The Impact of Missing Values on PLS, ML and FIML Model Fit

Malek Simon Grimm and Ralf Wagner

Abstract Structural equation modelling has become widespread in the marketing research domain due to the possibility of creating and investigating latent constructs. Today, several estimation methods are available, each with strengths and drawbacks. This study investigates how the established estimation methods of partial-least-squares (PLS), maximum likelihood (ML) and full-information maximum likelihood (FIML) perform with an increasing percentage of missing values (MVs). The research was conducted by investigating an adapted model of the European customer satisfaction index (ECSI). MVs were randomly generated with an algorithm. The performance of PLS, ML and FIML was tested with eight data sets that contained between 2.22% and 27.78% randomly generated MVs. It was shown that ML performs relatively poorly if the percentage of MVs exceeds 7%, while PLS performs satisfactorily if the percentage of MVs does not exceed 9%. FIML was shown to be mostly stable up to 17% MVs.

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1 Introduction

Structural equation modeling (SEM) is a set of powerful research methods applied in theory development and confirmatory theory testing (Richter et al, 2016). For fitting theoretical models to empirical data, researchers can choose between factor-analytic fitting algorithms based on the maximization of a log-likelihood function or composite-based partial-least-squares (PLS) minimizing residuals. Allison (2003) emphasized the disadvantages of case-wise or list-wise deletion that is common practice, and frequently, the default setting in software package covariance-based fitting of SEMs. Notably, this study provides evidence for the modern sophisticated missing value (MV) treatment (see Decker and Wagner, 2007 and Little and Rubin, 2019 for reviews), such as multiple imputations and the expectation-maximization algorithm which might lead to unbiased estimates in the case of randomly missing observations. However, in research practice these incidences are rare. In addition to the advantage of not being restricted by the means of the multivariate Gaussian distribution assumption for the observed indicators, PLS-based procedures are said to be robust against MVs (Tenenhaus et al, 2005). Parwoll and Wagner (2012) provide the first evidence that the performance of PLS-based fitting varies with the type of missingness and the extent of the MVs. Considering the need to provide researchers with systematic guidance, this study contributes the following:

- A discussion of patterns of missingness.
- A systematic comparison of the consequences of MVs of fitting an SEM with maximum likelihood (ML), full-information maximum likelihood (FIML) and PLS in a simulation experiment varying the proportion of MVs in the data set.

To pursue this purpose, the remainder of this manuscript is structured as follows. Next, we briefly discuss missingness patterns. Then, we introduce the research design of the simulation experiment. In the subsequent discussion of the results, we focus on global fit assessments. We conclude with a discussion of the results and an outline of promising avenues for further research.

2 Types of Missingness

MVs are distinguished between total non-response and item non-response. Total non-response considers the total dropout of a case within a data set. Item non-response describes the missingness of single aspects, questions or data points within a data set (Decker and Wagner, 2007). MVs are considered questions without answers or cases without cases (Koslowsky, 2002). However, an MV represents not only the missingness of a value, because three different patterns of MVs can be distinguished.

2.1 Missing at Random and Missing Completely at Random

Missing at random (MAR) refers to MVs where the probability of missingness on variable *Y* is related to other variables that are included within the measurement model, but not related to the variable *Y* itself (Enders, 2010). In other words, the other variables entail the mechanism to explain the missingness (Acock, 2005). The connotation of MAR might become misleading, because it implies that there is no relationship or mechanism that underlies the source of the missingness. However, missingness mechanisms are not random: The predisposition of MVs correlates with other study-related variables that are included in the data set (Baraldi and Enders, 2010).

The missing completely at random (MCAR) condition requires that a probability of MVs in variable *Y* is unrelated to all other measured variables, and to the probability of MVs in the variable *Y* itself (Enders, 2010). This condition represents a missingness mechanism that can be commonly comprehended under the term MV. However, the missingness pattern is not random; instead, the missingness does not depend on other variables (Little and Rubin, 2019). Although MCAR is a strict assumption, it represents a prominent MV mechanism that can be empirically tested (Little, 1988).

2.2 Missing Not at Random

Missing not at random (MNAR) or not missing at random means that the probability of missingness of data on variable *Y* is related to the variable

(Enders, 2010) or a non-empty set of other variables within the data set (Decker et al, 1998). Truncation and censoring are prominent in management and marketing research. MVs that are MNAR represent a problem, because almost all standard quantitative methods cannot cope with MVs that are MNAR (Molenberghs et al, 2014). Moreover, the MNAR patterns make up a permutative space of variations in the context of the simulation experiments. Due to page limitations, this study is limited to the MCAR scenario.

3 Simulation Study

A simulation study was conducted to investigate the estimation quality of the PLS, ML and FIML algorithms in scenarios with an increasing percentage of MVs. In Subsection 3.1, we illustrate how the MVs were implemented in a complete data set, and which global model fit criteria are considered in this study. In Subsection 3.2, we provide a brief discussion of differences between the PLS, ML and FIML algorithms that are relevant to this experiment. In Subsections 3.2.1 to 3.2.3, we outline the results of the simulation study.

3.1 Research Design

Adapting Parwoll and Wagner's (2012) procedure, we studied the performance of the PLS, ML and FIML algorithms using the example of the European customer satisfaction index (ECSI). We use a prominent ECSI benchmark data set with 250 complete observations that are provided by SmartPLS 3.0.

Studying the condition of MVs that are MCAR is of high interest, because MCAR is the most commonly considered missing value pattern within the relevant literature. Therefore, the investigation of the MCAR pattern assures the relevance of the study. Furthermore, investigating the MCAR pattern provides a certain comparability to the results in Parwoll and Wagner's (2012) study.

For generating MVs in an MCAR pattern, a *C*++ program was implemented that randomly selects MVs within a fixed array defined by the *N* and the total number of variables available. [1]

[1] The source code of the program is available from the authors upon request.

The initial data set consisted of 250 complete observations with 18 variables, which resulted in 4,500 entities. Following Parwoll and Wagner's (2012) study, data sets with 100 (2.22%), 200 (4.44%), 300 (6.67%), 400 (8.89%), 500 (11.11%), 600 (13.33%), 750 (16.67%) and 1,250 (27.78%) MVs were generated. Consequently, the data sets and the MV patterns were independent from one another. Meaning, eight different data sets were created and investigated.

To assess the impact of an increasing number of MVs, we considered several quality criteria. First, we examined the average variance extracted (AVE) and composite reliability (CR) which are defined by (cf. Fornell and Larcker, 1981; Parwoll and Wagner, 2012):

$$AVE = \frac{\sum \lambda_i^2}{\sum \lambda_i^2 + \sum Var(\varepsilon_i)} \tag{1}$$

$$CR = \frac{(\sum \lambda_i)^2}{(\sum \lambda_i)^2 + \sum Var(\varepsilon_i)} \tag{2}$$

λ_i^2 indicates the squared factor loading of the i^{th} manifest indicator, whereas λ_i represents the respective factor loading, and $Var(\varepsilon_i)$ denotes the observed error variance of the i^{th} indicator. Ideally, the AVE should remain stable with an increasing percentage of MVs to ensure measurement quality. AVE values can vary between 0 and 1. Values above 0.50 indicate sufficient measurement quality. CR should also remain stable if MVs are increasing. CR values can also vary between 0 and 1. The quality criterion is met with values above 0.70.

R^2 serves as a further criterion for the investigation of the performance and stability of the algorithms. R^2 refers to the amount of total variance explained by the respective independent variables. The definition is shown by equation 3. In this context, $\sum(y-\hat{y})^2$ represents the square sum of the residuals, and $\sum(y-\bar{y})^2$ represents the total square sum (Tjur, 2009). Similar to the AVE and CR, the R^2 values remain ideally identical if the percentage of MVs is increasing. However, the R^2 values should at least stay relatively constant if the MVs are increasing. There is no exact threshold level, but R^2 values range between 0 and 1, and should be possibly close to 1:

$$R^2 = 1 - \frac{\sum(y-\hat{y})^2}{\sum(y-\bar{y})^2} \tag{3}$$

The path coefficients are standardized estimates of the regression coefficients, and serve additionally as a further quality criterion (Bring, 1994). Standardized path coefficients can vary between 0 and 1, and should be stable if the percentage of MVs is increasing.

The indices standardized root means square residual (SRMR) and normed fit index (NFI) serve as absolute model fit quality criteria. Chen (2007) defines the SRMR model criteria as shown by the following equation:

$$SRMR = \sqrt{\frac{2\sum\sum[(s_{ij} - \sigma_{ij})/(s_{ii}s_{jj})]^2}{p(p+1)}} \tag{4}$$

In this regard, s_{ij} stands for the observed covariance, whereas σ_{ij} indicates the model-implied covariance. $s_{ii}s_{jj}$ are the standard deviations of the observed manifest variables. p equals the number of variables. The SRMR represents a standardized version of the root mean square residuals index (RMR or RMSR). One advantage is that the SRMR is relatively independent from sample size (Cangur and Ercan, 2015; Chen, 2007). Possible values can vary between 0 and 1. The respective threshold is ≤ 0.10. The NFI is defined by:

$$NFI = \frac{\chi_b^2 - \chi_m^2}{\chi_b^2} \tag{5}$$

χ_b^2 is the χ^2 estimate of the baseline or null model, and χ_m^2 is the χ^2 estimator of the assumed model. The NFI can range between 0 and 1. Bentler (1992) set the threshold above 0.9 for an excellent model fit. More recent literature suggests the threshold should be raised to 0.95 (Hu and Bentler, 1999).

The highlighted quality criteria (AVE, CR, R^2, standardized path estimates, SRMR and NFI) served as quality criteria for the investigation of the estimation methods.

3.2 PLS, ML and FIML Model Fit

To assess the model fit of the ECSI, we chose to estimate the SEM with the PLS and ML algorithms. PLS and ML can be seen as the most widely used estimation methods for SEM (Sharma and Kim, 2013). PLS and ML underlie different assumptions and methods. ML is the best-known representative of covariance-based approaches. PLS underlies the estimation method of component-based approaches (Dolce and Lauro, 2015). Each estimation method has its strengths and weaknesses. For example, PLS is considered to be better suited if the research has a predictive purpose. ML assumes that the observations are independent from one another, and normal distribution has to be assumed. PLS, in contrast, is free of those assumptions (O'Loughlin and Coenders, 2004). However, ML estimators are considered unbiased and PLS estimators lack accuracy, compared to ML estimators (Dolce and Lauro, 2015). In this vein, ML is often referred as "hard modelling" while PLS is referred to as "soft modelling" (Tenenhaus et al, 2005). FIML is a newer approach, and based on the ML estimation method. FIML allows MVs in some variables. During the FIML estimation, for each respondent, a log-likelihood function is calculated with the difference between the estimated and observed variables (Enders, 2001). The likelihood function is cumulatively computed for the entire sample (Enders and Bandalos, 2001).

The estimation methods of PLS, ML and FIML, therefore, seem as a suitable and comprehensive selection for investigating model fit accuracy with an increasing percentage of MVs. SmartPLS 3.0 was used for the PLS algorithm. We chose SmartPLS because the software is commonly used within other relevant studies, and we used, adapted and manipulated an initial data set that is provided by the software SmartPLS 3.0. We used SAS Studio 3.71 for the ML and FIML algorithms; because the software is licensed for clinical research, whereas R packages are mostly provided by third parties. However, using R and the respective packages would yield the same results and estimates as SmartPLS and SAS.

For all three estimation methods, the ECSI model was initially estimated with the data set that contained 0% MVs. However, the model did not fit with the ML estimator. Therefore, the model was iteratively reduced until it fitted with all estimation methods. Additionally, regression constraints had to be added for the ML and FIML estimation methods. The adapted ECSI model that was used for the model fit investigation is shown in Fig. 1.

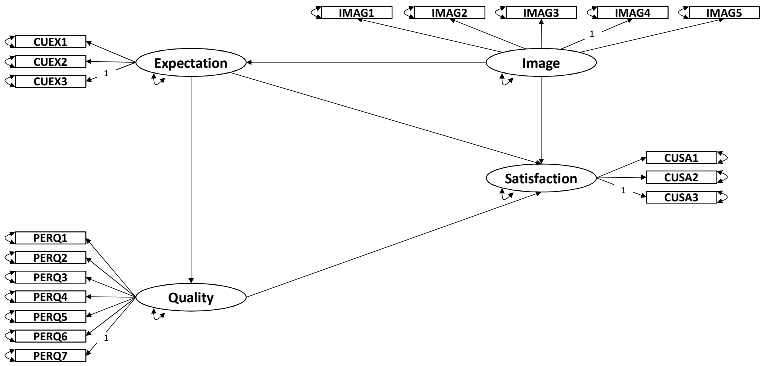


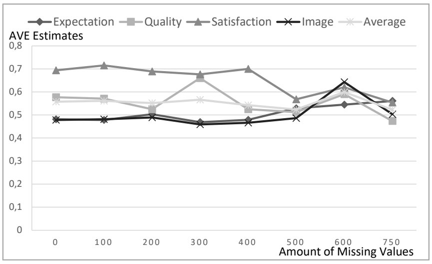
Figure 1: Adapted model of the ECSI; source: Based on Fornell et al (1996).

3.2.1 PLS Model Fit

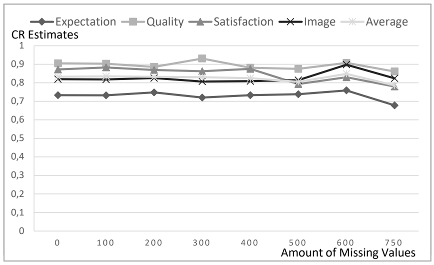
Figure 2 shows how the selected quality criteria, which were highlighted in Sect. 3.1, behave with an increasing percentage of MVs. The PLS algorithm was able to deal with up to 750 MVs within the data set, which equals 16.67% MVs.

The AVE (cf. Figure 2a) remains stable if the percentage of MVs increases. However, the variance is notably reduced if the MVs increase. It is very likely that this is because increasing MVs inevitably reduce the total information available, and fewer data points are available to estimate the AVE.

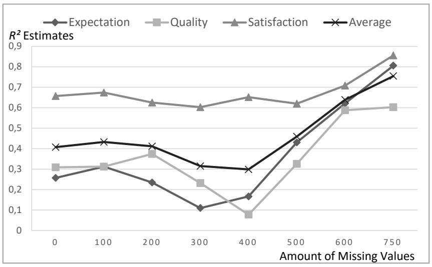
CR (cf. Figure 2b) remains stable with an increasing percentage of MVs. There are no notable changes for the total variance, values and point-to-point distances. These three indicators hint to a certain degree of unbiasedness of the CR estimates. More insightful is the revealed behaviour pattern of the R^2 estimates (cf. figure 2c): First, similar to the AVE estimates, the total variance is reduced. Second, it becomes obvious that the R^2 values are upwardly biased. This is might be problematic if researchers try to fit, derive or validate a model with the PLS algorithm, and if their data set contains a certain percentage of MVs. Possible results could be that single constructs might be used for a model, because the R^2 indicates a satisfactory level of explained or predicted variance, although the actual values are considerably upwardly biased. Regarding the path estimates (cf. Figure 2d), it can be concluded that there are slight changes in the overall values if the percentage of MVs increases.



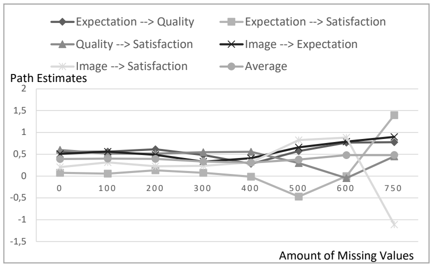
(a) PLS AVE estimates.



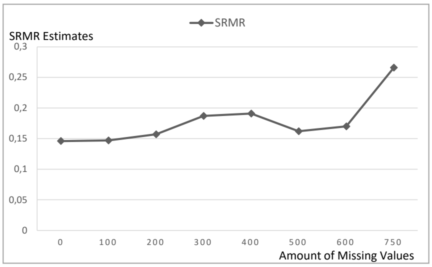
(b) PLS CR estimates.



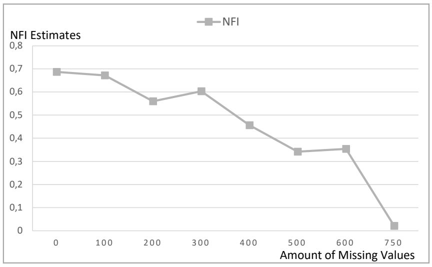
(c) PLS R^2 estimates.



(d) PLS path estimates.



(e) PLS SRMR estimates.



(f) PLS NFI estimates.

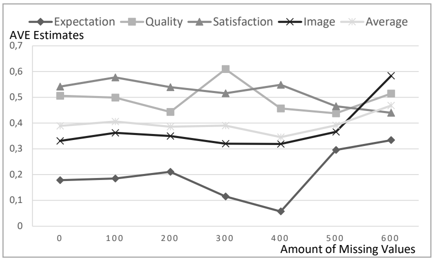
Figure 2: Impact of MVs on the model assessments with the PLS estimation method; source: own representations.

In total, the variance, or scattering, increases notably. Observing the behaviour of the model fit estimates SRMR (cf. Figure 2e) and NFI (cf. Figure 2f) reveals an interesting pattern: Both estimates are moving further away from their respective thresholds. Initially, both values do not meet their respective threshold level, meaning the SRMR is estimated too low and the NFI is estimated too high. If the percentage of MVs increases, both model fit estimates worsen considerably. This can lead to the rejection of a model if researchers encounter MVs.

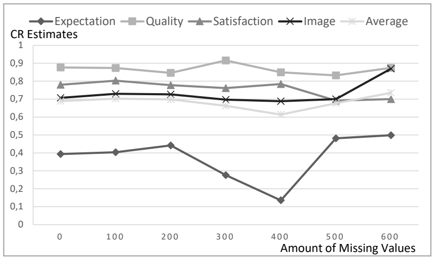
3.2.2 ML Model Fit

The results of the ML investigation are shown in Figure 3. As shown by the graphics Figures 3a to 3f, the ML estimation method was able to deal with a total of 600 MVs which equals 8.89% of MV.

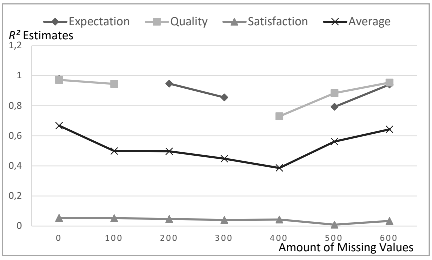
As indicated by Figure 3a, the AVE tends to become upwardly biased. Similar to the estimation with the PLS algorithm, the total variance is reduced. CR, however, remains overall relatively stable if the percentage of MVs increases, although the construct Expectation is slightly downward biased (cf. Figure 3b). Considerable calculation errors were encountered during the estimation of the R^2 estimates (cf. Figure 3c). This is critical, because R^2 values are crucial for the constructs' assessment within SEM. The ML algorithm initial error rate might make this estimation method unusable for certain studies. The path coefficients remain relatively stable if 500 MVs (11.11%) are not exceeded (cf. Figure 3d). After this point, the estimates are considerably downwardly biased. The model fit estimate SRMR (cf. Figure 3e) initially meets the required threshold of values below or equal 0.10. If the MVs increase, then the ML-estimated SRMR behaves similarly as the PLS-estimated SRMR index, and increases. However, the ML-estimated SRMR increases moderately while the PLS estimated SRMR increases drastically. Within this research, the respective threshold of 0.10 is exceeded if more than 400 (8.89%) MVs are encountered. In comparison to the PLS-estimated NFI model fit index, the calculation of the ML-estimated NFI index is initially relatively high, but does not meet its respective threshold of equal or above .95. Similar to the ML-calculated SRMR index, the ML-estimated NFI moves moderately far away from its respective threshold, and changes for the worse if the MVs increase.



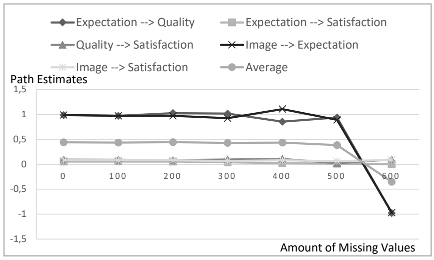
(a) ML AVE estimates.



(b) ML CR estimates.

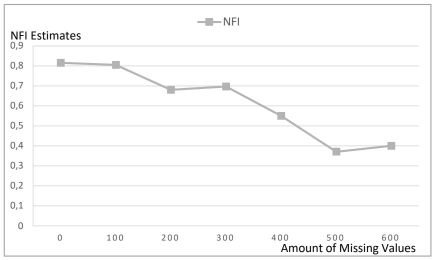


(c) ML R^2 estimates.



(d) ML path estimates.

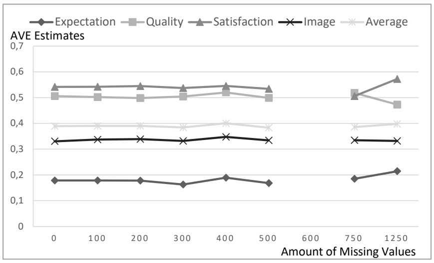
(e) ML SRMR estimates.



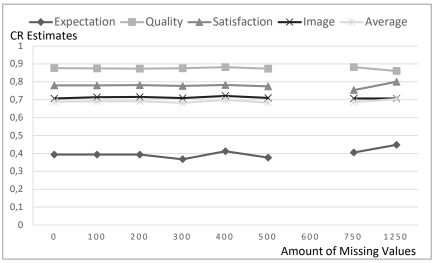
(f) ML NFI estimates.

Figure 3: Impact of MVs on the model assessments with the ML estimation method; source: own representations.

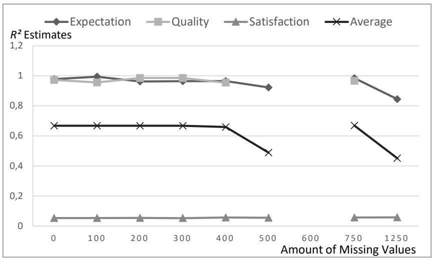
3.2.3 FIML Model Fit



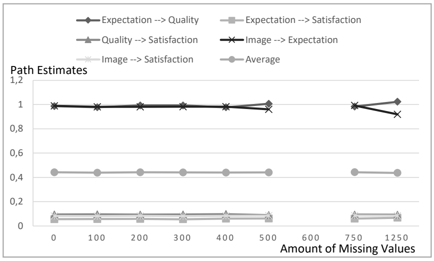
(a) FIML AVE estimates.



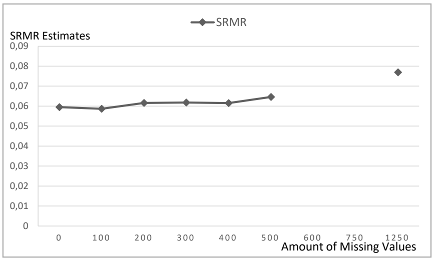
(b) FIML CR estimates.



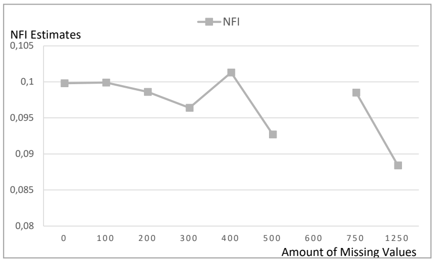
(c) FIML R^2 estimates.



(d) FIML path estimates.



(e) FIML SRMR estimates.



(f) FIML NFI estimates.

Figure 4: Impact of MVs on the model assessments with the FIML estimation method; source: own representations.

Figure 4 depicts the results of the FIML investigation. The pattern of the MVs for the data set with 600 MVs (13.33%) was not suitable for the FIML algorithm. Nonetheless, the FIML method was the only algorithm that was able to estimate the last data set with 1,250 MVs (27.78%).

FIML provides relatively stable results for the AVE (cf. Figure 4a). Variance between the points remains stable, as well as the point-to-point distance of the single estimates. CR (cf. Figure 4b) also remains stable if the percentage of MV increases. CR seems to be as well unbiasedly estimated even if 750 (16.67%) MVs are exceeded. R^2 estimates (cf. Figure 4c) are stable up to 400 (8.89%) MVs, and are only slightly downward biased. More interesting is that the variance between the points remains stable. The PLS estimation began at this point to lose total variance between the points (cf. Figure 2c) and the ML algorithm encountered problems calculating the R^2 values (cf. Figure 3c). The path coefficients also remain stable over time regarding the overall variance and point-to-point distances (cf. Figure 4d). No upwardly or downward biases become apparent. The SRMR index (cf. Figure 4e) is initially below its respective threshold. The SRMR remains even under its respective threshold if 1,250 MVs (27.78%) are estimated. Interesting are the estimates of the NFI (cf. Figure 4f): As assumed, all the initial estimates of the FIML equal those of the ML estimation method, with exception of the NFI. The index is considerably underestimated in comparison to the PLS estimation (cf. Figure 2f) and the ML estimation (cf. Figure 3f).

4 Conclusion and Outlook

This study provides insights into the performances of PLS, ML and FIML SEM estimation methods under varying proportions of MV in the data set. Results show that the performance and estimation accuracy vary substantially with the percentage of MVs. Within a data set that included 4,500 data points, 100 (2.22%), 200 (4.44%), 300 (6.67%), 400 (8.89%), 500 (11.11%), 600 (13.33%), 750 (16.67%) and 1,250 (27.78%) randomly generated MVs were induced. With an adapted ECSI model, the performance of the estimation methods was investigated with the AVE, CR, R^2, path estimates, SRMR and the NFI.

Based on this simulation study, we conclude that the estimation PLS method provides, in summary, unbiased estimates until 8.89% MVs. Upon this point, the AVE, CR, R^2, path estimates and SRMR remain relatively stable. Only the

NFI index is notably downward biased. If the level of 8.89% MVs is exceeded, the PLS algorithm reduces the estimation variance of the AVE and R^2 values. The CR remains stable. However, the variances of the path estimates increase notably. The SRMR remains stable, but the NFI estimation is downward biased. Consolidating all fit criteria considered, the PLS algorithm should not be used if the percentage of MVs exceeds 9%.

In addition, the calculation errors could have shown that the ML estimation method provides unbiased results up to a percentage of 7% MVs. The AVE tends to be stable until the percentage of MVs does not exceed 4%. After this point, an observable bias became apparent, leading to an upward bias and a variance reduction if the MVs further increase. However, the estimated CR (with the exception of the dimension Expectation) remains stable, as well as the path estimates. The global model fit indices change substantially if 7% of MVs are exceeded. This could lead to the rejection of a model. We suggest using the ML estimation method only if the level of 7% MVs is not exceeded.

The FIML estimation method failed because of numerical calculation issues for the 7% data set, but showed to provide stable results until a percentage of 17% MVs. Furthermore, FIML was the only algorithm that could cope with the maximum MV data set of almost 28% MVs. However, in the initial analysis the NFI was computed too low and SRMR too high (in comparison to the other estimation methods). Nonetheless, FIML provided evidence to provide unbiased estimates up to a percentage of 17% MVs.

In summary, it can be concluded that ML estimation seems to be biased if the percentage of MVs reaches 7%. Researchers are well advised to use the PLS algorithm if the percentage of MVs does not exceed 9%. FIML tends to be slightly more stable, and is able to provide unbiased estimates until a percentage of 17%.

This simulation study provides empirical evidence complementing Parwoll and Wagner's (2012) pioneering study in a more comprehensive in-depth look at the estimation accuracy and quality of the PLS, ML and FIML estimation methods in the presence of MVs. However, in this study, the performance of PLS, ML and FIML was investigated based solely on the case-wise deletion approach. Next steps are the consideration of other MV treatments, such as multiple imputations. Additionally, processes that generate missing values, such as censoring or truncation, should be considered. Furthermore, investigating various MV patterns could provide further insights into the performance, behavior, stability and estimation accuracy of well-known SEM estimation methods.

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