the different K_B. The largest value (per K_B) is printed in bold. For the values which appear equally more decimal places were checked. Apparently, the largest values appear sometimes for $K_B = 1,000$ and sometimes for $K_B = 300$, but most often for $K_B = 100$. Thus, the standard deviations appear on average not strictly larger as a larger number of bootstrap replications gets performed. Moreover, the differences between the estimates appear very low.
A change of the bootstrapped standard deviation implies a different value of the test statistic T. Therefore, the decision whether a null hypothesis gets rejected or not may be affected. For a larger number of bootstrap replications even a larger exceeding of the nominal size is possible: e.g. on the 10%-level for π_{10} and $K_B = 100$ the actual size is 14.93% and for $K_B = 300$ or 1,000 the respective size exceeds 15% (I do not show further tables for the different K_B). As the mean value of the respective standard deviations appears lower and the standard deviation appears in the denominator of the test statistic, this makes intuitively sense. However, I remark that a straightforward deduction from the change of the *mean value* of the bootstrapped standard deviations on actual power or actual size is not possible.

With regard to the different PLS inner schemes I show the results concerning actual size and actual power in table 3.22 and 3.23. The tables show only the results for the 5%-level. The values appear either equal or the difference confines to the fourth decimal place.

I detected for ML and PLS large differences concerning actual size and actual power as well as concerning accuracy of the coefficient estimates. I find it therefore useful to graphically illustrate some results. The figures 3.4 (page 101 et seq.), 3.5 (page 103) and 3.6 (page 104) show for variation G the density functions of the ML and PLS coefficient estimates, the corresponding standard deviations and the resulting test statistics referring to the π, the γ and the λ coefficients (π_1, π_7 and λ_1 are excluded, since these parameters are fixed for the ML estimation). I do this although I did not summarise the results of variation G with respect to accuracy. For all results see Appendix H tables H.17 and H.18 page 157 et seq. At this point I remark that the results approximate the

[72] A mean standard deviation equals the square root of the corresponding mean variance.

	$K_B = 100$	$K_B = 300$	$K_B = 1,000$
π_1	0.11597	**0.11602**	0.11598
π_2	0.11149	0.11150	**0.11151**
π_3	0.11818	**0.11828**	**0.11833**
π_4	**0.12038**	0.12036	0.12035
π_5	0.10959	**0.10967**	0.10961
π_6	**0.11419**	0.11412	0.11407
π_7	**0.10874**	0.10873	0.10873
π_8	**0.11363**	0.11361	0.11361
π_9	**0.11023**	0.11016	0.11017
π_{10}	**0.11769**	0.11763	0.11758
γ_1	0.06157	0.06158	**0.06158**
γ_2	0.06080	**0.06080**	0.06079
λ_1	0.03392	**0.03395**	0.03394
λ_2	0.03284	**0.03395**	0.03286
λ_3	**0.03709**	0.03709	0.03708
λ_4	0.04835	0.04838	**0.04838**

Table 3.21: PLS bootstrapped standard deviations (mean values) of all individual coefficient estimates (variation G).

	centroid	factorial	path
π_6	0.0628	0.0626	0.0624
π_{10}	0.0895	0.0892	0.0892
λ_4	0.0535	0.0530	0.0529

Table 3.22: Actual size for PLS applying different inner schemes (variation G), $\alpha = 0.05$.

	centroid	factorial	path
π_1	0.7987	0.7989	0.7989
π_2	0.8586	0.8587	0.8587
π_3	0.6961	0.6961	0.6960
π_4	0.4924	0.4927	0.4927
π_5	0.8372	0.8370	0.8369
π_7	0.9933	0.9932	0.9932
π_8	0.8426	0.8424	0.8425
π_9	0.9762	0.9762	0.9762
γ_1	1.0000	1.0000	1.0000
γ_2	1.0000	1.0000	1.0000
λ_1	1.0000	1.0000	1.0000
λ_2	1.0000	1.0000	1.0000
λ_3	1.0000	1.0000	1.0000

Table 3.23: Actual power for PLS applying different inner schemes (variation G), $\alpha = 0.05$.

results of the basic model in terms of accuracy.
The graphs (referring to the figures 3.4, 3.5 and 3.6) are sorted as follows: The first columns show the density functions of the coefficient estimates. Each population parameter is marked with a vertical line, respectively. The second columns show the density functions of the standard error estimates. Each dashed line represents the expected standard error of the respective ML or PLS coefficient estimator. Such value equals the square root of the average over all respective k estimated coefficient variances (9,990 for ML and 10,000 for PLS). The third columns of the graphs show the density of the corresponding test statistics.[73] The respective critical value(s) for the 5%-level, i.e. the 0.025 and/or the 0.975 quantile, is (are) marked with a grey line. Since the respective t- and z-values take on very close values, they graphically coincide.

Concerning the coefficient estimates, i.e. referring to the first column in all three figures, the ML results appear on average quite unbiased. In contrast, for PLS the coefficient estimates deviate for most coefficients clearly from the population parameter. Only with regard to the coefficients which are truly zero (π_6, π_{10} and λ_4) the PLS density functions appear unbiased, and only a slight shift appears for the coefficients which appertain to the second formative measurement model (π_8 and π_9). Also for the three coefficients for which I do not show any graphs the described results apply: the curve of the coefficient which appertains to the second formative measurement model (π_7) appears for PLS only slightly shifted, whereas for the other two coefficients (π_1 and λ_1) the curves appear apparently shifted compared to the true value. For ML the density functions I do not show appear unbiased.

In the second column of the respective figures (pages 101 to 104) I show the density functions of the ML and PLS standard deviations. For ML in the formative measurement models the curves appear right skewed and show larger variability than the respective PLS curves. Moreover, the corresponding curves lie to the left of the respective expected value for both approaches. Since the marks base on the squared standard deviations large values are weighted strongly, i.e. the more large values appear the more the mark lies to the right. Therefore, apparently for ML more large values appear. In general, ML yielded

[73] The density functions conform a test of $H_0 : \beta_j = 0$.

larger standard deviations than PLS. However, the described picture is different for the standard deviation density functions of π_6 and π_{10}, which are truly zero. The corresponding curves appear for ML less right skewed and show lower variability.

With respect to the structural model the variability of the standard deviations is apparently larger for ML than for PLS. Moreover, the ML curves appear again right skewed, although this is more difficult to identify from the scaled graphs. The PLS curves fit better their corresponding expected value, indicating that large estimates appear less often.

At this point I go more into detail concerning the ML standard deviation functions relating to the formative measurement models and the structural model. Giving a close look to the corresponding estimates, some conspicuous results can be detected, namely coefficient estimates that deviate strongly and reveal extremely large standard deviations. Such an inaccurate parameter estimate may occur, if several maxima exist, and the ML approach converges towards another maximum than the appropriate one. Although these estimates apparently are implausible, I did not discard these results from my analysis, as I did not define a threshold for rejecting such estimates. As an example I show in Appendix I a histogram of the $\sqrt{\widehat{\text{var}}\,(\hat{\gamma}_1)}$ estimates (figure I.1 page 160) and the corresponding density values (table I.1 page 161). The histogram reveals the right skewness and the density values reveal that outliers exist. However, as mentioned above, the results I present do include all estimates.

Referring again to the figures shown on page 101 et seqq. and thereby concerning the reflective measurement model (figure 3.6) the ML standard error estimates take on larger values compared to PLS. For both approaches the curves have a normal shape. Only for PLS the vertical mark indicates that PLS reveals some large values. With respect to the density function of $\sqrt{\widehat{\text{var}}\left(\hat{\lambda}_4\right)}$ ML shows lower variability than PLS.

Comparing the density functions of the PLS and ML standard deviations, the PLS curves lie in general to the left implying lower standard error estimates (excluding the graphs belonging to the coefficients which are truly zero, π_6, π_{10} and λ_4). In this regard I bring to mind that the PLS standard deviations do not result larger for a larger number of bootstrap replications K_B, but rather fairly coincide with the here presented results, see table 3.21 page 97.

Further, I investigated also the ML bootstrapped standard deviations, which becomes more reasonable as the ML approach apparently yielded some large standard deviations. But, the bootstrapping of the standard error appears not recommendable. Yet, I can eliminate a possible doubt, that I should have had to bootstrap the standard errors. However, at this point I omit further tables, but show some condensed findings in Appendix I table I.2 page 163.

In the third column of the figures (page 101 et seqq.) the resulting test statistics appear for PLS mainly larger, which is a consequence of the smaller standard deviations. But, obviously also the coefficient estimates influence the test statistics: when looking at the PLS estimates related to π_{10}, the right shift of the density curve of the test statistic appears to result from the overestimation of the coefficient. The PLS test statistic values show larger variability compared to ML, except for the values which are truly zero. The respective ML density curves lie to the left of the corresponding PLS curves, which especially in the formative measurement models leads to lower power for ML. Referring to the actual size the graphical assessment is difficult, because the graphs would need to be depicted much larger. Only for π_6 and π_{10} it is apparent that the rates are larger for PLS than for ML (the respective pink curves lie above the black curves). The precise values are given in the previously shown table 3.19 page 95.

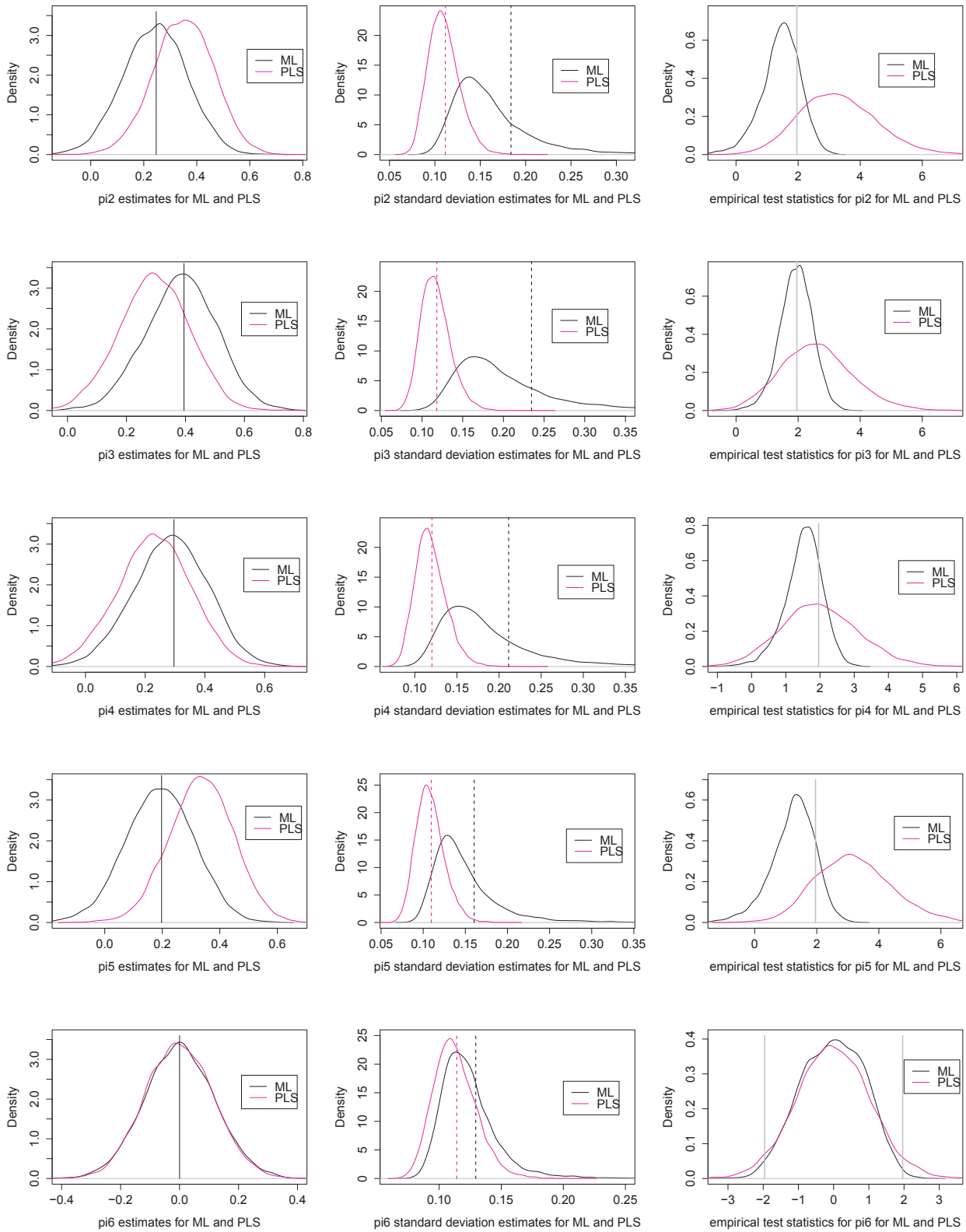

Figure 3.4 continues on the next page.

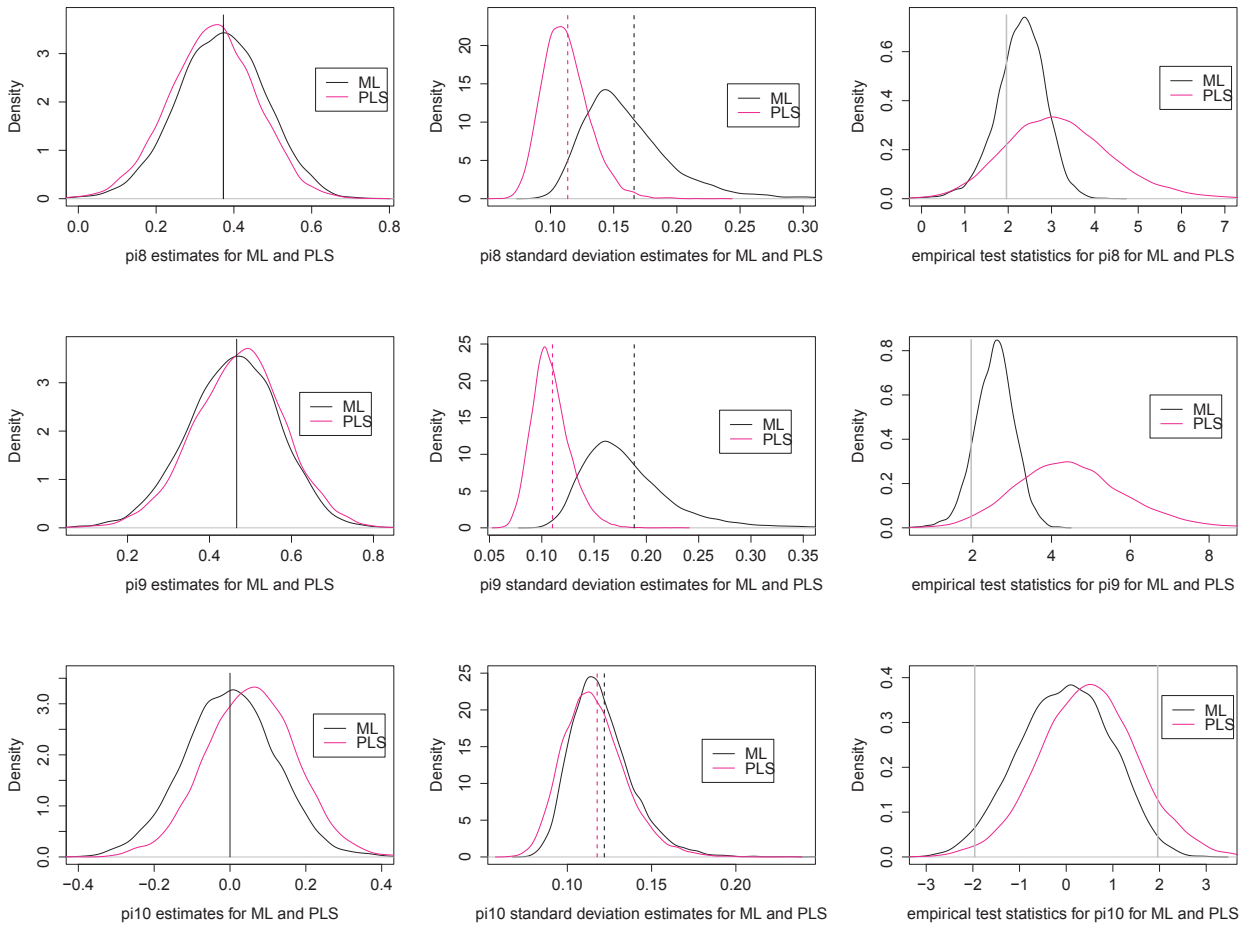

Figure 3.4: ML and PLS simulation results for the π coefficients (variation G, from page 101 on).

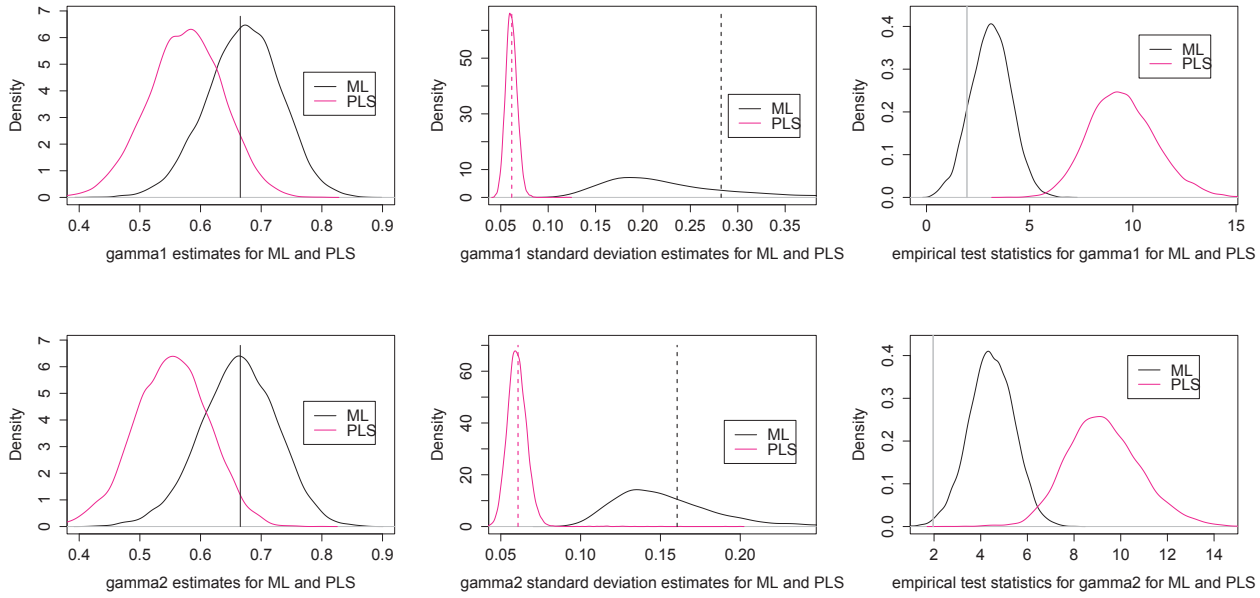

Figure 3.5: ML and PLS simulation results for the γ coefficients (variation G).

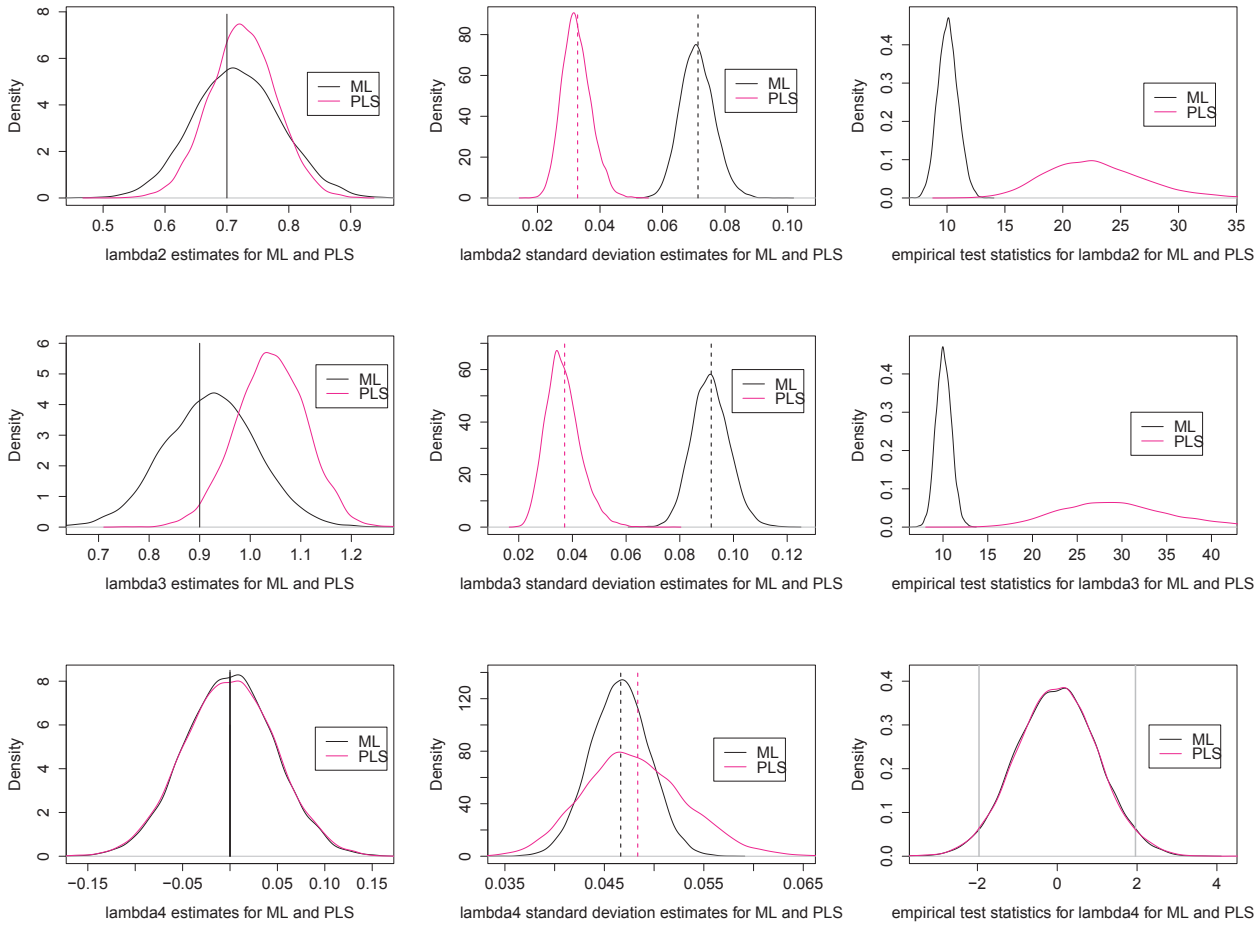

Figure 3.6: ML and PLS simulation results for the λ coefficients (variation G).

3.3.3 Conclusions

In this section I resume the simulation study results and draw conclusions. I ascribe differences in accuracy, that appear between the basic model and a specific variation, to the individual modification which characterises the specific variation. This is reasonable firstly, because I let all other specification aspects unchanged, respectively, and secondly, because I performed a very high number of Monte Carlo iterations ($K = 10,000$ for each specification).

My first topic is ML and PLS convergence. As expected PLS shows much lower non-convergence rates than ML does. More precisely for PLS no case is worth mentioning in the context of non-convergence, because the respective rates remain for all cases below 1%. But, I ascertain that PLS non-convergence can appear for a correctly specified model.[74] Concerning the ML approach the respective results are overall good, but I can outline three different factors that have an impact on its convergence: sample size, the underlying variance-covariance matrix of $\mathbf{x}$ and the incorporated explained variance (R^2). Sample size has the largest impact. Unsurprisingly the ML non-convergence rate is very high if n is very low, i.e. for $n = 15$ ML did not converge in almost 60% of all samples. I investigated four different sample sizes and the corresponding ML non-convergence rates appear to follow a declining curve, see figure 3.7. Already at $n = 50$ the non-convergence rate drops to less than 20% and drops further as n increases until it reaches zero. If the variance-covariance matrix of $\mathbf{x}$ represents an identity matrix (E1) ML has no convergence problems at all. In this regard my results do not conform the statement that ML non-convergence becomes more likely if covariances are close to zero (see section 2.1.2). This may be the case because the variance-covariance matrix $\mathbf{V}^{\mathrm{II}}$ does not involve any contradictories and its information content is maximal. Moreover, the underlying model specifications may facilitate convergence. Non-convergence increases strongly if the x variables are afflicted with (imperfect) multicollinearity (E2). It is intuitive that higher correlations imply lower information. If the model incorporates lower R^2, non-convergence appears more often, as a comparison of the basic model to variation A, AB1 and AB2 reveals. Non-normality does not have an impact on ML non-convergence, since

[74] Henseler (2010) revealed non-convergence cases for PLS solely for misspecified models.

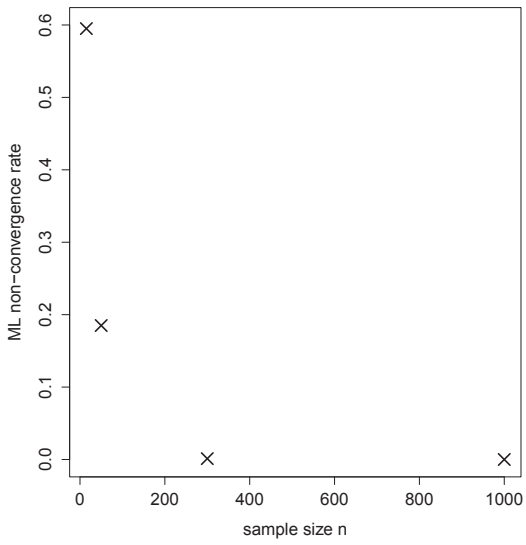

Figure 3.7: Relation between ML non-convergence and sample size.

the non-convergence rates remain constant when the basic model is changed into variation B1 or B2 as well as when variation A is changed into AB1 or AB2.

With respect to ML convergence I further want to point out an additional result I gained during some pre-studies. I observed that ML convergence can be influenced by the imposed restrictions without changing the number of restrictions, i.e. the number of fixed parameters. In the specified model the ML non-convergence rate could have been lower by imposing the restrictions $\gamma_1 = \gamma_2 = \lambda_1 = 1$ (instead of $\pi_1 = \pi_6 = \lambda_1 = 1$[75]). However, I did not choose this restriction in order to stick to the explanations in chapter 2.1 and the common practice. But, it may matter for practical applications that convergence can be influenced without imposing further restrictions.

OLS is not an iterative estimation procedure and thus, does not at all suffer from non-convergence, but it may mathematically occur that some $\hat{\lambda}$ parameters cannot be estimated, because the covariances between fitted values $\hat{y}_k^{\mathrm{OLS}}$ and $\hat{y}_s^{\mathrm{OLS}}$ $(k \neq s)$ behave such that a negative value appears under the square root, referring to equation 2.30 page 49. Even in such case $\hat{\lambda}$ estimates are available, namely those that result from the division of the total effect

[75]This restrictions apply to all variations, except variation G.

OLS coefficients. In my study negative values under the root do only occur for specifications where either the determination coefficients are low (all A variations) or where the sample size is small (variation C1). The largest rate appears for variation C1 ($n = 15$) with 687 missing $\hat{\lambda}_q$ values ($\forall\ q$) out of 10,000.[76] The maximum number of missing $\hat{\lambda}$ values for an A variation appears for AB1 with 102 missing values. I conclude that first of all the "scaling" of the y variables is responsible to obtain positive values under the respective square root. This is intuitive and underpinned by my results, because all remaining models do not at all suffer from this problem and the model incorporates solely positive relations. For a small n it is not unlikely that the sample may be atypical, and may thereby lead to atypical covariances between the y variables or rather between their fitted values. The same may appear if relatively large error terms impact the y variables. Since the error term is random it can either augment each observation positively or negatively and thereby possibly change the sign of the respective covariances.

In the following I proceed with the evaluation of the simulation study results concerning the accuracy of the coefficient estimators.
When looking at the *md* and *rmse* averages referring to the individual coefficient estimates the main picture can be described in the following way: For all specifications, apart from variation C1 and E2, the smallest *md* averages appear for ML, either regarding all values, or regarding all values except the one of the second formative measurement model. The lowest variability appears often for the OLS estimates. The corresponding measures appear similar for ML. On the contrary the respective PLS values appear clearly larger. In summary, I can ascertain that the PLS biases appear systematically and that they are solely small for models which incorporate many indicators and a large sample (D2, D3). Besides, the differences between the individual *md* and *rmse* values are for PLS much larger than for ML or OLS (see the individual results in Appendix H). Especially in the reflective measurement model extremely large values appear for PLS. Extremely large PLS biases in the re-

[76] The respective measurement model consists of three indicators. One unsolvable equation (according to equation 2.30 page 49) entails that all three λ coefficients cannot get estimated applying the covariances. In case more indicators operationalise the latent variable possibly some $\hat{\lambda}$ estimates may be obtained by using the respective covariances.

flective measurement model are in line with the results of prior simulation studies (see f.i. CASSEL ET AL., 1999, p. 442 et seq. or RINGLE ET AL., 2009, p. 28 et seq.). The fact that the PLS biases appear on average lower in the formative measurement model of ξ_2 than of ξ_1 is surprising, because ξ_2 is operationalised by less indicators than ξ_1. Since n is large ($n = 300$) the effect of more indicators should have had a positive impact on accuracy.
The main picture concerning the accuracy of the total effect estimates can be described in the following way: PLS reveals in general larger *md* values compared to ML and OLS, although the individual PLS biases cancel each other out to some degree. A different picture appears again for the case where n is very small (variation C1) and where the x variables show very high correlations (E2). For these cases PLS is able to keep up in terms of accuracy or appears even preferable. The largest total effect *rmse* values appear throughout for OLS, with the exception of C3. I assume this to be the case because the OLS total effect estimators do not use all information the models incorporates, namely the covariances between the y variables. Finally, when considering all results the most condensed conclusion is that the ML approach outperforms the other two approaches.

In the following I go more into details and illustrate what I can deduce from the variations, firstly concerning accuracy, referring to the variations A to F, and secondly concerning size and power of a test for significance of the coefficients, referring to variation G.

In case the model incorporates relatively low explained variance (A cases) all approaches react with an increase in bias and variability. The PLS *md* values concerning the $\hat{\gamma}$ and $\hat{\lambda}$ estimates stand out as much larger than the respective ML and OLS values. In effect, with respect to the results of variation A PLS gets clearly outperformed in terms of *md* and *rmse*. Nevertheless, PLS shows quite reasonable results concerning the total effect coefficients. In order to keep implications straightforward my overall conclusion is to prefer ML when the proportion of explained variance is relatively low.

On the basis of the B models I conclude that ML, PLS and OLS are robust towards non-normality, because the measures of accuracy appear almost identical when changing the basic model into B1 or B2 as well as when changing variation A into AB1 or AB2. Consequently, the approaches are also robust

towards the type of distribution since the results of the variations B1 and B2 as well as of the variations AB1 and AB2 appear similar. The respective cases include error terms which follow either a continuous uniform distribution or a chi-squared distribution. Finally, my conclusion referring to both B cases corresponds with the basic model and my conclusion concerning both AB cases corresponds with variation A: concerning the individual estimates PLS cannot be recommended, but ML should be favoured. Considering all respective estimation results I conclude that the ML approach can be preferred over the OLS approach, though the differences are rather small. If the total effect coefficients are of interest the PLS estimates are acceptable, but ML is the best choice again.

The C cases reveal the following: When the sample size is extremely low (in C1 $n = 15$) ML suffers not only from non-convergence, but also from large biases and variabilities. The large biases emerge in all measurement models. Concerning the structural model the ML approach yields the least biased estimates compared to the other approaches, which is astonishing given this extremely small sample size. For OLS all values are throughout bad. As sample sizes increases, the ML and OLS estimates become quickly more accurate. Already for $n = 50$ (C2) the accuracy measures concerning the individual coefficients appear noticeably lower for both approaches. Considering all respective measures PLS is outperformed by ML and OLS. If sample size increases further (it is $n = 300$ in the basic model and $n = 1,000$ in C3) the ML and OLS results become throughout better. Unsurprisingly, the PLS estimates appear inconsistent since its estimates do not become more accurate as sample size increases. In contrast, PLS results can even become less accurate as sample size increases.[77] I conclude that for a very low sample size PLS yields the most accurate, yet biased, estimates concerning the individual and the total effect coefficients. The variability of the estimates is very large. Therefore, the results need to be analysed carefully. For a moderate sample size (from 50 onwards) the most straightforward conclusion is to prefer ML over PLS and OLS. Admittedly also the PLS and OLS results are partially

[77] Regarding the reflective measurement model the mean bias appears lower in C1 and C2 compared to the basic model. Regarding the structural model the mean bias appears lower in C2 compared to the basic model.

acceptable, but I consider straightforward implications as relevant.

The PLS property "consistency at large" is assessed with the D models. The results ascertain the property that the PLS estimates become more accurate as both, sample size and number of indicators, increase. However, also the ML and OLS estimates become better. In summary, with regard to variation D2 and D3 ML outperforms OLS and PLS (concerning the individual coefficients and the total effects), although D3 features ideal PLS conditions.

The E variations vary with respect to the variance-covariance matrix of $\mathbf{x}$. PLS reveals the lowest biases if an identity matrix ($\mathbf{V}^{\mathrm{II}}$) is applied. However, the biases remain quite stable as correlations increase ($\mathbf{V}^{\mathrm{I}}$ in the basic model exhibits moderate correlations). Even in presence of multicollinearity ($\mathbf{V}^{\mathrm{III}}$) the biases increase only slightly. The OLS biases concerning the individual coefficients as well as the total effect coefficients are only slightly affected by the degree of the incorporated correlations. This is unsurprising, since OLS estimators, i.e. the total effect estimators, are robust towards imperfect multicollinearity and the individual estimates rely on these estimators. Concerning ML the *md* values of the $\hat{\pi}$ coefficients appear much larger for (imperfectly) multicollinear x indicators (E2). Unsurprisingly the *rmse* values concerning the formative measurement models increase for increasing correlations between the x variables with regard to all approaches. As the variance-covariance matrix in variation E2 comprises very sparse information, the *rmse* values appear extremely large. Referring to the accuracy of the individual and the total effect coefficients ML cannot be recommended because its $\hat{\pi}$ estimates suffer strongly under the (imperfectly) multicollinear formative indicators. A comparison between the PLS and OLS accuracies regarding E2 does not deliver a straightforward implication: OLS appears preferable in terms of bias but the variability is unacceptably high. At least PLS variability is a bit lower, but firstly, it is still high and secondly, the corresponding biases are higher. Consequently, at least the results concerning the formative measurement models must be assessed carefully no matter which approach gets applied. If the formative measurement models get excluded from the assessment, i.e. with regard to the other partial models, ML and OLS outperform PLS.

With respect to variation F, where $\mathbf{x}$ is discrete, for all three approaches the measures of accuracy appear very similar to those of the basic model. In other

words the information loss concerning the x variables did not have a large impact on parameter accuracy, so that I can conclude that the estimation quality does not suffer, if the exogenous indicators are discrete instead of continuous.

With respect to prediction I mainly assessed the accuracy of the predicted endogenous y variables. These values refer to the residuals, so that it is unsurprising that OLS shows in general the highest accuracy: firstly, because in the OLS approach each y variable gets directly regressed on $\mathbf{x}$ and thereby the sum of squared residuals (the residuals that get assessed) gets minimised and secondly, because the md is always zero as a characteristic of OLS. Regarding the cases which incorporate low determination coefficients (all A cases), ML, PLS and OLS show strictly large $rmse$ values. This is plausible because the incorporated lower R^2 values imply poorer fits of a linear regression to the data. According to my study PLS is not favourable to make predictions, as PLS reveals throughout the largest $rmse$ values. The most accurate predicted values appear for the OLS approach. The ML results approximate the OLS results in terms of accuracy.

An additional investigation was directed at the accuracy of the fitted values and scores. I remarked in the context of the accuracy of the scores that the fact that PLS estimates scores is not per se an advantage. Using formative indicators (these are exogenous and represent f.i. driver variables) fitted values can be computed according to the specified model. Whether the ML, PLS or OLS fitted values or the PLS scores are more accurate depends on certain model characteristics. It may occur that referring to PLS the fitted values are more precise than the scores. Further, the fitted values of ML or OLS may be even more precise. In a model where the causality flows only in one direction the endogenous y variables can only be predicted by the x variables. I explicitly stress this point again because indicators may never get predicted by applying the scores of their corresponding latent variable, because otherwise an indicator would be used to predict itself. In a model like the one shown in figure 3.8 the variables y_4 to y_6 may not get predicted applying the scores of η_1. On the contrary, if a specific y_q (for $q = 4$, 5, or 6) gets predicted applying the scores of ξ_1, the described error does not occur. Consequently, the variables y_1 to y_3 cannot at all be predicted without committing the described mistake, see hereto Wold (1982, p. 9 et seq.).

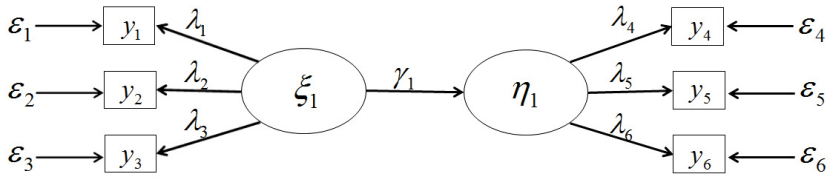

Figure 3.8: Simple model that incorporates solely reflective indicators.

Variation G served predominantly to investigate actual size and actual power referring to a significance test with $H_0 : \beta_j = 0$. I investigated on the 1%-, 5%- and 10%-level the individual coefficients for the ML and PLS approach and the total effect coefficients for the OLS approach. Regarding the individual coefficients I determined actual size in the formative and the reflective measurement models, while I determined actual power in all partial models. I enhanced the ML and PLS results by graphical illustrations.

My very condensed findings are the following: The ML actual size never exceeds the respective nominal size but rather undercuts it. ML actual power appears low to moderate in the formative measurement models, good in the structural model and reaches 1.0 in the reflective measurement model. PLS shows in general high actual power, but its actual size always exceeds the nominal size. Thus, PLS rejects a null hypothesis $H_0 : \beta_j = 0$ too often. Regarding OLS actual power is moderate to good and the α-level is kept (slight variations can be reasoned with random fluctuations).

In the following I elaborate these findings first concerning ML and PLS and thereafter concerning OLS. The graphical ML and PLS illustrations (figures 3.4 to 3.6 page 101 et seqq.) show for each coefficient the density function of the coefficient estimates, of the respective standard deviations and of the resulting test statistics.

With respect to ML the prior findings concerning the unbiasedness of the path coefficients can easily be recognised in the figures. Regarding the standard deviations some ML estimates are conspicuous bad, but nevertheless entered the assessment. These large values (outliers) result in a relatively large average over the k estimates (represented by the dashed line). So in case large values occur, the dashed line does not "fit" well the density curve. As the average represents the expected value of the corresponding estimator (k is very large)

the results appear (partially) distorted. Actually, standard deviation outliers do occur for the γ coefficients and those π coefficients which truly take on a non-zero number. Consequently no outliers appear for those π coefficients which truly are zero and all λ coefficients. It can be reasoned that I should have had to discard implausible results. However, despite the exclusion of implausible results, the density functions of the standard deviations appear right skewed in the formative measurement models and the structural model. Thus, the formative specifications are possibly problematic for ML when it comes to the estimation of the standard errors, affecting the estimates in the formative measurement models, and further affecting the estimates of the structural model as some latent variables are specified in a formative way (in my case $\boldsymbol{\xi}$). However, I assume a researcher would identify the very large standard deviations as implausible and discard them. Notwithstanding, I did not define a certain threshold within my Monte Carlo study for an automatic discarding, since it is difficult to reason one concrete value. I assess the ML standard deviations further applying exemplary $\sqrt{\widehat{\text{var}}\,(\hat{\gamma}_1)}$. A histogram of the standard deviations reveals that values greater 0.5 appear relatively seldom (see Appendix I figure I.1 page 160). The corresponding densities are given in table I.1 (page 161) and reveal that starting from a value of 0.550 the densities for the classified standard error estimates are throughout lower than 0.1. Figure I.2 (page 162) shows how the picture changes when all estimates greater 0.550 get discarded.[78] As the "large" estimates got removed the dashed line, i.e. the expected estimator value, fits the density function clearly better.

Concerning the actual power the corresponding test statistic density curves illustrate that actual power is lower for ML compared to PLS, referring to the (non-zero) π coefficients and the γ coefficients.[79] Numerically this is intuitive, because the respective ML coefficients appear unbiased and the standard deviations larger. With respect to the reflective specifications the ML results are absolutely inconspicuous. Ultimately, although formative specifications lead apparently for ML to difficulties with regard to the estimation of the standard errors (outliers and skewness), the nominal size is never exceeded.

The additionally estimated ML bootstrapped standard deviations are not con-

[78] I do not claim that 0.550 is the best threshold, but use this value as an example.

[79] The 5%-significance level is marked with a grey vertical line.

vincing. Unsurprisingly they imply that for my case, in which multinormality is given, the original standard deviations from the estimation procedure shall be preferred over the bootstrapped values (see Appendix I table I.2 page 163).

Concerning PLS the biases that appear for most coefficient estimates become visible in the respective figures (page 101 et seqq.). The bootstrapped PLS standard deviations show low variability compared to the respective ML curves. The corresponding dashed lines lie to the right compared to the density curves and the density curves appear slightly right skewed.

The bootstrapping can be modified in terms of the number of bootstrap replications (K_B). For PLS I investigated three different cases including 100, 300 or 1,000 bootstrap replications. The resulting standard deviations do not strictly appear larger. On the contrary the largest values appear mainly for the lowest K_B. These values refer mainly to the formative measurement models. But also for the structural model and the reflective measurement model more values appear higher for $K_B = 300$ than for $K_B = 1,000$. Moreover, the differences between the values are very low so that the impact on the test decision is only marginal. I did not show further ratios, but pointed out that the actual size may even become larger as the number of bootstrap replication increases. Consequently, the appearing exceeding of the nominal size may even increase for a higher K_B. This makes intuitively sense, when the mean values of standard deviations appear lower. Finally, I cannot conclude that the PLS bootstrapped standard deviations become larger with a higher number of bootstrap replications.

The test statistic density functions illustrate that PLS leads to higher power than ML does. However, the PLS test statistic always exceeds the determined α-level. The graphs only hint at that problem, the precise values in table 3.19 (page 95) give evidence. For example regarding π_{10} the actual size reaches nearly 9% on the 5%-level. Finally, the fact that PLS exceeds the respective α-levels can only lead to the conclusion that the PLS test statistic is not appropriate to serve its purpose.

I conclude that ML is suitable to determine significance of path coefficients, although the results appear conservative within formative measurement models. On the contrary the PLS test statistic is not appropriate to test coefficients on their significance.

Concerning OLS I investigated actual size and actual power referring to the total effect coefficients, because the population parameters which equal a value of zero distort the division of a total effect coefficient into single coefficients. The simulation results ascertain that OLS power depends on the magnitude of the respective population parameter. It makes statistically sense that a population parameter close to zero is much more difficult to distinguish from zero, or in other words it becomes more difficult to reject the null hypothesis $H_0 : \beta_j = 0$. In summary, the results for OLS power are inconspicuous. When it comes to the rejection of a true null hypothesis my simulation study confirms that the presented OLS approach accurately determines significance since the actual sizes correspond with the respective nominal sizes - the small variations can be ascribed to random fluctuation. Therefore, the practical implication arises that an estimated total effect which is detected as significant (conservatively on the 1%-level) may be divided into single coefficients. If the total effect is composed of (at least) one coefficient which truly equals zero the estimates would be distorted in approximately 1% of all cases (α). Therefore, researchers should investigate the results with respect to plausibility. Inflated estimates may indicate the implausibility and a researcher may consider whether partial effect(s) may be zero.

Finally, I complemented my study by assessing the three different PLS inner schemes, firstly in terms of accuracy (for the basic model) and secondly with respect to significance of the path coefficients (for case G). Concerning accuracy my results ascertain that the differences are marginally low. Concerning actual size and actual power only marginal differences appear, too.[80] Hence, the PLS estimates appear in general for each weighting scheme the least accurate and the respective α-level is not kept. Consequently I do not conclude that a certain weighting scheme must be preferred over another one.

[80] To be precise the actual size appears marginally smaller when the path weighting scheme is applied, yet the respective nominal size is clearly exceeded.

Chapter 4

Critical Appraisal

The two approaches ML and PLS have a very different proceeding and both are not trivial. The literature reveals several inconsistencies that can make it even harder to understand the methods, especially for researchers who just begin to work with structural equation models or who work application oriented. This situation plus mainly the two facts that formative measurement models in ML studies as well as actual test size[81] in PLS studies are up to date only rarely investigated, led to my research motivation.

The purpose of this work was to present a comprehensible introduction to ML and PLS, as well as to introduce an approach which contributes by its simplicity. I named this latter approach the OLS approach. I purposed to assess for all three approaches estimator properties as well as the test size beside statistical power, particularly applying a model which incorporates formative indicators. By performing a Monte Carlo simulation I purposed to contribute to the confusions which appear in the PLS literature and present reliable results and implications.

My general proceeding was the following. In chapter 1 I introduced to structural equation modelling with latent variables in general and further introduced inconsistencies that appear in the literature. With chapter 2 I contributed a comprehensible introduction to ML and PLS. To contrast the classical ML approach with the currently popular PLS approach, I gave an overview of simulation study results with regard to consistency, bias, power and convergence (or improper solutions). Further, I introduced the OLS approach and

[81] Referring to $H_0 : \beta_j = 0$.

presented in detail the estimation procedure as I propose it. Chapter 3 is dedicated to my extensive simulation study. With regard to all three approaches I assessed the accuracy of the individual coefficient estimates, of the total effect coefficient estimates and of the predicted values. I measured accuracy in terms of mean deviation (md) and variability ($rmse$) for many different specifications. Specifically I assessed the effect of the degree of correlations between formative indicators, of the incorporated ratio of unexplained variance, of the error term distribution, of sample size and of available data (in terms of number of indicators and sample size). Furthermore, I investigated for all three approaches the frequency a type I error gets committed (test size) and the frequency a null hypothesis gets correctly rejected (statistical power) referring to a test for significance of the coefficients.

The simulation study results led to the following conclusion. Concerning the confusions which appear in the literature I ascertain that with respect to accuracy ML is in general the better approach compared to PLS, even if formative measurement models are applied and if the data is non-normally distributed. My study ascertains that the PLS estimators systematically deliver biased values. These biases appear to be quite stable, even under bad conditions, such as (imperfectly) multicollinear formative indicators or as extraordinary small sample sizes. I remark that very high correlations between formative indicators imply low information and consequently lead to high variability in the estimators. Extremely small sample sizes are in general critical and can only be justified with circumstances that made it impossible to gather more observations (including immense costs). ML non-convergence becomes problematic under the same circumstances under which accuracy suffers, i.e. extremely small sample size and (imperfectly) multicollinear formative indicators. Though it is remarkable that at a sample size of $n = 15$ the ML estimators concerning the structural model appear the least biased.
With respect to the OLS approach I can ascertain that its estimators for the individual coefficients are unbiased and consistent. In general OLS yields slightly less accurate results than ML. Clear differences between these two approaches appear for the case of multicollinearity, because OLS estimators are robust towards imperfect multicollinearity. Consequently the individual estimates, which base on the OLS estimates (i.e. on the total effects), appear unbiased.

Despite their unbiasedness, the estimates reveal large deviations from the true value, as the *rmse* values appear large. Further, if the sample size is extremely small the estimators suffer strongly in terms of bias.

In table 4.1 I summarise the results of my Monte Carlo study, saying which approach overall seems preferable. For a few table cells I could have referred also to another approach because the differences are small, or one approach was slightly better in terms of *md* and the other one in terms of *rmse*. In such cases I display the more straightforward approach. The table shows some question marks which indicate that the interpretation of such estimates needs generally be considered with caution. With respect to prediction the OLS approach seems to be a good alternative in general, but the differences to ML were rather small, i.e. ML was in general second best. As to the rest ML appears as good and robust approach.

	With respect to...		
	Coeff.	TE	Prediction
· R^2 relatively high, normal data, $n = 300$, 3 to 5 indicators per latent variable, low to moderate correlated formative indicators	ML	ML	OLS
· R^2 low	ML	ML	OLS
· data non-normally distributed	ML	ML	OLS
· extremely few observations ($n = 15$)	PLS?	PLS?	OLS
· from few ($n = 50$) observations onwards	ML	ML	OLS
· at least 6 per latent variable and large n	ML	ML	OLS
· low (zero) correlated formative indicators	ML	ML	OLS
· imperfectly multicollinear formative indicators, accuracy concerning the fMM	?	PLS	OLS
· imperfectly multicollinear formative indicators, accuracy concerning the SM and the rMM	ML		
· exogenous indicators ($\mathbf{x}$) are discrete	ML	ML	OLS

Table 4.1: The overall preferable approach in terms of accuracy for different cases.

The investigation of the test for significance of the path coefficients revealed the following: PLS shows larger actual power than ML, but does that at the cost of an exceeded nominal size, when the null hypothesis is true. The actual test size of PLS exceeds throughout the respective nominal size for each α-level.

Especially in the formative measurement models the actual size appears clearly too large. Consequently, the PLS test statistic is not appropriate to determine significance of the path coefficients. Admittedly the expected values of the PLS standard errors of the path coefficients appear relatively low, but this is not very meaningful as the α-level is not kept. The ML standard errors do, however, suffer from formative specifications, but the ML test statistic appears rather conservative, i.e. the respective α-levels get clearly undercut. ML power depends strongly on the magnitude of the coefficient. The same is true for OLS (with respect to the total effect coefficients), which also keeps the α-level.

Finally I outline some pros and cons concerning my study.
I consider the introductions to the methods comprehensible. Thereby the introduced OLS approach constitutes a great benefit in the field of structural equation modelling. To my best knowledge up to date no studies apply the presented estimation procedure, which works in a straightforward way, is very easy to comprehend and thus easy to replicate. Further, the Monte Carlo set-up is described very transparent and the specifications vary systematically. All specified cases incorporate formative measurement models, whereby I contribute to a research need. In total I performed remarkably 230,000 Monte Carlo iterations (excluding all bootstrap replications in the course of a single Monte Carlo iteration). Thus, my study appears very extensive and since I performed 10,000 iterations for each particular specification the results can be considered reliable.

Cons of my study are the following. First of all I need to remark that I cannot conclude that the presented results are valid for other specifications. However, other ML and PLS studies reveal similar pictures, underpinning the reliability of my results.
My specified model can be considered as inadequate with respect to complexity.[82] I am aware that more complex models are more relevant for practical applications. However, to present the OLS approach I chose on purpose a model of low complexity to exemplify the estimation procedure and later on applied the same model in my simulation study. I find this charming because it makes my study transparent and easy to replicate.
In my model the $\boldsymbol{\xi}$ variables were defined error-free. Therefore, these variables

[82] Only in the in the D2 and D3 variations I augmented further indicators.

are in any case normally distributed, even with respect to my non-normality cases, i.e. all B cases. However, with respect to ML and OLS identification it was not an option to specify all error terms free, but some error terms had to be restricted to a value of zero.
My simulation study covers certain specifications, but more specifications are possible. I did not simulate a model that f.i. incorporates a misspecification or uses solely reflective operationalisations.
I investigated test size and power of a test for significance of the individual path coefficients for ML and PLS. This investigation is limited to the measurement models. The specified model (referring to variation E, see figure 3.2 page 61) is not appropriate to assess the actual size in the inner model. The model shown in figure 4.1 corresponds with variation G, but incorporates a third exogenous latent variable ξ_3, whose structural coefficient $\gamma_3 = 0$. Accordingly ξ_3 is separated from the rest of the model and further the covariances between the corresponding indicators (x_{11} to x_{13}) are not explained by the model (see section 2.1.2). Consequently, such a model is not identified in terms of ML. To assess the actual size in the inner model the model may incorporate f.i. a causality leading from ξ_2 to ξ_3.
Moreover, I did not investigate a Count Data Model, i.e. a model which incorporates endogenous discrete variables. The presented OLS approach is not suitable to estimate the respective coefficients (representing the total effects), because OLS ignores that the data is discrete and does not ensure integer outcome values. Under certain circumstances the OLS estimates may even be inconsistent (Winkelmann, 2008, p. 65 et seq.). The respective coefficients (representing the total effects) of such Count Data Model need to get estimated with a suitable approach such as Poisson Regression or Negative Binomial Regression (for an application see f.i. Koch, 2009).[83]

For future research I recommend further ML, PLS and OLS comparisons applying models which incorporate formative indicators. Regarding OLS I propose to divide the total effect estimates only if they are significant, but

[83]However, the presented data generation was not suitable to assess such a model, because applying the population parameters would not have led to discrete $\mathbf{y}$ values and an aggregation after their generation to discrete values would not have matched the population coefficients.

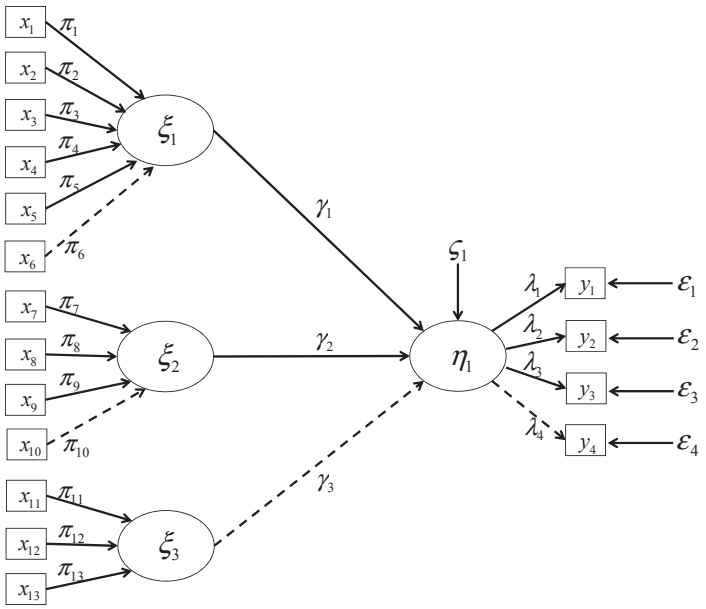

Figure 4.1: Model which is in terms of ML not identified.

to assess the results in terms of their plausibility. Implausible results may indicate that the total effect is composed of (at least) one coefficient which equals zero. Further, I suggest to capture in general the actual size referring to the significance testing of path coefficients, but to capture it in particular in the inner model. With respect to OLS I recommend to assess the significance of the individual coefficient estimates, applying the bootstrap technique for the estimation of the corresponding standard errors. Moreover, I recommend to specify a case applying exclusively discrete indicators ($\mathbf{x}$ and $\mathbf{y}$) and e.g. to vary the coefficient patterns (homogeneous vs. heterogeneous). Further, I recommend to extend the different specifications, applying f.i. more complex models or models which incorporate misspecifications.

Appendix

Appendix A

PLS Applications

In table A.1 PLS application studies are listed together with their individual reason(s) for applying PLS (if reasons are given).[84] The studies are interdisciplinary, i.e. they cover several business areas, such as (international) Marketing and Strategic Management. The list is partially based on Henseler et al. (2009) and Reinartz et al. (2009), but includes also others application studies (such as published after 2009). Since a large number of PLS application studies has been published - according to Hair et al. (2012b, p.414) 204 articles were published solely referring to marketing journals until 2010 - this is only a selection, which gives a condensed overview.

[84] In the header "MS" is the abbreviation for misspecification and "MC" for multicollinearity.

Study	Indicator distribution	Sample size	Model complexity	Research stage	Formative Indicators	Prediction orientation	Identification/convergence	MS/MC	Source
Fornell/Robinson, 1983	x	x							Journal of Consumer Research
Birkinshaw et al., 1995	x	x				x			Strategic Management Journal
Dawes et al., 1998	x	x							Journal of Marketing
Milberg et al., 2000	x					x			Organization Science
Lee, 2001		x							Journal of Business Research
White et al., 2003					x	x			Journal of Marketing
Eskildsen et al., 2004	x					x		x	Total Quality Management
Mintu-Wimsatt/Graham, 2004	x	x							Journal of the Academy of Marketing Science
Reinartz et al., 2004					x		x		Journal of Marketing Research
Venaik et al., 2005	x	x	x	x	x				Journal of International Business Studies
Hennig-Thurau et al., 2006	x								Journal of Marketing
Johnson et al., 2006			x						Journal of Marketing
Ulaga/Eggert, 2006					x				Journal of Marketing
Hennig-Thurau et al., 2007					x				Journal of Marketing
Hsu/Wang, 2008	x					x		x	Total Quality Management
McFarland et al., 2008					x				Journal of Marketing
Harmancioglu et al., 2009			x						Journal of Product and & Brand Management
Wu et al., 2009					x				Social Indicators Research
Ernst et al., 2010	x				x				Journal of Marketing
Lam et al., 2010					x				Journal of Marketing
Anderson/Swaminathan, 2011	x		x					x	Journal of Marketing Theory and Practice
Arazy/Gellatly, 2012	x								Journal of Management Information Systems
Brady et al., 2012									Journal of Marketing
San José-Cabezudo/Camarero-Izquierdo, 2012					x				Journal of Advertising
Bicen/Madhavaram, 2013	x								Journal of Marketing Theory and Practice
Garnefeld et al., 2013	x						x		Journal of Marketing
Landau/Bock, 2013	x	x	x		x	x			Long Range Planning
Nell/Ambos, 2013	x	x	x	x					Strategic Management
Calvo-Mora et al., 2014									Journal of Business Research
Surienty et al., 2014									Social Indicators Research

Table A.1: Reasons for applying PLS (studies are sorted by date).

Appendix B

Derivation of the implied variance-covariance matrix

The derivation is presented by Bollen (1989, p. 324 et seq.) and Trinchera (2007, p. 69 et seqq.) among others. Usually for simplicity the variables $\boldsymbol{\eta}$, $\boldsymbol{\xi}$, $\mathbf{y}$ and $\mathbf{x}$ enter als deviations from their means. Furthermore, the error terms are uncorrelated. Both assumptions are not necessary, but they simplify the notation.

For

$$\boldsymbol{\Sigma}(\boldsymbol{\theta}) = \begin{bmatrix} \boldsymbol{\Sigma}_{yy}(\boldsymbol{\theta}) & \boldsymbol{\Sigma}_{yx}(\boldsymbol{\theta}) \\ \boldsymbol{\Sigma}_{xy}(\boldsymbol{\theta}) & \boldsymbol{\Sigma}_{xx}(\boldsymbol{\theta}) \end{bmatrix}$$

the "partial" covariance matrices need to be derived. They are $\boldsymbol{\Sigma}_{yy}(\boldsymbol{\theta})$, $\boldsymbol{\Sigma}_{xx}(\boldsymbol{\theta})$, $\boldsymbol{\Sigma}_{yx}(\boldsymbol{\theta})$ and $\boldsymbol{\Sigma}_{xy}(\boldsymbol{\theta})$. Recall that $\mathrm{E}(\mathbf{y}) = \mathrm{E}(\mathbf{x}) = 0$ and uncorrelated error terms $\boldsymbol{\epsilon}$ and $\boldsymbol{\delta}$ are assumed.

With $\mathrm{E}(\mathbf{y}) = 0$ the first one is

$$\begin{aligned} \boldsymbol{\Sigma}_{yy}(\boldsymbol{\theta}) &= \mathrm{E}(\mathbf{y}\mathbf{y}') \\ &= \mathrm{E}\left[(\boldsymbol{\lambda}_y\boldsymbol{\eta} + \boldsymbol{\epsilon})(\boldsymbol{\eta}'\boldsymbol{\lambda}_y' + \boldsymbol{\epsilon}')\right] \\ &= \boldsymbol{\lambda}_y \mathrm{E}(\boldsymbol{\eta}\boldsymbol{\eta}')\boldsymbol{\lambda}_y' + \boldsymbol{\Theta}_\epsilon. \end{aligned}$$

Furthermore, $\mathrm{E}(\boldsymbol{\eta}\boldsymbol{\eta}')$ can be derived (recall $\boldsymbol{\eta} = \mathbf{B}\boldsymbol{\eta}+\boldsymbol{\Gamma}\boldsymbol{\xi}+\boldsymbol{\zeta} = (\mathbf{I}-\mathbf{B})^{-1}\boldsymbol{\Gamma}\boldsymbol{\xi}+\boldsymbol{\zeta}$):

$$\begin{aligned}\mathrm{E}(\boldsymbol{\eta}\boldsymbol{\eta}') &= \mathrm{E}\left(\left[(\mathbf{I}-\mathbf{B})^{-1}\boldsymbol{\Gamma}\boldsymbol{\xi}+\boldsymbol{\zeta}\right]\ \left[\boldsymbol{\xi}'\boldsymbol{\Gamma}'[(\mathbf{I}-\mathbf{B})^{-1}]'+\boldsymbol{\zeta}'\right]\right)\\ &= (\mathbf{I}-\mathbf{B})^{-1}(\boldsymbol{\Gamma}\boldsymbol{\Phi}\boldsymbol{\Gamma}'+\boldsymbol{\Psi})\left[(\mathbf{I}-\mathbf{B})^{-1}\right]'\end{aligned}$$

With this information $\boldsymbol{\Sigma}_{yy}(\boldsymbol{\theta})$ can be transformed to

$$\boldsymbol{\Sigma}_{yy}(\boldsymbol{\theta}) = \boldsymbol{\Lambda}_y(\mathbf{I}-\mathbf{B})^{-1}(\boldsymbol{\Gamma}\boldsymbol{\Phi}\boldsymbol{\Gamma}'+\boldsymbol{\Psi})[(\mathbf{I}-\mathbf{B})^{-1}]'\boldsymbol{\Lambda}_y'+\boldsymbol{\Theta}_\epsilon.$$

The second partial covariance matrix is:

$$\begin{aligned}\boldsymbol{\Sigma}_{xx}(\boldsymbol{\theta}) &= \mathrm{E}(\mathbf{x}\mathbf{x}')\\ &= \mathrm{E}\left[(\boldsymbol{\Lambda}_x\boldsymbol{\xi}+\boldsymbol{\delta})(\boldsymbol{\xi}'\boldsymbol{\Lambda}_x'+\boldsymbol{\delta}')\right]\\ &= \boldsymbol{\Lambda}_x\mathrm{E}(\boldsymbol{\xi}\boldsymbol{\xi}')\boldsymbol{\Lambda}_x'+\boldsymbol{\Theta}_\delta\\ &= \boldsymbol{\Lambda}_x\boldsymbol{\Phi}\boldsymbol{\Lambda}_x'+\boldsymbol{\Theta}_\delta\end{aligned}$$

The third partial covariance matrix is:

$$\begin{aligned}\boldsymbol{\Sigma}_{yx}(\boldsymbol{\theta}) &= \mathrm{E}(\mathbf{y}\mathbf{x}')\\ &= \mathrm{E}[(\boldsymbol{\Lambda}_y\boldsymbol{\eta}+\boldsymbol{\epsilon})(\boldsymbol{\xi}'\boldsymbol{\Lambda}_x'+\boldsymbol{\delta}')]\\ &= \boldsymbol{\Lambda}_y\mathrm{E}(\boldsymbol{\eta}\boldsymbol{\xi}')\boldsymbol{\Lambda}_y'\\ &= \boldsymbol{\Lambda}_y\mathrm{E}\left[(\mathbf{I}-\mathbf{B})^{-1}(\boldsymbol{\Gamma}\boldsymbol{\xi}+\boldsymbol{\zeta})\boldsymbol{\xi}'\right]\boldsymbol{\Lambda}_x'\\ &= \boldsymbol{\Lambda}_y(\mathbf{I}-\mathbf{B})^{-1}\boldsymbol{\Gamma}\boldsymbol{\Phi}\boldsymbol{\Lambda}_x'\end{aligned}$$

The remaining partial covariance matrix corresponds with the latter one in the way

$$\boldsymbol{\Sigma}_{xy}(\boldsymbol{\theta}) = \left[\boldsymbol{\Sigma}_{yx}(\boldsymbol{\theta})\right]',$$

because the main diagonal mirrors the two matrices.

Appendix C

Bootstrapping

The estimate $\hat{\theta}$ of a parameter of interest θ is estimated on the basis of a sample $\mathbf{x}$ of size n. The data set has been drawn from a probability distribution F. The purpose is to estimate the standard error of $\hat{\theta}$, i.e. $\sqrt{\widehat{\text{var}}_F(\hat{\theta})}$. The bootstrap technique constitutes the simplest non-parametric approach to do so.

A bootstrap sample $\mathbf{x^b}$ of size n gets drawn with replacement from the empirical distribution $\hat{F}$, while each observed value $x_1, x_2, ..., x_n$ has the probability $\frac{1}{n}$ to get drawn. In other words the observed data is treated as population. Hence, $\mathbf{x^b}$ consists only of data points of $\mathbf{x}$, whereby some values appear 0, 1, 2,... times. This bootstrap sample serves subsequently to estimate the parameter of interest (θ), which I name $\hat{\theta}^b$. This procedure is repeated K_B times, so that finally K_B estimates $\hat{\theta}^b$ are available.

The bootstrap estimate of $\sqrt{\text{var}_F(\hat{\theta})}$ applies the empirical distribution $\hat{F}$ instead of F and is called "plug-in estimate" (Efron/Tibshirani, 1993, p. 46). Accordingly, the bootstrap estimate for the standard error of the statistic $\hat{\theta}$ is

$$\sqrt{\widehat{\text{var}}_{\hat{F}}(\hat{\theta}^b)} = \frac{1}{K_B - 1} \sum_{b=1}^{K_B} \left(\hat{\theta}^b - (\bar{\hat{\theta}^b})^2 \right)$$

where $(\bar{\hat{\theta}^b})^2$ represents the average of the bootstrap parameter estimates. "In other words, the bootstrap estimate of [...] $\left[\sqrt{\text{var}_F(\hat{\theta})}\right]$ is the standard error of $\hat{\theta}$ for data sets of size n randomly sampled from $\hat{F}$" (Efron/Tibshirani, 1993, p. 46).

With K_B going to infinity the ideal bootstrap estimate of $\sqrt{\text{var}_{\hat{F}}(\hat{\theta}^b)}$ is

$$\lim_{(K_B)\to\infty} \sqrt{\widehat{\text{var}}_{K_B}} = \sqrt{\widehat{\text{var}}_{\hat{F}}(\hat{\theta}^b)}.$$

Accordingly, the empirical standard deviation approximates the population standard deviation as the number of replications K_B goes to infinity.

Efron/Tibshirani (1993, p. 48) suggest that 25-200 replications are sufficient to estimate a standard error. Fox et al. (2013) states in his reference manual (p. 4) that 100 replications "should be enough for computing standard errors, but not confidence interval". Consequently the default number of replications regarding his *sem* package (Fox et al., 2013) is 100, which pertains also in the *plspm* package (Sanchez et al., 2013). Both packages appertain to the free software R (R Core Team, 2014).

Appendix D

Simulation studies summary

In this section I summarise prior findings gained from Monte Carlo simulation studies concerning the PLS and ML estimators. Thereby I focus on those parts of the studies, which correspond with my research interest (f.i. I do not refer to other methods which were investigated in the respective studies). With respect to estimator consistency see tables D.1. Results referring to estimator biases and their robustness towards sample size, data distribution or misspecification are tabulated in table D.2. Moreover, I summarise simulation results concerning the special aspects of power in table D.3, and concerning non-convergence / improper solutions in table D.4.
The findings differ to some extent and depend on the individual study set-up, e.g. model complexity or sample size. I describe the main characteristics of the individual study set-ups in table D.5. The table shows study characteristics I consider advantageously or disadvantageously.
Within each table the articles are sorted by date of publication.

Source	Consistency
Hui/Wold, 1982	With both increasing, the number of indicators per latent variable and the sample size, all **PLS** estimates and the fitted values of the latent variables become more accurate. PLS is consistent at large.
Cassel et al., 1999	"The biases for the estimates seem to be unaffected by the increasing sample size" (p. 443). Hence, **PLS** estimators are inconsistent. In the inner model the estimates can even become more biased as sample size increases.
Chin/Newsted, 1999	**PLS** structural coefficient estimations do not become more accurate with an increasing sample size. Hence, they are inconsistent. But, they become more accurate with both increasing, sample size and number of indicators per latent variable. Thus, they are consistent at large. "For sample sizes of 150 or 200, the mean PLS estimate yielded the population parameter at indicator level of 16 and 32 [...]" (p. 333).
Chin et al., 2003	Concerning the **PLS** structural coefficients: "Increasing the sample size [...] does not improve on these estimations and, in fact, can make them worse" (p. 204).
Reinartz et al., 2009	As sample size increases accuracy of **ML** estimators improves. "[...] if consistency matters, ML-based CBSEM should be preferred over **PLS**" (p. 338).

Table D.1: Simulation study results concerning estimator consistency.

Source	Bias
Areskoug, 1982	With two indicators per construct "unacceptable estimates may result even with large samples" (p. 110) for **ML** and **PLS**. For this extreme biases, however, no clear pattern is recognisable, either ML or PLS coefficient estimates are on average less biased. Apart from that case ML is usually more accurate than PLS. With adding indicators the results become better.
Boomsma, 1982	**ML** estimation quality depends on the size of the coefficients in the measurement models. Large coefficient sizes are especially advantageously in the case of a relative small sample size (i.e. for $n = 25$ or 50).
Chou/Bentler, 1995	In general **ML** generates reliable statistical results, even if the data is non-normally distributed. (ML "consistently provided the most unbiased estimates", p. 53.)
Cassel et al., 1999	**PLS** estimators are biased even under optimal assumptions. The biases of the coefficient estimates increase as skewness of the indicators increases. Concerning PLS correlations between formative indicators or exogenous latent variables have no systematic consequences on the biases. Multicollinearity can even lead to better estimation results. If a latent variable is missing (i.e. the model is misspecified) especially the coefficients in the inner model are biased (the bias increases accordingly to the relevance of the missing construct). The scores of the endogenous latent variable are quite accurate, even with skewed data, multicollinearity and misspecification.
Chin/Newsted, 1999	A greater number of latent variables does not lead to more accurate **PLS** estimates concerning the coefficients in the measurement models. "At best, the standard error dropped slightly as the number of LVs increased, but only when the number of indicators was at four or eight" (p. 333). Estimations are comparably accurate if constructs are operationalised by eight or more indicators.

Table D.2 continues on the next page.

Source	Bias
Chin et al., 2003	Given a measurement model with one single indicator the **PLS** coefficients in the inner model are always strongly biased (no matter how large the sample size is). Concerning the coefficients in the measurement models "it is not until we use 10 to 12 indicators that a more accurate loading estimate is reached" (p. 205). Less indicators lead to comparable results when the sample size is larger. 20 observations lead always to bad results, no matter how many indicators are incorporated. Heterogeneous coefficient sizes in the measurement models improve the estimation of the corresponding structural coefficient.
Reinartz et al., 2009	Under optimal assumptions **ML** estimators are accurate. "PLS path coefficients systematically deviate from the true parameter values" (p. 339). For samples smaller than 250 observations **PLS** estimators are less biased than ML estimators. Non-normality of the data does not have an impact on PLS and ML estimator biases. The higher the product *sample size* times *the size of the measurement model coefficients* the less are the PLS and ML structural coefficients biased. The inner ML coefficient estimates can be considered accurate with a sample of only 100 observations when the coefficients in the measurement model are large. But, when the coefficients in the measurement model are low a sample of 500 observations is required (this result is based on four indicators per latent variable). Overall ML bias is lower than PLS bias.

Table D.2 continues on the next page.

Source	Bias
Ringle et al., 2009	In the inner model **ML** estimators are as a general rule more accurate than **PLS** estimators. The same is true for all measurement models. But, ML shows some outliers in terms of mean squared error. That is the case when formative indicators within one block show very heterogeneous correlations (strong and close to zero correlations). ML mse appears also large in a reflective measurement model if the indicators are highly correlated. A homogeneous correlation pattern between formative indicators is an advantage for the PLS estimation. ML estimations show some extreme outliers when indicators show low correlations while they operationalise the same construct (mse outliers). There is no systematic change between normal and non-normal data concerning accuracy, not for PLS nor for ML. ML estimates are as a general rule more accurate than PLS estimates even with non-normally distributed data.

Table D.2: Simulation study results concerning estimator bias (from page 131 on).

Source	Power
Chin/Newsted, 1999	Small coefficients (0.2) in **PLS** measurement models are only detected when the sample size is at least 150-200. Large coefficients (0.6, 0.8) are already detected with a sample of 20 observations.
Chin et al., 2003	Concerning **PLS**: "[...] both sample size and the number of indicators are influential in determining significance for interaction terms" (p. 203; this results holds for all coefficients in the inner model). However, at least 100-150 observations and 4-6 indicators are required to identify significance in the inner model. Moreover, the larger a structural coefficient is, the more likely is its detection.
Reinartz et al., 2009	**PLS** clearly shows higher power than **ML**. Concerning both methods, but especially for ML, statistical power is positively influenced by sample size. Moreover, the size of the coefficients in the measurement models and the number of indicators per latent variable are important for statistical power with respect to ML.

Table D.3: Simulation study results concerning power.

Source	Non-convergence and improper solutions
Boomsma, 1982	**ML** non-convergence "depends heavily on the population covariances [...] and the sample size [...]" (p. 155). The first issue implies that "inconsistencies" such as positive correlated indicators, but whose coefficients (between them and the latent variable) are positive and negative, may not appear. The second issue implies a negative impact of sample size on non-convergence frequency. The lower the sample the more likely is non-convergence. Depending on the respective model good or acceptable convergence rates appear for samples greater or equal 100 and in a few cases even for lower sample sizes.
Boomsma/ Hoogland, 2001	**ML** non-convergence or improper solutions are likely to occur when the sample size is lower than 200. Moreover, convergence depends positively on the number of indicators per construct and the size of the respective coefficients. Non-convergence and the appearance of improper solutions are not affected by the degree of non-normality. The more complex a model is, the more often non-convergence or improper solutions occur.
Reinartz et al., 2009	**ML** non-convergence is not affected by the data distribution. ML convergence is positively influenced by the size of the coefficients in the measurement models as well as by the number of indicators per latent variable. The less indicators are available the more important is the size of the indicator coefficients with respect to convergence. For ML convergence the sample size should comprise at least 200 observations.

Table D.4 continues on the next page.

Source	Non-convergence and improper solutions
Henseler, 2010	The **PLS** algorithm may not converge when a model is misspecified. Occurrence of convergence can then be influenced by the chosen weighting scheme (the weighting scheme favours convergence) and the chosen starting values. Furthermore, convergence can be achieved if the misspecification is corrected. The author advises to choose a small convergence criterion (e.g. 0.00001) because the change of the outer weights can get very small and then grow again and (for example) converge to a non-zero constant value.

Table D.4: Simulation study results concerning non-convergence and improper solutions (from page 135 on).

Source	Study characteristics	Pros (+) and Cons (-)
Areskoug, 1982	ML and PLS, two latent variables, solely reflective operationalisation, one sample per case, variation of: number of items per construct (2-16), sample size (25-800). Examination of all coefficients (inner model and measurement models).	- Very simple model, only one sample per case, only reflective measurement models.
Boomsma, 1982	Factor analysis model (ML estimation), 300 samples per case, multivariate normal distribution, variation of: sample size (25-400), number of indicators per construct (3-4), loading pattern, correlation between the latent variables (0, 0.3). Examination of parameter estimates, standard errors, the goodness-of-fit statistic χ^2 and as a side product convergence frequency and rate of inadmissible solutions.	- Simple factor analysis model, solely ML.
Hui/Wold, 1982	PLS, two latent variables, solely reflective operationalisation, normally distributed indicators, variation of: number of items per construct (4-32), sample size (25-100). Examination of all coefficients (inner model and measurement models) and of all fitted values of the latent variables.	- Very simple model, number of replications unknown, only reflective measurement models, solely PLS.

Table D.5 continues on the next page.

Source	Study characteristics	Pros (+) and Cons (-)
Chou/Bentler, 1995	ML, confirmatory factor analysis, two correlated factors, three indicators per factor, sample size of 200, two different assumptions (all parameters are free or all six loadings are fixed), variation of: data distribution, standard errors (robust, not robust). Examination of accuracy, explicitly of all parameters, standard errors and the goodness-of-fit statistic χ^2.	- Only 100 replications per case, the results are not presented numerically, solely ML.
Cassel et al., 1999	PLS, four latent variables, formative and reflective operationalisation, $R^2 = 0.7$ in each partial model, error terms in measurement models are continuous uniform distributed, error term in inner model is normally distributed, 500 samples per case, variation of: sample size (50-1000), distribution of the exogenous indicators, degree of multicollinearity, different cases of misspecifications (missing variable in the inner model with either large or small coefficient). Examination of all coefficients (inner model and measurement models) and of the fitted values of the endogenous latent variable.	+ Incorporation of formative measurement models, detailed and systematic presentation of the results. - Only 500 samples per case, solely PLS.

Table D.5 continues on the next page.

Source	Study characteristics	Pros (+) and Cons (-)
Chin/Newsted, 1999	PLS, three latent variables, heterogeneous coefficients in each measurement model (i.e. one half of the indicators is good, one fourth is adequate and one fourth is useless), variation of: sample size (20-200), 100 samples per case, number of latent variables (2-16), number of items per construct (4-32). Examination of all coefficients (inner model and measurement models) and statistical power.	- Only 100 samples per case, solely reflective measurement models, solely PLS. Only Power was investigated without the type I error. The simulation results are only put into words, no tables are given.
Boomsma/ Hoogland, 2001, citing Boomsma, 1983, and Boomsma, 1985, and Hoogland, 1999	Different studies (original sources were partly not accessible), variation of: sample size (22-1,600), size of coefficients, correlation of latent variables, number of items per latent variable, number of latent variables. Examination of non-convergence and improper solutions.	- Partly not accessible (unpublished dissertation), only ML, solely reflective indicators.
Chin et al., 2003	PLS, four latent variables (one is an interaction variable), solely reflective operationalisation, 500 samples per case, variation of: size of coefficients (in the measurement models), sample size (20-500), number of items per construct (1-12), degree of measurement error (R^2 in the measurement models). Examination of coefficients in the inner model (accuracy and statistical power).	- Only reflective measurement models, only 500 samples per case, solely PLS. Only Power was investigated without the type I error. One table is missing to which the authors refer.

Table D.5 continues on the next page.

Source	Study characteristics	Pros (+) and Cons (-)
Reinartz et al., 2009	ML and PLS, six latent variables, solely reflective operationalisation, 200 samples per case, variation of: sample size (100-10,000), number of items per construct (2-8), data distribution, size of coefficients (in the measurement models) and their pattern (equal or different). Examination of convergence rate, parameter accuracy in the inner model and its drivers, statistical power.	+ Simulation of many cases, very systematically. - No formative measurement models, only 200 replications per case. Only Power was investigated without the type I error.
Ringle et al., 2009	ML and PLS, five latent variables, formative and reflective operationalisation, 1,000 samples per case, $n = 300$, variation of the data distribution. Examination of all coefficients (inner model and measurement models) with focus on the formative measurement models (i.e. correlation pattern of the formative indicators).	+ Incorporation of formative measurement models, detailed presentation of the results. - The interpretation of the results appears relatively pro PLS and contra ML.

Table D.5 continues on the next page.

Source	Study characteristics	Pros (+) and Cons (-)
Henseler, 2010	PLS, four latent variables but one is omitted (misspecification), the remaining three latent variables are operationalised by two indicators respectively, the error term in the inner model is normally distributed, 500 samples per case, variation of: sample size (20-500), weighting scheme and starting values. Examination of PLS convergence.	- Very simple model, only reflective measurement models, solely PLS, only 500 samples per case.

Table D.5: Design of simulation studies, sorted by date (from page 137 on).

Appendix E

OLS for SEM applying solely reflective indicators

In a model where all latent variables are specified reflective it is not possible to perform regressions with $\mathbf{x}$ as exogenous variables. An example for such kind of model is shown in figure 2.9 page 52. According to the model each y_q could get regressed on the two ξ variables, but the ξ variables are latent. One way to handle this case is to first estimate fitted values for the latent variables. This can be done applyiing the parameter estimates $\hat{\boldsymbol{\pi}}$.

In section 2.4.2 I showed how to estimate the λ coefficients applying the fitted values of the (reflective) endogenous indicators $\hat{y}$ (see equation 2.28 page 48). The case described here, however, is different since no fitted values for the dependent indicators (here $\mathbf{x}$) are available. Therefore, the observed $\mathbf{x}$ get applied. With uncorrelated error terms and $\text{var}(\hat{\xi}_1) = 1$ the relation is f.i.

$$\begin{aligned} \text{cov}(x_1, x_2) &= \text{cov}(\hat{\pi}_1\hat{\xi}_1 + \hat{\epsilon}_{x1},\ \hat{\pi}_2\hat{\xi}_1 + \hat{\epsilon}_{x2}) \\ &= \hat{\pi}_1\hat{\pi}_2 \underbrace{\text{var}(\hat{\xi}_1)}_{\overset{!}{=}1} \\ \hat{\pi}_2 &= \frac{\text{cov}(x_1, x_2)}{\hat{\pi}_1} \end{aligned} \tag{E.1}$$

With at least three indicators per latent variable ξ_g (for $g = 1, 2$) the corresponding $\hat{\pi}$ coefficients can get solved analogous to section 2.4.2 (page 48 et seqq.), but using the $\text{cov}(x_k, x_s)$ as in equation E.1.

Fitted values for the latent variable $\hat{\xi}_1$ can be estimated with the corresponding set of observed indicators $\mathbf{x}$ and estimated $\hat{\boldsymbol{\pi}}$ coefficients. The relationship between one indicator and its latent variable is

$$x_l = \pi_l \xi_1 + \epsilon_{xl}.$$

Usually in a linear regression both, the independent (x) and dependent variable (y) are observable. The estimated linear relation results as $y = \hat{\beta}x + \hat{\epsilon}$. The respective fitted values for y are $\hat{y} = \hat{\beta}x$ and lie on a line. Here, ξ is not observed, no fitted values for neither x_l (the dependent variable) nor ϵ_{xl} are available, but estimates $\hat{\pi}_l$ are available. Hence,the fitted values for the latent variable can only be estimated as

$$\hat{\xi}_g = \frac{1}{\hat{\pi}_l} x_l$$

(for x_l appertaining to ξ_g), which is not utterly accurate. Since one measurement model is composed of several indicators, all corresponding information gets incorporated by taking the mean over all sets of fitted values.

$$\hat{\xi}_1 = \frac{1}{5} \sum_{i=1}^{5} \frac{1}{\hat{\pi}_i} x_i \tag{E.2}$$

$$\hat{\xi}_2 = \frac{1}{3} \sum_{i=6}^{8} \frac{1}{\hat{\pi}_i} x_i \tag{E.3}$$

Equation E.2 and E.3 refer to the model shown in figure 2.9 page 52.
Each y_q can then be regressed on $\hat{\boldsymbol{\xi}}$. Analogous to the procedure described in section 2.4.2 the OLS parameters can be divided to obtain $\hat{\boldsymbol{\lambda}}$ and $\hat{\boldsymbol{\gamma}}$. The λ coefficients can moreover get estimated using again the covariances between the corresponding indicators ($\mathbf{y}$).

Appendix F

The error term distributions

In this passage the details regarding the error term distributions are described. In the A specifications the error term is not normally distributed, but either non-central chi-squared or continuous uniform distributed. This implementation is realised as follows.

A non-normal chi-squared distribution is specified by three parameters. These are

- n, the number of observations,
- df, the degrees of freedom and
- ncp, the non-centrality parameter.

The mean and variance of a non-central chi-squared distribution are

$$\mu = df + ncp$$

and

$$\sigma^2 = 2 \cdot (df + 2 \cdot ncp).$$

The shape of the distribution, i.e. the density, is defined by df and ncp. To get a highly skewed density I determine $df = 2.5$ and $ncp = 0.5$. This distribution has $\mu = 3.0$ and $\sigma^2 = 7$ (see figure F.1). From this distribution the error terms ζ^{prel} and $\varepsilon^{\text{prel}}$ are drawn (each with sample size n).[85] So far μ and σ^2 differ from the desired values. To render the mean equal to a value of zero

[85] In the data generation process I set different seeds for each drawing.

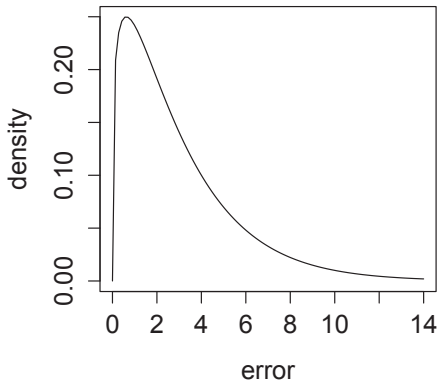

Figure F.1: The density of the applied chi-squared distribution.

and the variance equal to the value that corresponds with the respective R^2 an adjustment is necessary. The mean adjustment is simply done by subtracting the mean (3.0). For the variance adjustment first the desired variance needs to be determined. It can be computed in general as

$$\text{RSS} = \text{ESS}\left(\frac{1}{R^2} - 1\right)$$

with RSS standing for the residual variance and ESS standing for the explained variance. The mean and variance adjustment can be realised with

$$\varepsilon = \left(\varepsilon^{\text{prel}} - \mu\right) \cdot \sqrt{\frac{RSS^{\text{rMM}}}{\sigma^2}}$$

(ε appertains to the reflective measurement model and is used as an example).

The drawing for the uniform distributed error term works like the following. Again three parameters need to be set:

- n, the number of observations,
- the minimum min and
- the maximum max.

It is

$$\mu = \frac{1}{2} \cdot (min + max)$$

and

$$\sigma^2 = \frac{1}{12}(max - min)^2.$$

Setting $max = -min$ leads to a mean equal to zero. In order to obtain a variance which corresponds with the defined R^2 the maximum ought to be

$$max = \frac{\sqrt{12 \cdot RSS}}{2}.$$

With the determined parameters the samples can get drawn from the respective distribution.

Appendix G

Total Effect Coefficients

The total effect coefficients result as $\mathbf{TE_{xy}} = \boldsymbol{\pi}^{\text{true}}\boldsymbol{\gamma}^{\text{true}}\boldsymbol{\lambda}'$. The population values are shown in table G.1.

	y_1	y_2	y_3	per x_l
x_1	0.26289	0.18402	0.23660	0.22784
x_2	0.16431	0.11501	0.14788	0.14240
x_3	0.26289	0.18402	0.23660	0.22784
x_4	0.19717	0.13802	0.17745	0.17088
x_5	0.13144	0.09201	0.11830	0.11392
x_6	0.37238	0.26066	0.33514	0.32273
x_7	0.24825	0.17378	0.22343	0.21515
x_8	0.31031	0.21722	0.27928	0.26894
per y_q	0.24370	0.17059	0.21933	

Table G.1: The total effect population parameters.

These values are valid for the basic model and variations A, B and C.

Appendix H

Individual simulation study results

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.39500	0.38856	0.33620	0.38037	-0.00644	-0.05880	-0.01462	0.11823	0.13182	0.11692
π_2	0.24687	0.24077	0.35030	0.23568	-0.00610	0.10343	-0.01119	0.11706	0.15085	0.11481
π_3	0.39500	0.38665	0.29336	0.37922	-0.00834	-0.10163	-0.01577	0.11968	0.15645	0.11772
π_4	0.29625	0.28872	0.23163	0.28295	-0.00752	-0.06462	-0.01329	0.12446	0.13741	0.12219
π_5	0.19750	0.19223	0.33515	0.18819	-0.00527	0.13765	-0.00930	0.12143	0.17763	0.11884
π_6	0.55950	0.55347	0.54486	0.54775	-0.00604	-0.01464	-0.01175	0.10865	0.10790	0.10803
π_7	0.37300	0.36969	0.35506	0.36597	-0.00331	-0.01794	-0.00703	0.11401	0.11454	0.11298
π_8	0.46625	0.46178	0.48401	0.45652	-0.00448	0.01776	-0.00974	0.11060	0.11021	0.10981
γ_1	0.66555	0.66928	0.57411	0.67248	0.00373	-0.09144	0.00693	0.06019	0.11047	0.05854
γ_2	0.66555	0.66290	0.55203	0.65974	-0.00265	-0.11351	-0.00581	0.06339	0.12862	0.06196
λ_1	1.00000	1.01846	1.22801	1.02378	0.01846	0.22801	0.02378	0.10403	0.23965	0.10885
λ_2	0.70000	0.71298	0.72623	0.71639	0.01298	0.02623	0.01639	0.07302	0.06078	0.07608
λ_3	0.90000	0.91649	1.04114	0.92025	0.01649	0.14114	0.02025	0.09480	0.15805	0.09894

Table H.1: Individual simulation study results for the basic model.

	md			***rmse***		
	centroid	factorial	path	centroid	factorial	path
missing results	0	0	0			
$\pi_1 - \pi_5$	0.09322	0.09322	0.09322	0.15083	0.15083	0.15083
$\pi_6 - \pi_8$	0.01678	0.01678	0.01678	0.11088	0.11088	0.11089
γ_1, γ_2	0.10248	0.10250	0.10251	0.11954	0.11963	0.11967
$\lambda_1 - \lambda_3$	0.13180	0.13179	0.13178	0.14678	0.14681	0.14683
TE per y_1	0.04097	0.04097	0.04097	0.09852	0.09854	0.09855
TE per y_2	0.04011	0.04012	0.04013	0.06495	0.06496	0.06497
TE per y_3	0.03994	0.03995	0.03995	0.08518	0.08519	0.08520
prediction $y_1 - y_3$	0.00029	0.00029	0.00029	1.49572	1.49572	1.49572

Table H.2: Simulation study results for PLS applying different inner schemes (for the basic model).

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.39500	0.40611	0.30184	0.29157	0.01112	-0.09316	-0.10342	0.21832	0.27287	0.25441
π_2	0.24687	0.19392	0.31817	0.17673	-0.05295	0.07130	-0.07014	0.27148	0.25045	0.23821
π_3	0.39500	0.32585	0.26020	0.28893	-0.06915	-0.13480	-0.10607	0.27903	0.28994	0.25430
π_4	0.29625	0.22814	0.20551	0.21363	-0.06811	-0.09073	-0.08262	0.28900	0.27895	0.25507
π_5	0.19750	0.15809	0.30364	0.14008	-0.03941	0.10615	-0.05741	0.27840	0.26526	0.24130
π_6	0.55950	0.53885	0.51117	0.45849	-0.02066	-0.04833	-0.10101	0.23395	0.24594	0.26207
π_7	0.37300	0.33355	0.33400	0.30734	-0.03946	-0.03900	-0.06567	0.27972	0.25890	0.25959
π_8	0.46625	0.41397	0.45630	0.38133	-0.05228	-0.00996	-0.08493	0.27412	0.24761	0.26207
γ_1	0.66555	0.69069	0.49474	0.70994	0.02514	-0.17081	0.04439	0.12031	0.20507	0.10307
γ_2	0.66555	0.64469	0.45248	0.63078	-0.02086	-0.21307	-0.03477	0.13428	0.24151	0.11278
λ_1	1.00000	1.12504	1.74367	1.16397	0.12504	0.74367	0.16397	0.29646	0.78226	0.34273
λ_2	0.70000	0.78979	0.80283	0.81554	0.08979	0.10283	0.11554	0.20950	0.18810	0.43433
λ_3	0.90000	1.01440	1.36060	1.04319	0.11440	0.46060	0.14319	0.27070	0.52088	0.30334

Table H.3: Individual simulation study results for variation A.

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.39500	0.38729	0.33444	0.37888	-0.00771	-0.06055	-0.01612	0.11794	0.13145	0.11694
π_2	0.24687	0.23947	0.34906	0.23453	-0.00740	0.10219	-0.01234	0.11873	0.15125	0.11675
π_3	0.39500	0.38712	0.29441	0.37972	-0.00787	-0.10058	-0.01528	0.11950	0.15520	0.11793
π_4	0.29625	0.29094	0.23391	0.28565	-0.00530	-0.06234	-0.01060	0.12399	0.13761	0.12192
π_5	0.19750	0.19205	0.33471	0.18800	-0.00545	0.13721	-0.00950	0.11825	0.17605	0.11632
π_6	0.55950	0.55558	0.54684	0.55001	-0.00392	-0.01266	-0.00949	0.10844	0.10875	0.10786
π_7	0.37300	0.36892	0.35406	0.36479	-0.00408	-0.01894	-0.00821	0.11223	0.11426	0.11136
π_8	0.46625	0.46047	0.48288	0.45532	-0.00579	0.01663	-0.01093	0.11181	0.11052	0.11138
γ_1	0.66555	0.67087	0.57545	0.67398	0.00532	-0.09010	0.00843	0.06095	0.11049	0.05929
γ_2	0.66555	0.66132	0.55086	0.65824	-0.00423	-0.11469	-0.00731	0.06394	0.13058	0.06255
λ_1	1.00000	1.01779	1.22775	1.02200	0.01779	0.22775	0.02200	0.10593	0.24342	0.11044
λ_2	0.70000	0.71177	0.72500	0.71566	0.01177	0.02500	0.01566	0.07318	0.06572	0.07690
λ_3	0.90000	0.91671	1.04161	0.92085	0.01671	0.14161	0.02085	0.09477	0.16210	0.09890

Table H.4: Individual simulation study results for variation B1.

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.39500	0.38886	0.33608	0.38031	-0.00613	-0.05892	-0.01469	0.11675	0.13004	0.11601
π_2	0.24687	0.24071	0.35016	0.23581	-0.00616	0.10329	-0.01107	0.11977	0.15195	0.11749
π_3	0.39500	0.38393	0.29117	0.37659	-0.01107	-0.10383	-0.01840	0.12008	0.15800	0.11820
π_4	0.29625	0.29077	0.23307	0.28513	-0.00547	-0.06317	-0.01111	0.12201	0.13626	0.11973
π_5	0.19750	0.19389	0.33669	0.18979	-0.00361	0.13919	-0.00771	0.11642	0.17653	0.11398
π_6	0.55950	0.55416	0.54586	0.54843	-0.00535	-0.01364	-0.01107	0.10666	0.10711	0.10581
π_7	0.37300	0.36942	0.35415	0.36523	-0.00358	-0.01886	-0.00777	0.11168	0.11340	0.11048
π_8	0.46625	0.46171	0.48396	0.45673	-0.00454	0.01771	-0.00953	0.10966	0.10950	0.10867
γ_1	0.66555	0.66934	0.57317	0.67258	0.00379	-0.09238	0.00703	0.06141	0.11146	0.05956
γ_2	0.66555	0.66228	0.55058	0.65912	-0.00327	-0.11497	-0.00643	0.06479	0.13026	0.06333
λ_1	1.00000	1.01644	1.22762	1.02105	0.01644	0.22762	0.02105	0.10356	0.23843	0.10865
λ_2	0.70000	0.71101	0.72497	0.71452	0.01101	0.02497	0.01452	0.07297	0.05896	0.07642
λ_3	0.90000	0.91508	1.04117	0.91904	0.01508	0.14117	0.01904	0.09427	0.15639	0.09848

Table H.5: Individual simulation study results for variation B2.

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.39500	0.40259	0.29833	0.28834	0.00760	-0.09667	-0.10666	0.21502	0.27126	0.25419
π_2	0.24687	0.19367	0.31512	0.17669	-0.05320	0.06824	-0.07018	0.27531	0.25125	0.24104
π_3	0.39500	0.32769	0.26287	0.29095	-0.06731	-0.13212	-0.10405	0.27695	0.28919	0.25616
π_4	0.29625	0.23515	0.20983	0.21985	-0.06110	-0.08642	-0.07640	0.28492	0.27831	0.25209
π_5	0.19750	0.15777	0.30391	0.14152	-0.03973	0.10641	-0.05598	0.26920	0.26127	0.23565
π_6	0.55950	0.54163	0.51462	0.46199	-0.01788	-0.04488	-0.09752	0.23109	0.24791	0.26126
π_7	0.37300	0.33194	0.33258	0.30436	-0.04106	-0.04042	-0.06864	0.27521	0.25852	0.25852
π_8	0.46625	0.41454	0.45408	0.37871	-0.05171	-0.01217	-0.08754	0.27406	0.24651	0.26413
γ_1	0.66555	0.69269	0.49629	0.71160	0.02714	-0.16926	0.04605	0.12410	0.20586	0.10545
γ_2	0.66555	0.64106	0.44938	0.62782	-0.02449	-0.21617	-0.03773	0.13754	0.24563	0.11588
λ_1	1.00000	1.12345	1.73789	1.15675	0.12345	0.73789	0.15675	0.29956	0.78598	0.32880
λ_2	0.70000	0.78487	0.80091	0.81347	0.08487	0.10091	0.11347	0.20823	0.19480	0.32891
λ_3	0.90000	1.01267	1.36597	1.04579	0.11267	0.46597	0.14579	0.26947	0.53228	0.29664

Table H.6: Individual simulation study results for variation AB1.

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.39500	0.40712	0.30295	0.29115	0.01213	-0.09205	-0.10384	0.21389	0.26941	0.25375
π_2	0.24687	0.19056	0.31749	0.17642	-0.05631	0.07062	-0.07045	0.27765	0.25302	0.24290
π_3	0.39500	0.31783	0.25398	0.28384	-0.07716	-0.14102	-0.11116	0.28084	0.29426	0.25761
π_4	0.29625	0.23703	0.20901	0.21814	-0.05922	-0.08724	-0.07810	0.28589	0.27704	0.25056
π_5	0.19750	0.16285	0.30820	0.14355	-0.03465	0.11070	-0.05395	0.27050	0.25956	0.23225
π_6	0.55950	0.54003	0.51421	0.45881	-0.01947	-0.04529	-0.10069	0.23015	0.24465	0.25893
π_7	0.37300	0.33248	0.33283	0.30440	-0.04052	-0.04018	-0.06860	0.27697	0.25664	0.25594
π_8	0.46625	0.41452	0.45563	0.37916	-0.05174	-0.01062	-0.08709	0.27510	0.24399	0.26057
γ_1	0.66555	0.69067	0.49296	0.71071	0.02512	-0.17259	0.04516	0.12511	0.20764	0.10519
γ_2	0.66555	0.64245	0.44821	0.62870	-0.02310	-0.21734	-0.03685	0.13967	0.24631	0.11630
λ_1	1.00000	1.12095	1.74117	1.15436	0.12095	0.74117	0.15436	0.29577	0.77918	0.32652
λ_2	0.70000	0.78310	0.80076	0.80737	0.08310	0.10076	0.10737	0.20846	0.18482	0.22962
λ_3	0.90000	1.00829	1.36321	1.04140	0.10829	0.46321	0.14140	0.26829	0.51952	0.32134

Table H.7: Individual simulation study results for variation AB2.

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.39500	0.54401	0.23404	0.17996	0.14902	-0.16096	-0.21504	0.39879	0.55763	0.49420
π_2	0.24687	0.08277	0.24812	0.12338	-0.16411	0.00125	-0.12349	0.57382	0.51577	0.45125
π_3	0.39500	0.17346	0.19490	0.18164	-0.22153	-0.20010	-0.21336	0.60201	0.57938	0.50353
π_4	0.29625	0.07681	0.17172	0.14781	-0.21944	-0.12453	-0.14844	0.61140	0.56974	0.47819
π_5	0.19750	0.08456	0.23266	0.08839	-0.11293	0.03516	-0.10911	0.56532	0.51090	0.44170
π_6	0.55950	0.66127	0.43584	0.29137	0.10177	-0.12366	-0.26813	0.38429	0.55451	0.54788
π_7	0.37300	0.16563	0.29265	0.19335	-0.20738	-0.08035	-0.17965	0.63202	0.53956	0.50540
π_8	0.46625	0.18301	0.39818	0.24480	-0.28324	-0.06807	-0.22145	0.67106	0.54156	0.52960
γ_1	0.66555	0.76602	0.70187	0.88259	0.10047	0.03632	0.21704	0.42288	0.42500	0.28205
γ_2	0.66555	0.66447	0.49286	0.76053	-0.00108	-0.17269	0.09498	0.42895	0.39203	0.23059
λ_1	1.00000	1.26752	1.14556	1.42488	0.26752	0.14556	0.42488	0.60009	0.40936	0.73834
λ_2	0.70000	0.87496	0.66885	0.98953	0.17496	-0.03115	0.28953	0.43723	0.26320	0.44531
λ_3	0.90000	1.12297	0.96120	1.27766	0.22297	0.06120	0.37766	0.57180	0.35591	0.74644

Table H.8: Individual simulation study results for variation C1.

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.39500	0.41798	0.29964	0.30571	0.02298	-0.09535	-0.08928	0.23208	0.30283	0.27618
π_2	0.24687	0.19049	0.31492	0.18800	-0.05638	0.06805	-0.05888	0.29384	0.27881	0.26422
π_3	0.39500	0.32738	0.25966	0.30727	-0.06761	-0.13534	-0.08772	0.30346	0.32190	0.28024
π_4	0.29625	0.23210	0.21111	0.23170	-0.06414	-0.08514	-0.06455	0.30882	0.30828	0.27770
π_5	0.19750	0.16336	0.30563	0.15569	-0.03414	0.10813	-0.04180	0.29348	0.29134	0.26258
π_6	0.55950	0.55881	0.51586	0.47857	-0.00070	-0.04364	-0.08093	0.24989	0.28275	0.28472
π_7	0.37300	0.33055	0.33240	0.31803	-0.04245	-0.04060	-0.05497	0.30410	0.29009	0.28077
π_8	0.46625	0.41423	0.46313	0.40080	-0.05202	-0.00312	-0.06545	0.30467	0.28191	0.28609
γ_1	0.66555	0.70020	0.62964	0.71565	0.03465	-0.03591	0.05010	0.14198	0.15387	0.12253
γ_2	0.66555	0.64877	0.55296	0.64195	-0.01678	-0.11259	-0.02360	0.15099	0.19018	0.12978
λ_1	1.00000	1.10656	1.21020	1.12766	0.10656	0.21020	0.12766	0.28455	0.28220	0.28642
λ_2	0.70000	0.77247	0.71152	0.78883	0.07247	0.01152	0.08883	0.19725	0.13855	0.19823
λ_3	0.90000	0.99399	1.02385	1.01408	0.09399	0.12385	0.11408	0.25405	0.21552	0.25668

Table H.9: Individual simulation study results for variation C2.

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.39500	0.39275	0.33940	0.39041	-0.00225	-0.05560	-0.00458	0.06401	0.08436	0.06360
π_2	0.24687	0.24521	0.35476	0.24368	-0.00166	0.10789	-0.00319	0.06463	0.12408	0.06427
π_3	0.39500	0.39200	0.29780	0.38964	-0.00299	-0.09720	-0.00535	0.06577	0.11735	0.06549
π_4	0.29625	0.29436	0.23632	0.29256	-0.00189	-0.05993	-0.00369	0.06709	0.08940	0.06678
π_5	0.19750	0.19611	0.34022	0.19484	-0.00139	0.14272	-0.00266	0.06540	0.15491	0.06507
π_6	0.55950	0.55715	0.54772	0.55546	-0.00235	-0.01179	-0.00405	0.05853	0.05962	0.05830
π_7	0.37300	0.37157	0.35754	0.37044	-0.00143	-0.01546	-0.00256	0.06164	0.06378	0.06144
π_8	0.46625	0.46580	0.48797	0.46431	-0.00045	0.02172	-0.00195	0.06015	0.06305	0.05998
γ_1	0.66555	0.66693	0.56679	0.66789	0.00138	-0.09876	0.00234	0.03405	0.10464	0.03376
γ_2	0.66555	0.66433	0.54947	0.66333	-0.00122	-0.11608	-0.00222	0.03539	0.12091	0.03515
λ_1	1.00000	1.00578	1.23053	1.00714	0.00578	0.23053	0.00714	0.05636	0.23403	0.05950
λ_2	0.70000	0.70384	0.72785	0.70492	0.00384	0.02785	0.00492	0.03972	0.04111	0.04159
λ_3	0.90000	0.90499	1.04347	0.90622	0.00499	0.14347	0.00622	0.05130	0.14858	0.05375

Table H.10: Individual simulation study results for variation C3.

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.55874	0.51117	0.47607	0.44605	-0.04757	-0.08268	-0.11270	0.21770	0.27132	0.24162
π_2	0.34922	0.30180	0.29767	0.27756	-0.04741	-0.05154	-0.07166	0.25523	0.27845	0.23693
π_3	0.55874	0.48779	0.47327	0.44680	-0.07095	-0.08548	-0.11195	0.24855	0.27295	0.24269
π_4	0.41906	0.36738	0.35997	0.33648	-0.05168	-0.05909	-0.08258	0.25669	0.27799	0.23899
π_5	0.27937	0.24746	0.24088	0.22727	-0.03191	-0.03850	-0.05210	0.26205	0.28177	0.23817
π_6	0.68376	0.64990	0.63131	0.59928	-0.03387	-0.05245	-0.08448	0.22225	0.25756	0.23614
π_7	0.45584	0.42209	0.41738	0.39876	-0.03375	-0.03846	-0.05709	0.27070	0.28542	0.24972
π_8	0.56980	0.53549	0.53021	0.50367	-0.03431	-0.03959	-0.06613	0.25583	0.27378	0.24323
γ_1	0.70711	0.73161	0.64459	0.73936	0.02450	-0.06252	0.03226	0.13338	0.18981	0.11470
γ_2	0.70711	0.68035	0.58821	0.66959	-0.02676	-0.11889	-0.03752	0.14496	0.20283	0.12800
λ_1	1.00000	1.10140	1.21073	1.12772	0.10140	0.21073	0.12772	0.28288	0.28291	0.28658
λ_2	0.70000	0.76951	0.71073	0.78872	0.06951	0.01073	0.08872	0.19569	0.13882	0.19787
λ_3	0.90000	0.99018	1.02347	1.01424	0.09018	0.12347	0.11424	0.25254	0.21625	0.25692

Table H.11: Individual simulation study results for variation D1.

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.39509	0.38210	0.37625	0.34968	-0.01299	-0.01884	-0.04541	0.08917	0.10290	0.09396
π_2	0.24693	0.23769	0.23378	0.21781	-0.00924	-0.01315	-0.02912	0.09212	0.10712	0.08907
π_3	0.39509	0.38011	0.37545	0.34640	-0.01498	-0.01964	-0.04869	0.08894	0.10285	0.09205
π_4	0.29632	0.28654	0.28250	0.26013	-0.00978	-0.01382	-0.03619	0.09237	0.10614	0.08933
π_5	0.19755	0.19092	0.18728	0.17498	-0.00663	-0.01026	-0.02257	0.09361	0.10816	0.08869
π_6	0.39509	0.38236	0.37735	0.35036	-0.01273	-0.01774	-0.04473	0.08886	0.10249	0.09289
π_7	0.24693	0.23782	0.23499	0.21793	-0.00911	-0.01195	-0.02900	0.09175	0.10581	0.08900
π_8	0.39509	0.38043	0.37447	0.34871	-0.01466	-0.02063	-0.04638	0.09008	0.10459	0.09469
π_9	0.29632	0.28497	0.28205	0.26118	-0.01135	-0.01427	-0.03514	0.09120	0.10520	0.09060
π_{10}	0.19755	0.19025	0.18777	0.17440	-0.00730	-0.00978	-0.02315	0.09258	0.10695	0.08780
π_{11}	0.48349	0.47508	0.47039	0.43917	-0.00841	-0.01310	-0.04432	0.08750	0.10125	0.09385
π_{12}	0.32233	0.31499	0.31188	0.29135	-0.00734	-0.01045	-0.03098	0.09205	0.10555	0.09107
π_{13}	0.40291	0.39450	0.39219	0.36188	-0.00841	-0.01072	-0.04103	0.08956	0.10317	0.08899
π_{14}	0.48349	0.47486	0.47140	0.43910	-0.00863	-0.01209	-0.04439	0.08807	0.10138	0.09507
π_{15}	0.32233	0.31654	0.31358	0.29059	-0.00579	-0.00874	-0.03174	0.09149	0.10489	0.08845
π_{16}	0.40291	0.39587	0.39371	0.36597	-0.00704	-0.00920	-0.03694	0.09032	0.10378	0.09252
γ_1	0.70711	0.71281	0.65973	0.75134	0.00570	-0.04738	0.04423	0.05349	0.07418	0.06955
γ_2	0.70711	0.70063	0.64359	0.73569	-0.00648	-0.06352	0.02859	0.05505	0.08573	0.06421
λ_1	1.00000	1.03174	1.11869	1.04833	0.03174	0.11869	0.04833	0.10202	0.14050	0.11639
λ_2	0.70000	0.72104	0.70989	0.73238	0.02104	0.00989	0.03238	0.07126	0.05369	0.08075
λ_3	0.90000	0.92803	0.97154	0.94273	0.02803	0.07154	0.04273	0.09150	0.09860	0.10437
λ_4	1.00000	1.03086	1.11764	1.04718	0.03086	0.11764	0.04718	0.10098	0.13968	0.11602
λ_5	0.70000	0.72190	0.71065	0.73388	0.02190	0.01065	0.03388	0.07155	0.05357	0.08195
λ_6	0.90000	0.92649	0.96998	0.94210	0.02649	0.06998	0.04210	0.09058	0.09723	0.10357

Table H.12: Individual simulation study results for variation D2.

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.27937	0.27407	0.27153	0.26542	-0.00530	-0.00784	-0.01395	0.04678	0.05550	0.04708
π_2	0.17461	0.17058	0.16906	0.16515	-0.00403	-0.00555	-0.00945	0.04797	0.05705	0.04721
π_3	0.27937	0.27400	0.27154	0.26532	-0.00537	-0.00783	-0.01405	0.04655	0.05527	0.04689
π_4	0.20953	0.20497	0.20317	0.19850	-0.00455	-0.00636	-0.01103	0.04749	0.05651	0.04707
π_5	0.13969	0.13628	0.13526	0.13198	-0.00340	-0.00442	-0.00771	0.04831	0.05690	0.04728
π_6	0.27937	0.27349	0.27120	0.26483	-0.00589	-0.00817	-0.01454	0.04751	0.05641	0.04786
π_7	0.17461	0.17038	0.16921	0.16500	-0.00423	-0.00539	-0.00961	0.04794	0.05664	0.04723
π_8	0.27937	0.27400	0.27101	0.26533	-0.00538	-0.00836	-0.01404	0.04754	0.05649	0.04777
π_9	0.20953	0.20607	0.20394	0.19953	-0.00346	-0.00559	-0.01000	0.04786	0.05647	0.04728
π_{10}	0.13969	0.13600	0.13458	0.13169	-0.00369	-0.00511	-0.00800	0.04851	0.05702	0.04752
π_{11}	0.27937	0.27299	0.27085	0.26433	-0.00638	-0.00853	-0.01504	0.04756	0.05613	0.04805
π_{12}	0.17461	0.17084	0.16967	0.16543	-0.00377	-0.00494	-0.00918	0.04789	0.05633	0.04705
π_{13}	0.27937	0.27378	0.27137	0.26511	-0.00559	-0.00801	-0.01426	0.04658	0.05554	0.04697
π_{14}	0.20953	0.20545	0.20322	0.19903	-0.00408	-0.00631	-0.01049	0.04770	0.05676	0.04735
π_{15}	0.13969	0.13639	0.13531	0.13202	-0.00330	-0.00437	-0.00767	0.04795	0.05677	0.04686
π_{16}	0.27937	0.27345	0.27066	0.26480	-0.00592	-0.00871	-0.01457	0.04694	0.05616	0.04735
π_{17}	0.17461	0.17099	0.16909	0.16555	-0.00362	-0.00551	-0.00906	0.04817	0.05683	0.04733
π_{18}	0.27937	0.27385	0.27150	0.26518	-0.00552	-0.00787	-0.01419	0.04693	0.05560	0.04730
π_{19}	0.20953	0.20452	0.20280	0.19805	-0.00501	-0.00672	-0.01148	0.04783	0.05617	0.04743
π_{20}	0.13969	0.13687	0.13586	0.13253	-0.00282	-0.00382	-0.00716	0.04778	0.05570	0.04672
π_{21}	0.34188	0.33791	0.33633	0.33124	-0.00397	-0.00555	-0.01064	0.04698	0.05512	0.04708
π_{22}	0.22792	0.22517	0.22391	0.22070	-0.00276	-0.00401	-0.00722	0.04766	0.05594	0.04720
π_{23}	0.28490	0.28097	0.27935	0.27542	-0.00393	-0.00555	-0.00948	0.04760	0.05624	0.04744
π_{24}	0.34188	0.33855	0.33664	0.33185	-0.00333	-0.00525	-0.01003	0.04676	0.05507	0.04675
π_{25}	0.22792	0.22532	0.22434	0.22088	-0.00260	-0.00358	-0.00704	0.04753	0.05652	0.04703
π_{26}	0.28490	0.28095	0.27937	0.27541	-0.00395	-0.00553	-0.00949	0.04765	0.05574	0.04751
π_{27}	0.34188	0.33789	0.33556	0.33124	-0.00399	-0.00632	-0.01064	0.04647	0.05525	0.04657
π_{28}	0.22792	0.22520	0.22468	0.22073	-0.00272	-0.00324	-0.00719	0.04753	0.05635	0.04706
π_{29}	0.28490	0.28174	0.28106	0.27616	-0.00316	-0.00384	-0.00874	0.04769	0.05607	0.04741
π_{30}	0.34188	0.33807	0.33606	0.33142	-0.00381	-0.00582	-0.01046	0.04658	0.05480	0.04666
π_{31}	0.22792	0.22451	0.22305	0.22009	-0.00342	-0.00487	-0.00783	0.04764	0.05658	0.04721
π_{32}	0.28490	0.28106	0.27965	0.27550	-0.00384	-0.00525	-0.00940	0.04704	0.05513	0.04685
γ_1	0.70711	0.70970	0.67934	0.71336	0.00260	-0.02777	0.00625	0.02806	0.04104	0.02716
γ_2	0.70711	0.70421	0.67103	0.69926	-0.00289	-0.03608	-0.00785	0.02872	0.04722	0.02838
λ_1	1.00000	1.01681	1.06072	1.02979	0.01681	0.06072	0.02979	0.05443	0.07290	0.06586
λ_2	0.70000	0.71255	0.70603	0.72140	0.01255	0.00603	0.02140	0.03800	0.02828	0.04610
λ_3	0.90000	0.91562	0.93728	0.92666	0.01562	0.03728	0.02666	0.04883	0.05200	0.05865
λ_4	1.00000	1.01716	1.06107	1.03015	0.01716	0.06107	0.03015	0.05442	0.07319	0.06598
λ_5	0.70000	0.71219	0.70567	0.72127	0.01219	0.00567	0.02127	0.03827	0.02868	0.04652
λ_6	0.90000	0.91620	0.93787	0.92784	0.01620	0.03787	0.02784	0.04939	0.05257	0.06004
λ_7	1.00000	1.01734	1.06126	1.03016	0.01734	0.06126	0.03016	0.05423	0.07317	0.06581
λ_8	0.70000	0.71232	0.70583	0.72136	0.01232	0.00583	0.02136	0.03827	0.02871	0.04605
λ_9	0.90000	0.91602	0.93770	0.92777	0.01602	0.03770	0.02777	0.04877	0.05192	0.05936
λ_{10}	1.00000	1.01781	1.06173	1.03056	0.01781	0.06173	0.03056	0.05413	0.07355	0.06571
λ_{11}	0.70000	0.71214	0.70563	0.72096	0.01214	0.00563	0.02096	0.03842	0.02883	0.04638
λ_{12}	0.90000	0.91577	0.93745	0.92763	0.01577	0.03745	0.02763	0.04929	0.05219	0.05952

Table H.13: Individual simulation study results for variation D3.

		mean			*md*			*rmse*		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.55874	0.54958	0.54622	0.53994	-0.00916	-0.01253	-0.01880	0.09214	0.10468	0.09172
π_2	0.34922	0.34263	0.34101	0.33642	-0.00659	-0.00821	-0.01280	0.09906	0.11287	0.09764
π_3	0.55874	0.54843	0.54445	0.53885	-0.01032	-0.01430	-0.01989	0.09162	0.10427	0.09138
π_4	0.41906	0.41046	0.40723	0.40310	-0.00860	-0.01183	-0.01595	0.09919	0.11214	0.09813
π_5	0.27937	0.27392	0.27089	0.26908	-0.00545	-0.00848	-0.01030	0.10509	0.12010	0.10326
π_6	0.68376	0.67754	0.67576	0.67130	-0.00622	-0.00801	-0.01246	0.08454	0.09457	0.08445
π_7	0.45584	0.45244	0.45008	0.44839	-0.00340	-0.00576	-0.00745	0.09840	0.11184	0.09767
π_8	0.56980	0.56540	0.56340	0.56011	-0.00441	-0.00641	-0.00970	0.09130	0.10400	0.09076
γ_1	0.70711	0.70883	0.61343	0.71048	0.00173	-0.09368	0.00337	0.05838	0.11101	0.05666
γ_2	0.70711	0.70301	0.60600	0.69872	-0.00410	-0.10110	-0.00838	0.05900	0.11730	0.05804
λ_1	1.00000	1.01860	1.22824	1.02391	0.01860	0.22824	0.02391	0.10391	0.23984	0.10878
λ_2	0.70000	0.71296	0.72609	0.71640	0.01296	0.02609	0.01640	0.07302	0.06075	0.07606
λ_3	0.90000	0.91657	1.04113	0.92034	0.01657	0.14113	0.02034	0.09470	0.15798	0.09876

Table H.14: Individual simulation study results for variation E1.

		mean			*md*			*rmse*		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.27372	0.63947	0.36047	0.24863	0.36575	0.08675	-0.02510	0.55412	0.39856	0.59415
π_2	0.17108	-0.07995	0.10791	0.16771	-0.25103	-0.06316	-0.00337	0.44325	0.25275	0.44117
π_3	0.27372	0.41607	0.04367	0.26974	0.14235	-0.23005	-0.00398	0.66208	0.54240	0.65472
π_4	0.20529	0.01890	0.18692	0.18350	-0.18639	-0.01837	-0.02179	0.48721	0.38752	0.50079
π_5	0.13686	0.01921	0.34021	0.11241	-0.11765	0.20335	-0.02445	0.59151	0.47513	0.58008
π_6	0.41092	0.70586	0.33580	0.40054	0.29494	-0.07512	-0.01038	0.52094	0.33359	0.55364
π_7	0.27395	0.32243	0.17871	0.27256	0.04848	-0.09524	-0.00139	0.36277	0.25331	0.35680
π_8	0.34243	-0.02609	0.50300	0.30400	-0.36852	0.16057	-0.03843	0.66396	0.35974	0.64987
γ_1	0.58460	0.60509	0.51174	0.61083	0.02049	-0.07286	0.02624	0.07654	0.10089	0.07526
γ_2	0.58460	0.58499	0.49846	0.59705	0.00039	-0.08614	0.01245	0.07286	0.11096	0.07372
λ_1	1.00000	1.01881	1.22786	1.02367	0.01881	0.22786	0.02367	0.10379	0.23951	0.10889
λ_2	0.70000	0.71415	0.72633	0.71631	0.01415	0.02633	0.01631	0.07323	0.06077	0.07610
λ_3	0.90000	0.91615	1.04110	0.92008	0.01615	0.14110	0.02008	0.09473	0.15802	0.09918

Table H.15: Individual simulation study results for variation E2.

		mean			***md***			***rmse***		
	true	ML	PLS	OLS	ML	PLS	OLS	ML	PLS	OLS
π_1	0.39500	0.38123	0.33410	0.37342	-0.01376	-0.06089	-0.02157	0.11023	0.12612	0.10984
π_2	0.24687	0.23708	0.33449	0.23224	-0.00980	0.08762	-0.01464	0.11013	0.13630	0.10819
π_3	0.39500	0.37966	0.29731	0.37257	-0.01534	-0.09768	-0.02243	0.11171	0.14822	0.11052
π_4	0.29625	0.28382	0.23293	0.27836	-0.01242	-0.06332	-0.01789	0.11602	0.13072	0.11437
π_5	0.19750	0.18902	0.31750	0.18537	-0.00848	0.12000	-0.01213	0.11397	0.16062	0.11173
π_6	0.55950	0.53972	0.53198	0.53440	-0.01978	-0.02752	-0.02510	0.10219	0.10355	0.10239
π_7	0.37300	0.36062	0.34741	0.35716	-0.01238	-0.02559	-0.01584	0.10660	0.10929	0.10609
π_8	0.46625	0.45064	0.47046	0.44593	-0.01562	0.00421	-0.02032	0.10407	0.10215	0.10398
γ_1	0.66555	0.66851	0.58073	0.67165	0.00296	-0.08481	0.00610	0.05926	0.10477	0.05769
γ_2	0.66555	0.66696	0.56478	0.66371	0.00141	-0.10077	-0.00184	0.06170	0.11717	0.06020
λ_1	1.00000	1.03813	1.23615	1.04330	0.03813	0.23615	0.04330	0.11005	0.24741	0.11533
λ_2	0.70000	0.72678	0.73296	0.73016	0.02678	0.03296	0.03016	0.07716	0.06407	0.08056
λ_3	0.90000	0.93411	1.04889	0.93773	0.03411	0.14889	0.03773	0.10007	0.16495	0.10459

Table H.16: Individual simulation study results for variation F.

		mean		***md***		***rmse***	
	true	ML	PLS	ML	PLS	ML	PLS
(missing results)		(0.00100)	(0)				
π_1	0.39500	0.38375	0.33130	-0.01125	-0.06370	0.11665	0.13236
π_2	0.24687	0.24178	0.34937	-0.00509	0.10250	0.12051	0.15242
π_3	0.39500	0.38532	0.29359	-0.00968	-0.10141	0.12092	0.15643
π_4	0.29625	0.28588	0.22885	-0.01036	-0.06740	0.12415	0.14053
π_5	0.19750	0.19139	0.33470	-0.00611	0.13720	0.11899	0.17634
π_6	0.00000	0.00023	-0.00080	0.00023	-0.00080	0.11874	0.11524
π_7	0.55950	0.55140	0.53480	-0.00811	-0.02470	0.10780	0.10979
π_8	0.37300	0.36746	0.34476	-0.00554	-0.02824	0.11328	0.11577
π_9	0.46625	0.45801	0.47217	-0.00824	0.00592	0.11204	0.11118
π_{10}	0.00000	-0.00091	0.05556	-0.00091	0.05556	0.12093	0.13085
γ_1	0.66555	0.67067	0.57480	0.00512	-0.09075	0.06146	0.10999
γ_2	0.66555	0.66223	0.55195	-0.00332	-0.11360	0.06358	0.12908
λ_1	1.00000	1.02345	1.22863	0.02345	0.22863	0.10399	0.24006
λ_2	0.70000	0.71654	0.72584	0.01654	0.02584	0.07257	0.05963
λ_3	0.90000	0.92098	1.04060	0.02098	0.14060	0.09413	0.15679
λ_4	0	-0.00041	-0.00039	-0.00041	-0.00039	0.04696	0.04793

Table H.17: Simulation study results for variation G with respect to the individual ML and PLS path coefficients.

		OLS		
	true	*mean*	*md*	*rmse*
$TE_{x_1y_1}$	0.26289	0.26171	-0.00118	0.11274
$TE_{x_2y_1}$	0.16431	0.16576	0.00145	0.11268
$TE_{x_3y_1}$	0.26289	0.26494	0.00205	0.11491
$TE_{x_4y_1}$	0.19717	0.19533	-0.00184	0.11637
$TE_{x_5y_1}$	0.13144	0.13246	0.00102	0.10980
$TE_{x_6y_1}$	0	0.00108	0.00108	0.10787
$TE_{x_7y_1}$	0.37238	0.37293	0.00055	0.11066
$TE_{x_8y_1}$	0.24825	0.24916	0.00091	0.10701
$TE_{x_9y_1}$	0.31031	0.30939	-0.00092	0.11196
$TE_{x_{10}y_1}$	0	-0.00106	-0.00106	0.10736
$TE_{x_1y_2}$	0.18402	0.18334	-0.00068	0.07856
$TE_{x_2y_2}$	0.11501	0.11616	0.00115	0.07892
$TE_{x_3y_2}$	0.18402	0.18427	0.00025	0.08096
$TE_{x_4y_2}$	0.13802	0.13777	-0.00024	0.08043
$TE_{x_5y_2}$	0.09201	0.09205	0.00004	0.07712
$TE_{x_6y_2}$	0	-0.00038	-0.00038	0.07565
$TE_{x_7y_2}$	0.26066	0.26102	0.00035	0.07775
$TE_{x_8y_2}$	0.17378	0.17373	-0.00004	0.07614
$TE_{x_9y_2}$	0.21722	0.21824	0.00102	0.07710
$TE_{x_{10}y_2}$	0	0.00023	0.00023	0.07564
$TE_{x_1y_3}$	0.23660	0.23707	0.00047	0.10135
$TE_{x_2y_3}$	0.14788	0.14978	0.00190	0.09994
$TE_{x_3y_3}$	0.23660	0.23720	0.00060	0.10310
$TE_{x_4y_3}$	0.17745	0.17659	-0.00086	0.10489
$TE_{x_5y_3}$	0.11830	0.11749	-0.00081	0.10017
$TE_{x_6y_3}$	0	0.00030	0.00030	0.09649
$TE_{x_7y_3}$	0.33514	0.33581	0.00067	0.09859
$TE_{x_8y_3}$	0.22343	0.22415	0.00072	0.09705
$TE_{x_9y_3}$	0.27928	0.27755	-0.00173	0.09882
$TE_{x_{10}y_3}$	0	-0.00041	-0.00041	0.09851
$TE_{x_1y_4}$	0	0.00047	0.00047	0.06599
$TE_{x_2y_4}$	0	0.00030	0.00030	0.06474
$TE_{x_3y_4}$	0	0.00017	0.00017	0.06657
$TE_{x_4y_4}$	0	-0.00101	-0.00101	0.06669
$TE_{x_5y_4}$	0	0.00005	0.00005	0.06430
$TE_{x_6y_4}$	0	-0.00004	-0.00004	0.06252
$TE_{x_7y_4}$	0	0.00024	0.00024	0.06303
$TE_{x_8y_4}$	0	-0.00067	-0.00067	0.06158
$TE_{x_9y_4}$	0	-0.00046	-0.00046	0.06379
$TE_{x_{10}y_4}$	0	-0.00073	-0.00073	0.06267

Table H.18: Simulation study results for variation G with respect to the OLS total effect coefficients.

Appendix I

ML standard error estimates

I classified the continuous ML standard errors estimates of $\hat{\gamma}_1$ and show in figure I.1 the corresponding histogram. The abscissa in the graph is restricted to values between 0.1 and 0.6, although the estimates vary between 0.09319 and 3.00844. However, the missing bars would appear very low. Applying this scale the skewness of the estimates is better identifiable than in figure 3.5 page 103. Table I.1 (page 161) reveals the densities for the classified data. The ML approach shows a few large standard deviations. From a value of 0.550 onwards the density is strictly lower than 0.1. In less than 2.5% (247 counts divided by k=9,990) the value exceeds an estimation value of 0.550.
In practical applications a researcher would assess the results individually, identify conspicuous results and discard them. Such a proceeding is reasonable since the ML approach may converge towards another maximum if several maxima exist. I did not define a threshold to discard results automatically within my Monte Carlo study, but show with figure I.2 (page 162) how the results change, if standard deviations which are larger than 0.550 get discarded: the green density curve appears very similar to the original (black) one. In contrast, the mark which represents the expected value of the ML standard error estimator lies much more to the left - since the values enter squared to calculate the expected value, the discarding of large values has a strong impact.

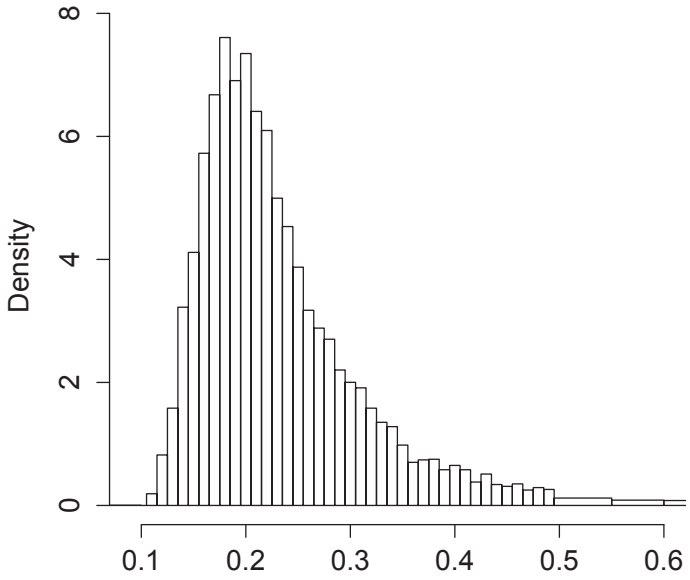

Figure I.1: Histogram of the ML standard deviations of $\hat{\gamma}_1$.

Additionally I estimated the standard deviations also by applying the bootstrap technique with 300 bootstrap replications (K_B). Table I.2 (page 163) reveals that it is favourable to apply the original estimates. The table shows for the classified estimates the absolute number of estimates within one class and the corresponding densities. With respect to the latter table the data is classified such that results appear quite condensed, but large values (outliers) can be identified. The table reveals that compared to the original estimates the bootstrapping produces many more outliers.

lower bound	upper bound	counts	density	lower bound	upper bound	counts	density
0	0.050	0	0	0.345	0.355	98	0.98098
0.050	0.100	1	0.00200	0.355	0.365	70	0.70070
0.100	0.105	0	0	0.365	0.375	74	0.74074
0.105	0.115	19	0.19019	0.375	0.385	75	0.75075
0.115	0.125	82	0.82082	0.385	0.395	58	0.58058
0.125	0.135	158	1.58158	0.395	0.405	65	0.65065
0.135	0.145	322	3.22322	0.405	0.415	58	0.58058
0.145	0.155	411	4.11411	0.415	0.425	38	0.38038
0.155	0.165	572	5.72573	0.425	0.435	51	0.51051
0.165	0.175	667	6.67668	0.435	0.445	34	0.34034
0.175	0.185	760	7.60761	0.445	0.455	31	0.31031
0.185	0.195	690	6.90691	0.455	0.465	35	0.35035
0.195	0.205	734	7.34735	0.465	0.475	25	0.25025
0.205	0.215	640	6.40641	0.475	0.485	29	0.29029
0.215	0.225	609	6.09610	0.485	0.495	26	0.26026
0.225	0.235	499	4.99499	0.495	0.550	66	0.12012
0.235	0.245	453	4.53453	0.550	0.600	43	0.08609
0.245	0.255	387	3.87387	0.600	0.650	40	0.08008
0.255	0.265	317	3.17317	0.650	0.700	28	0.05606
0.265	0.275	288	2.88288	0.700	0.750	17	0.03403
0.275	0.285	270	2.70270	0.750	0.800	25	0.05005
0.285	0.295	220	2.20220	0.800	1.000	44	0.02202
0.295	0.305	2	2.00200	1.000	1.200	17	0.00851
0.305	0.315	191	1.91191	1.200	1.700	21	0.00420
0.315	0.325	158	1.58158	1.700	2.200	5	0.00100
0.325	0.335	135	1.35135	2.200	2.700	4	0.00080
0.335	0.345	128	1.28128	2.700	3.200	2	0.00040

Table I.1: Classified ML standard deviations of $\hat{\gamma}_1$.

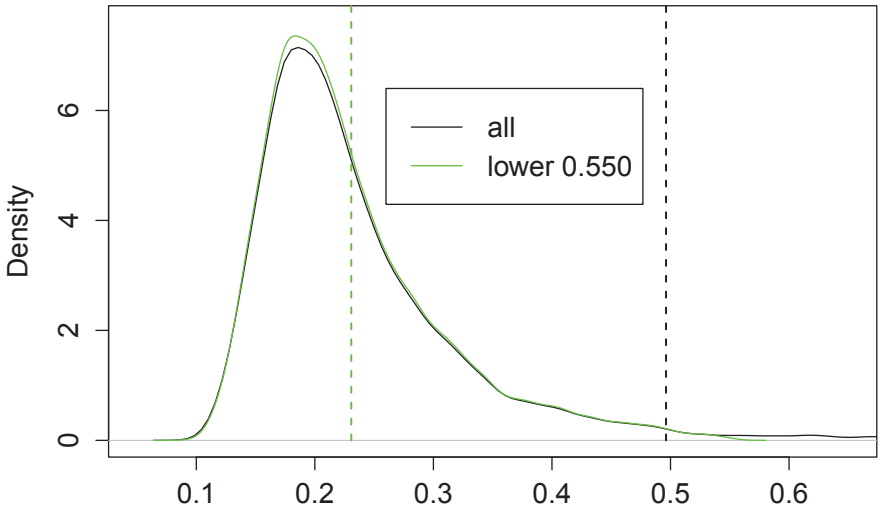

Figure I.2: Density function of the ML standard deviations of $\hat{\gamma}_1$ including all or a selection of estimates.

		Original		$K_B = 300$	
lower bound	upper bound	counts	density	counts	density
0	0.1	1	0.00100	4	0.00400
0.1	0.2	4071	4.07508	3704	3.70771
0.2	0.3	4128	4.13213	4398	4.40240
0.3	0.4	1120	1.12112	1248	1.24925
0.4	0.5	366	0.36637	301	0.30130
0.5	0.6	101	0.10110	103	0.10310
0.6	0.8	110	0.05506	91	0.04555
0.8	1.0	44	0.02202	12	0.00601
1.0	1.2	17	0.00851	9	0.00450
1.2	1.7	21	0.00420	14	0.00280
1.7	2.2	5	0.00100	6	0.00120
2.2	2.7	4	0.00080	0	0
2.7	3.2	2	0.00040	0	0
3.2	10.0	0	0	17	0.00025
10.0	20.0	0	0	11	0.00011
20.0	30.0	0	0	11	0.00011
30.0	40.0	0	0	10	0.00010
40.0	50.0	0	0	8	0.00008
50.0	60.0	0	0	7	0.00007
60.0	70.0	0	0	3	0.00003
70.0	80.0	0	0	1	0.00001
80.0	90.0	0	0	3	0.00003
90.0	100.0	0	0	1	0.00001
100.0	150.0	0	0	3	0.00001
150.0	200.0	0	0	0	0
200.0	400.0	0	0	4	0.00000
400.0	700.0	0	0	8	0.00000
700.0	1000.0	0	0	7	0.00000
1000.0	15500.0	0	0	6	0.00000

Table I.2: Classified ML standard deviations (original and bootstrapped) of $\hat{\gamma}_1$.

Bibliography

Ahrholdt, Dennis (2010): Erfoglsfaktoren einer E-Commerece Website - Empirische Identifikation vertrauensfördernder Signale im Internet Einzelhandel, Gabler Verlag / Springer Fachmedien, Wiesbaden.

Albers, Sönke / Hildebrandt, Lutz (2006): Methodische Probleme bei der Erfolgsfaktorenforschung - Messfehler, formative versus reflektive Indikatoren und die Wahl des Strukturlgeichungs-Modells, in: Zeitschrift für betriebswirtschaftliche Forschung, 58(2), pp. 2–33.

Alfons, Andreas (2014): simFrame: Simulation framework, URL: `http://cran.r-project.org/web/packages/simFrame/index.html`, r package version 0.5.2.

Anderson, Rolph E. / Swaminathan, Srinivasan (2011): Customer Satisfaction and Loyalty in E-Markets: A PLS Path Modeling Approach, in: Journal of Marketing Theory and Practice, 19(2), pp. 221–234.

Arazy, Ofer / Gellatly, Ian R. (2012): Corporate Wikis: The Effects of Owners´ Motivation and Behavior on Group Members´ Engagement, in: Journal of Management Information Systems, 29(3), pp. 87–116.

Areskoug, B. (1982): The first Canonical Correlation: Theoretical PLS Analysis and Simulation Experiments, in: Jöreskog, Karl G. / Wold, Herman (Eds), Systems Under Indirect Observation, Part I, pp. 95–118, North-Holland Publications, Amsterdam.

Balzano, Simona / Trinchera, Laura (2011): Structural Equation Models and Student Evaluation of Teaching: A PLS Path Modeling Study, in: Attanasio, Massimo / Capursi, Vincenza (Eds), Statistical Methods

for the Evaluation of University Systems, Contributions to Statistics, pp. 55–66, Physica-Verlag - A Springer Company, Berlin.

Barroso, Carmen / Cepeda Carrion, Gabriel / Roldan, Jose L. (2010): Applying Maximum Likelihood and PLS on Different Sample Sizes: Studies on SERVQUAL Model and Employee Behavior Model, in: Vinzi, Vincenzo Esposito / Chin, Wynne W. / Henseler, Jörg / Wang, Huiwen (Eds), Handbook of Partial Least Squares, pp. 427–448, Springer, Berlin.

Bentler, Peter M. / Chou, Chih-Ping (1987): Practical Issues in Structural Modeling, in: Sociological Methods & Research, 16(1), pp. 78–117.

Bicen, Pelin / Madhavaram, Sreedhar (2013): Research on Smart Shopper Feelings: An Extension, in: The Journal of Marketing Theory and Practice, 21(2), pp. 221–234.

Birkinshaw, Julian / Hood, Neil / Jonsson, Stefan (1998): Building Firm-Specific Advantages in Multinational Corporations: The Role of Subsidiary Initiative, in: Strategic Management Journal, 19(3).

Birkinshaw, Julian / Morrison, Allen / Hulland, John (1995): Structural and Competitive Determinants of a Global Integration Strategy, in: Strategic Management Journal, 16(8).

Bollen, Kenneth A. (1987): Total, Direct, and Indirect Effects in Structural Equation Models, in: Clogg, Clifford (Ed), Sociological Methodology, pp. 37–69, American Sociological Association, Washington, DC.

Bollen, Kenneth A. (1989): Structural Equations with Latent Variables, John Wiley & Sons, New York.

Bollen, Kenneth A. (2013): Eight myths about causality and structural equation models, in: Morgan, Stephen L. (Ed), Handbook of Causal Analysis for Social Research, Springer, URL: `http://ftp.cs.ucla.edu/pub/stat_ser/r393.pdf`.

Bollen, Kenneth A. / Lennox, Richard (1991): Conventional Wisdom on Measurement: A Structural Equation Perspective, in: Psychological Bulletin, 110(2), pp. 305–314.

Boomsma, Anne (1982): The Robustness of LISREL against Small Sample Sizes in Factor Analysis Models, in: Jöreskog, Karl G. / Wold, Herman O. (Eds), Systems Under Indirect Observation, Part I, pp. 149–173, North Holland Publishing, Amsterdam.

Boomsma, Anne (1983): On the robustness of LISREL (maximum likelihood estimation) against small sample size and nonnormality, Dissertation, University of Groningen, The Netherlands.

Boomsma, Anne (1985): Nonconvergence, improper solutions, and starting values in LISREL maximum likelihood estimation, in: Psychometrika, 50(2), pp. 229–242.

Boomsma, Anne / Hoogland, Jeffrey J. (2001): The robustness of LISREL modeling revisited, in: Cudeck, Robert / Du Toit, S. H. C. / Sörbom, Dag (Eds), Structural equation models: Present and future. A Festschrift in honor of Karl Jöreskog, pp. 139–168, Scientific Software International, Lincolnwood and IL, URL: `http://www.gmw.rug.nl/~boomsma/ssi.pdf`, accessed: 30.11.2012.

Brady, Michael K. / Voorhees, Clay M. / Brusco, Michael J. (2012): Service Sweethearting: Its Antecedents and Customer Consequences, in: Journal of Marketing, 76(2), pp. 81–98, ISSN 0022-2429, doi: 10.1509/jm.09.0420.

Calvo-Mora, Arturo / Ruiz-Moreno, Carolina / Picón-Berjoyo, Araceli / Cauzo-Bottala, Lourdes (2014): Mediation effect of TQM technical factors in excellence management systems, in: Journal of Business Research, 67(5), pp. 769–774.

Cassel, Claes / Hackl, Peter / Westlund, Anders H. (1999): Robustness of partial least-squares method for estimating latent variable quality structures, in: Journal of Applied Statistics, 26(4), pp. 435–446.

Chin, Wynne W. (1998a): Issues and Opinion on Structural Equation Modeling, in: MIS Quarterly, 22(1), pp. vii–xvi.

Chin, Wynne W. (1998b): The partial least squares approach for structural equation modeling, in: Marcoulides, George A. (Ed), Modern Methods for Business Research, pp. 295–336, Lawrence Erlbaum Associates, London.

Chin, Wynne W. / Marcolin, Barbara L. / Newsted, Peter R. (2003): A Partial Least Squares Latent Variable Modeling Approach for Measuring Interaction Effects: Results from a Monte Carlo Simulation Study and an Electronic-Mail Emotion/Adoption Study, in: Informations Systems Research, 14(2), pp. 189–217.

Chin, Wynne W. / Newsted, Peter R. (1999): Structural Equation Modeling Analysis with Small Samples Using Partial Least Squares, in: Hoyle, Rick H (Ed), Statistical Strategies for Small Sample Research, pp. 307–341, Sage Publications, Thousands Oak.

Chou, Chih-Ping / Bentler, Peter M. (1995): Estimates and Tests in Structural Equation Modeling, in: Hoyle, Rick H (Ed), Structural Equation Modeling: Concepts, Issues, and Applications, pp. 37–55, Sage Publications, Thousands Oak.

Dawes, Philip L. / Lee, Don Y. / Dowling, Grahame R. (1998): Information Control and Influence in Emergent Buying Centers, in: Journal of Marketing, 62(3), pp. 55–68.

Diamantopoulos, Adamantios / Riefler, Petra / Roth, Katharina P. (2007): Advancing Formative Measurement Models, Discussion Paper, University of Vienna, URL: `http://homepage.univie.ac.at/katharina.roth/research/Formative_Measurement_JBR.pdf`, accessed: 26.11.2012.

Diamantopoulos, Adamantios / Siguaw, Judy A. (2000): Introduction LISREL, Sage, Thousand Oaks.

DiCiccio, Thomas J. / Efron, Bradley / Hall, Peter / Martin, Michael A. / Canty, A. J. / Davison, A. C. / Hinkley,

D. V. / Gleser, Leon Jay / Lee, Stephen M. S. / Young, G. Alastair (1996): Bootstrap confidence intervalsCommentComment-CommentCommentRejoinder, in: Statistical Science, 11(3), pp. 189–228, doi:10.1214/ss/1032280214.

Dijkstra, Theo K. (2010): Latent Variables and Indices: Herman Wold´s Basic Design and Partial Least Squares, in: Vinzi, Vincenzo E. / Chin, Wynne W. / Henseler, Jörg / Wang, Huiwen (Eds), Handbook of Partial Least Squares, pp. 23–46, Springer, Berlin.

Djikstra, Theo (1983): Some Comments on Maximum Likelihood and Partial Least Squares Methods, in: Journal of Econometrics, 22(1-2), pp. 67–90.

Efron, Bradley / Tibshirani, Robert J. (1993): An Introduction to the Bootstrap, Chapman & Hall, New York.

Ernst, Holger / Hoyer, Wayne D. / Rübsaamen, Carsten (2010): Sales, Marketing, and Research-and-Development Cooperation Across New Product Development Stages: Implications for Success, in: Journal of Marketing, 74(5), pp. 80–92.

Eskildsen, Jacob / Kristensen, Kai / Juhl, Hans J. / Østergaard, Peder (2004): The Drivers of Customer Satisfaction and Loyalty. The Case of Denmark 2000-2002, in: Total Quality Management, 15(5-6), pp. 859–868.

Fornell, Claes (1982): A second generation of multivariate analysis, Praeger, New York.

Fornell, Claes / Bookstein, Fred L. (1982): Two Structural Equation Models: LISREL and PLS Applied to Consumer Exit-Voice Theory, in: Journal of Marketing Research, 19(4), pp. 440–452.

Fornell, Claes / Robinson, William T. (1983): Industrial Organization and Consumer Satisfaction/Dissatisfaction, in: Journal of Consumer Research, 9(4), URL: 403-412.

Fox, John / Nie, Zhenghua / Byrnes, Jarrett (2013): sem: Structural Equation Models, URL: http://CRAN.R-project.org/package=sem, r package version 3.1-3.

Garnefeld, Ina / Eggert, Andreas / Helm, Sabrina V. / Tax, Stephen S. (2013): Growing Existing Customers´ Revenue Streams Through Customer Referral Programs, in: Journal of Marketing, 77(4), pp. 17–32.

Gefen, David / Straub, Detmar W. / Boudreau, Marie-Claude (2000): Structural Equation Modeling and Regression: Guidelines for Research Practice, in: Communications of the Association for Information Systems, 4(7).

Goodhue, Dale / Lewis, William / Thompson, Ronald (2007): Statistical Power in Analyzing Interaction Effects: Questioning the Advantage of PLS with Product Indicators, in: Informations Systems Research, 18(2), pp. 211–227.

Götz, Oliver / Liehr-Gobbers, Kerstin / Krafft, Manfred (2010): Evaluation of Structural Equation Models Using the Partial Least Squares (PLS) Approach, in: Vinzi, Vincenzo E. / Chin, Wynne W. / Henseler, Jörg / Wang, Huiwen (Eds), Handbook of Partial Least Squares, Springer Handbooks of Computational Statistics, pp. 691–711, Springer, Berlin/Heidelberg.

Haenlein, Michael / Kaplan, Andreas M. (2004): A Beginner's Guide to Partial Least Squares Analysis, in: Understanding Statistics, 3(4), pp. 283–297.

Hair, Joe F. / Ringle, Christian M. / Sarstedt, Marko (2011): PLS-SEM: Indeed a Silver Bullet, in: Journal of Marketing Theory and Practice, 19(2), pp. 139–151.

Hair, Joseph F. / Sarstedt, Marko / Pieper, Torsten M. / Ringle, Christian M. (2012a): The Use of Partial Least Squares Structural Equation Modeling in Strategic Management Research: A Review of Past Practices and Recommendations for Future Applications, in: Long Range Planning, 45, pp. 320–340.

Hair, Joe F. / Sarstedt, Marko / Ringle, Christian M. / Mena, Jeannette A. (2012b): An assessment of the use of partial least squares

structural equation modeling in marketing research, in: Journal of the Academy of Marketing Science, 40(3), pp. 414–433.

Harmancioglu, Nukhet / Finney, R. Zachary / Joseph, Mathew (2009): Impulse purchase of new products: an empirical analysis, in: Journal of Product and & Brand Management, 18(1).

Hennig-Thurau, Thorsten / Groth, Markus / Paul, Michael / Gremler, Dwayne D. (2006): Are All Smiles Created Equal? How Emotional Contagion and Emotional Labor Affect Service Relationships, in: Journal of Marketing, 70(3), pp. 58–73.

Hennig-Thurau, Thorsten / Henning, Victor / Sattler, Henrik (2007): Consumer File Sharing of Motion Pictures, in: Journal of Marketing, 71(4), pp. 1–18.

Henseler, Jörg (2010): On the convergence of the partial least squares path modeling algorithm, in: Computational Statistics, 25(1), pp. 107–120.

Henseler, Jörg / Dijkstra, Theo K. / Sarstedt, Marko / Ringle, Christian M. / Diamantopoulos, Adamantios / Straub, Detmar W. / Ketchen Jr., David J. / Hair, Joseph F. / Hult, G. Tomas M. / Calantone, Roger J. (2014): Common Beliefs and Reality About PLS: Comments on Rönkkö and Evermann (2013), in: Organizational Research Methods, 17(2), pp. 182–209.

Henseler, Jörg / Ringle, Christian M. / Sinkovics, Rudolf R. (2009): The Use of Partial Least Squares Path Modeling in International Marketing, in: Advances in International Marketing, 20, pp. 277–320.

Hoogland, Jeffrey J. (1999): The robustness of estimation methods for covariance structure analysis, Dissertation, University of Groningen, Netherlands, unpublished.

Hsu, Sheng-Hsun / Chen, Wun-Hwa / Hsieh, Ming-Jyh (2006): Robustness Testing of PLS, LISREL, EQS and ANN-based SEM for Measuring Customer Satisfaction, in: Total Quality Management and Business Excellence, 17(3), pp. 355–371.

Hsu, Sheng-Hsun / Wang, Yu-Che (2008): The development and empirical validation of the Employee Satisfaction Index model, in: Total Quality Management and Business Excellence, 19(4), pp. 353–366.

Huber, Frank / Herrmann, Andreas / Meyer, Frederik / Vogel, Johannes / Vollhardt, Kai (2007): Kausalmodellierung mit Partial Least Squares: Eine anwendungsorientierte Einführung, Gabler, Wiesbaden.

Hui, Baldawin S. (1982): On building partial least squares models with interdependent inner relations, in: Jöreskog, Karl G. / Wold, Herman (Eds), Systems Under Indirect Observation, Part I, pp. 249–271, North-Holland Publications, Amsterdam.

Hui, Baldwin S. / Wold, Herman (1982): Consistency and Consistency at large of Partial Least Squares Estimates, in: Jöreskog, Karl G. / Wold, Herman (Eds), Systems Under Indirect Observation, Part II, pp. 119–130, North-Holland Publications, Amsterdam.

Hult, G. Tomas M. / Neese, William T. / Bashaw, R. Edward (1997): Faculty Perceptions of Marketing Journals, in: Journal of Marketing Education, 19(1), pp. 37–52.

Jarvis, Cheryl Burke / MacKenzie, Scott B. / Podsakoff, Philip (2003): A Critical Review of Construct Indicators and Measurement Model Misspecification in Marketing and Consumer Research, in: The Journal of Consumer Research, 30(2), pp. 199–218.

Johnson, Michael D. / Herrmann, Andreas / Huber, Frank (2006): The Evolution of Loyalty Intentions, in: Journal of Marketing, 70(2), pp. 122–132.

Jöreskog, Karl G. (1982): The LISREL Approach to Causal Model-Building in the Social Sciences, in: Jöreskog, Karl G. / Wold, Herman O. (Eds), Systems Under Indirect Observation, Part I, pp. 81–99, North Holland Publishing, Amsterdam.

Jöreskog, Karl G. / Sörbom, Dag / du Toit, Stephen / du Toit, Mathilda (2000): LISREL 8: New Statistical Features, SSI Scientific Software International, USA.

Kaplan, David (1989): A Study of the Sampling Variability and z-Values of Parameter Estimates from Misspecified Structural Equation Models, in: Multivariate Behavioral Research, 24(1), pp. 41–57.

Kaplan, David (2000): Structural Equation Modeling, No. 10 in Advanced Quantitative Techniques in the Social Sciences Series, Sage Publications, Thousands Oak.

Koch, Anke (2009): Regionale Verteilung der Beschäftigung in Deutschland: Panel- und Zähldatenmodelle, vol. Bd. 14ofSchriften zur empirischen Wirtschaftsforschung, Lang, Frankfurt, M. and Berlin and Bern and Bruxelles and New York, NY and Oxford and Wien, ISBN 3631597665.

Lam, Son K. / Ahearne, Michael / Hu, Ye / Schillewaert, Niels (2010): Resistance to Brand Switching When a Radically New Brand is Introduced: A Social Identity Theory Perspective, in: Journal of Marketing, 74(6), pp. 128–146.

Landau, Christian / Bock, Carolin (2013): Value Creation through Vertical Intervention of Corporate Centres in Single Business Units of Unrelated Diversified Portfolios – The Case of Private Equity Firms, in: Long Range Planning, 46(1-2), pp. 97–124.

Lee, Don Y. (2001): Power, conflict, and satisfaction in IJV supplier - Chinese distributor channels, in: Journal Business Research, 52(2), pp. 149–160.

Lohmöller, Jan-Bernd (1989): Latent variable path modelling with partial least squares, Physica-Verlag, Heidelberg.

MacCallum, Robert C. / Browne, Michael W. (1993): The Use of Causal Indicators in Covariance Structure Models: Some Practical Issues, in: Psychological Bulletin, 114(3), pp. 533–541.

McDonald, Roderick P. (1996): Path Analysis with Composite Variables, in: Multivariate Behavioral Research, 31(2), pp. 239–270.

McFarland, Richard G. / Bloodgood, James M. / Payan, Janice M. (2008): Suppy Chain Contagion, in: Journal of Marketing, 72(2), pp. 63–79.

Mels, Gerhard (2006): LISREL for Windows: Getting Started Guide, URL: http://www.ssicentral.com/lisrel/techdocs/GSWLISREL.pdf, accessed: 15.11.2012.

Milberg, Sandra J. / Smith, H. Jeff / Burke, Sandra J. (2000): Information Privacy: Corporate Management and National Regulation, in: Organization Science, 11(1), pp. 35–57.

Mintu-Wimsatt, Alma / Graham, John L. (2004): Testing a Negotiation Model on Canadian Anglophone and Mexican Exporters, in: Journal of the Academy of Marketing Science, 32(3).

Morgan, Stephen L. / Winship, Christopher (2007): Counterfactuals and Causal Inference, Cambridge, New York.

Nell, Phillip C. / Ambos, Björn (2013): Parenting advantage in the MNC: An embeddedness perspective on the value added by headquarters, in: Strategic Management Journal, 34(9), pp. 1086–1103.

Nevitt, Jonathan / Hancock, Gregory R. (2001): Performance of Bootstrapping Approaches to Model Test Statistics and Parameter Standard Error Estimation in Structural Equation Modeling, in: Structural Equation Modeling, 8(3), pp. 353–377.

Noonan, Richard / Wold, Herman O. (1982): PLS path modeling with indirectly observed variables: A comparison of alternative estimates for latent variables, in: Jöreskog, Karl G. / Wold, Herman (Eds), Systems Under Indirect Observation, Part II, pp. 75–94, North-Holland, Amsterdam.

R Core Team (2014): R: A Language and Environment for Statistical Computing, R Foundation for Statistical Computing, Vienna, Austria, URL: http://www.R-project.org/.

Reinartz, Werner / Haenlein, Michael / Henseler, Jörg (2009): An empirical comparison of the efficacy of covariance-based and variance-based SEM, in: International Journal of Research in Marketing, 26, pp. 332–344.

Reinartz, Werner / Krafft, Manfred / Hoyer, Wayne D. (2004): The Customer Relationship Management Process: Its Measurement and Impact on Performance, in: Journal of Marketing Research, 41(3), pp. 293–305.

Rigdon, Edward E. (1995): A Necessary and Sufficient Identification Rule for Structural Models Estimated in Practice, in: Multivariate Behavioral Research, 30(3), pp. 359–383.

Ringle, Christian M. / Götz, Oliver / Wetzels, Martin / Wilson, Bradley (2009): On the Use of Formative Measurement Specifications in Structural Equation Modeling: A Monte Carlo Simulation Study to Compare Covariance-Based and Partial Least Squares Model Estimation Methodologies, Discussion Paper MPRA Paper No. 15390, Maastricht University, Maastricht Research School of Economics of Technology and Organization (METEOR), URL: `http://mpra.ub.uni-muenchen.de/15390/`, accessed: 29.11.2012.

Rönkkö, Mikko / Evermann, Joerg (2013): A Critical Examination of Common Beliefs About Partial Least Squares Path Modeling, in: Organizational Research Methods, 16(3), pp. 425–448.

Rubin, Donald B. (1986): Statistics and Causal Inference: Comment: Which Ifs Have Causal Answers, in: Journal of the American Statistical Association, 81(396), pp. 961–962.

San José-Cabezudo, Rebeca / Camarero-Izquierdo, Carmen (2012): Determinants of Opening-Forwarding E-Mail Messages, in: Journal of Advertising, 41(2), pp. 97–112.

Sanchez, Gaston / Trinchera, Laura / Russolillo, Giorgio (2013): plspm: Tools for Partial Least Squares Path Modeling (PLS-PM), URL: `http://CRAN.R-project.org/package=plspm`, r package version 0.4.1.

Satorra, Albert / Bentler, Peter M. (1994): Corrections to test statistics and standard errors in covariance structure analysis, in: von Eye, Alexander / Clogg, Clifford C. (Eds), Latent variables analysis: Applications for developmental research, pp. 399–419, Sage, Thousand Oaks.

Savalei, Victoria / Bentler, Peter M. (2006): Structural Equation Modeling, in: Grover, Rajiv / Vriens, Marco (Eds), The Handbook of Marketing Research, pp. 330–364, Sage Publications, Thousand Oaks.

Schermelleh-Engel, Karin / Moosbrugger, Helfried / Müller, Hans (2003): Evaluating the Fit of Structural Equation Models: Tests of Significance and Descriptive Goodness-of-Fit Measures, in: Methods of Psychological Research, 8(2), pp. 23–73.

Schneeweiss, Hans (1993): Consistency at Large in Models with Latent Variables, in: Haagen, Klaus / Bartholomew, David / Deistler, Manfred (Eds), Statistical Modelling with Latent Variables, pp. 299–320, Elsevier Science Pubishers, Amsterdam.

Sobel, Michael E. (1987): Direct and Indirect Effect in Linear Structural Equation Models, in: Sociological Methods & Research, 16(1), pp. 155–176.

Sörbom, Dag (2001): Karl Jöreskog and LISREL: a personal story, in: Cudeck, Robert / Toit, Stephen Du / Sörbom, Dag (Eds), Structural Equation Modeling: Present and Future, pp. 3–10, SSI Scientific Software International, Lincolnwood.

Stapleton, David C (1978): Analyzing political participation data with a MIMIC Model, in: Sociological Methodology, pp. 52–74.

Surienty, Lilis / Ramayah, T. / Lo, May-Chiun / Tarmizi, Azlin Natasha (2014): Quality of Work Life and Turnover Intention: A Partial Least Square (PLS) Approach, in: Social Indicators Research, 119(1), pp. 405–420.

Tenenhaus, Michael (2008): Component-based Structural Equation Modelling, in: Total Quality Management and Business Excellence, 19(7/8), pp. 871–886.

Tenenhaus, Michel / Vinzi, Vincenzo E. / Chatelin, Yves-Marie / Lauro, Carlo (2005): PLS path modeling, in: Computational Statistics & Data Analysis, 48, pp. 159–205.

Trinchera, Laura (2007): Unobserved Heterogeneity in SEM: a new approach to latent class detection in PLS Path Modeling, Dissertation, Dipartimento di Matematica e Statistica, Università degli Studi di Napoli "Federico II".

Ulaga, Wolfgang / Eggert, Andreas (2006): Value-Based Differentiation in Business Relationships: Gaining and Sustaining Key Suppliers Status, in: Journal of Marketing, 70(1), pp. 119–136.

Venaik, Sunil / Midgley, David F. / Devinney, Timothy M. (2005): Dual Paths to Performance: The Impact of Global Pressures on MNC Subsidiary Conduct and Performance, in: Journal of International Business Studies, 36(6), pp. 655–675.

Vilares, Manuel J. / Almeida, Maria H. / Coelho, Pedro S. (2010): Comparison of Likelihood and PLS Estimators for Structural Equation Modeling: A Simulation with Customer Satisfaction Data, in: Vinzi, Vincenzo Esposito / Chin, Wynne W. / Henseler, Jörg / Wang, Huiwen (Eds), Handbook of Partial Least Squares, pp. 289–305, Springer, Berlin.

Völckner, Frankziska / Sattler, Henrik / Henning-Thurau, Thorsten / Ringle, Christian M. (2010): The Role of Parent Brand Quality for Service Brand Extension Success, in: Journal of Service Research, 13(4), pp. 379–396.

White, J. Chris / Varadarajan, P. Rajan / Dacin, Peter A. (2003): Market Situation Interpretation and Response: The Role of Cognitive Style, Organizational Culture, and Information Use, in: Journal of Marketing, 67(3), pp. 63–79.

Winkelmann, Rainer (2008): Econometric analysis of count data, 5. ed., Springer, Berlin, ISBN 3540776486.

Winklhofer, Heidi M. / Diamantopoulos, Adamantios (2002): Managerial evaluation of sales forecasting effectiveness: A MIMIC modeling approach, in: International Journal of Research in Marketing, 19(2), pp. 151–166.

Wold, Herman O. (1979): Model Construction and Evaluation when Theoretical Knowledge is Scarce: an Example of the Use of Partial Least Squares, Cahiers du Département d'Économétrie 79.06, Département d'Économétrie, Faculté des Sciences a Économiques et Sociales, Université de Genève, Genève.

Wold, Herman O. (1982): Soft modeling: the basic design and some extensions, in: Jöreskog, Karl G. / Wold, Herman (Eds), Systems Under Indirect Observation, Part II, pp. 1–54, North-Holland, Amsterdam.

Wold, Herman O. (1985a): Partial least squares, in: Kotz, Samuel / Johnson, Norman L. (Eds), Encyclopedia of Statistical Sciences, vol. 6, pp. 581–591, Wiley, New York.

Wold, Herman O. (1985b): Systems analysis by partial least squares, in: Nijkamp, P. / Leitner, H. / Wrigley, N. (Eds), Measuring the unmeasurable, pp. 221–251, Martinus Nijhoff, Dordrecht/Boston/Lancaster.

Woods, Carol M. / Oltmanns, Thomas F. / Turkheimer, Eric (2009): Illustration of MIMIC-Model DIF Testing with the Schedule for Nonadaptive and Adaptive Personality, in: Journal of Psychopathology and Behavioral Assessment, 31(4), pp. 320–330, URL: `http://link.springer.com/article/10.1007%2Fs10862-008-9118-9/fulltext.html`.

Wu, Chia-Huei / Chen, Lung Hung / Tsai, Ying-Mei (2009): Investigating Importance Weighting of Satisfaction Scores from a Formative Model with Partial Least Squares Analysis, in: Social Indicators Research, 90(3), URL: `http://www.springerlink.com/content/dj58085238q0576k/`.

Yuan, Ke-Hai / Wu, Ruilin / Bentler, Peter M. (2011): Ridge structural equation modelling with correlation matrices for ordinal and continuous data, in: The British journal of mathematical and statistical psychology, 64(1), pp. 107–133.

Yung, Yia F. / Bentler, Peter M. (1998): Bootstrapping techniques in analysis of mean and covariance structure, in: Marcoulides, George A. (Ed), Modern Methods for Business Research, pp. 195–226, Lawrence Erlbaum Associates, London.