Introduction

Methods

A Framework for Adversarial Collaboration

Methods of Individual Simulation Studies

Studies by Kriegmair

The methodological setup of my individual simulation studies follows the structure we established for our *adversarial simulation* framework to facilitate stepwise collaboration. In the initial phase of our case study, I independently conducted two separate simulation studies without my collaborator's involvement with the goal to conceptually replicate the findings regarding SAM compared to standard SEM estimation of Rosseel & Loh (2022) and Dhaene & Rosseel (2023). However, there are several differences in the design and setup of the studies compared to the original studies as outlined below.

Aims, objectives and research questions

Both studies aimed to evaluate the performance of vanilla SEM (with maximum likelihood) compared to global SAM (gSAM), local SAM with maximum likelihood (lSAM-ML), and local SAM with unweighted least squares (lSAM-ULS) under various conditions. The two research questions we jointly established prior to conducting the studies served as general basis for both studies:

1. How do SAM and traditional SEM methods (including ML and ULS) compare in terms ofbias, Mean Squared Error (MSE), and convergence rates in small to moderate samples?
2. What is the impact of model misspecifications, such as residual correlations and cross-loadings, on the performance of SAM compared to traditional SEM methods?

Population Models and Data Generation Mechanisms

Study 1

Data were generated based on a 5-factor population structural model with 3 indicators for each factor. Four different models were simulated (see figure 1-4). In line with Rosseel & Loh (2022) this model design was chosen to represent a realistic model with sufficient complexity to pose a challange for the estimation methods, especially in the presence of misspecifications:

- Model 1.1: Correctly specified model.
- Model 1.2: Misspecified with cross-loadings in the population model that are ignored in the estimation model (model 1.1)
- Model 1.3: Misspecified with correlated residuals and a reversed structural path between the third and fourth latent factors in the population model that are ignored in the estimation model (model 1.1)
- Model 1.4: Misspecified with a bidirectional structural relation between factors 3 and 4 specified as only one directional

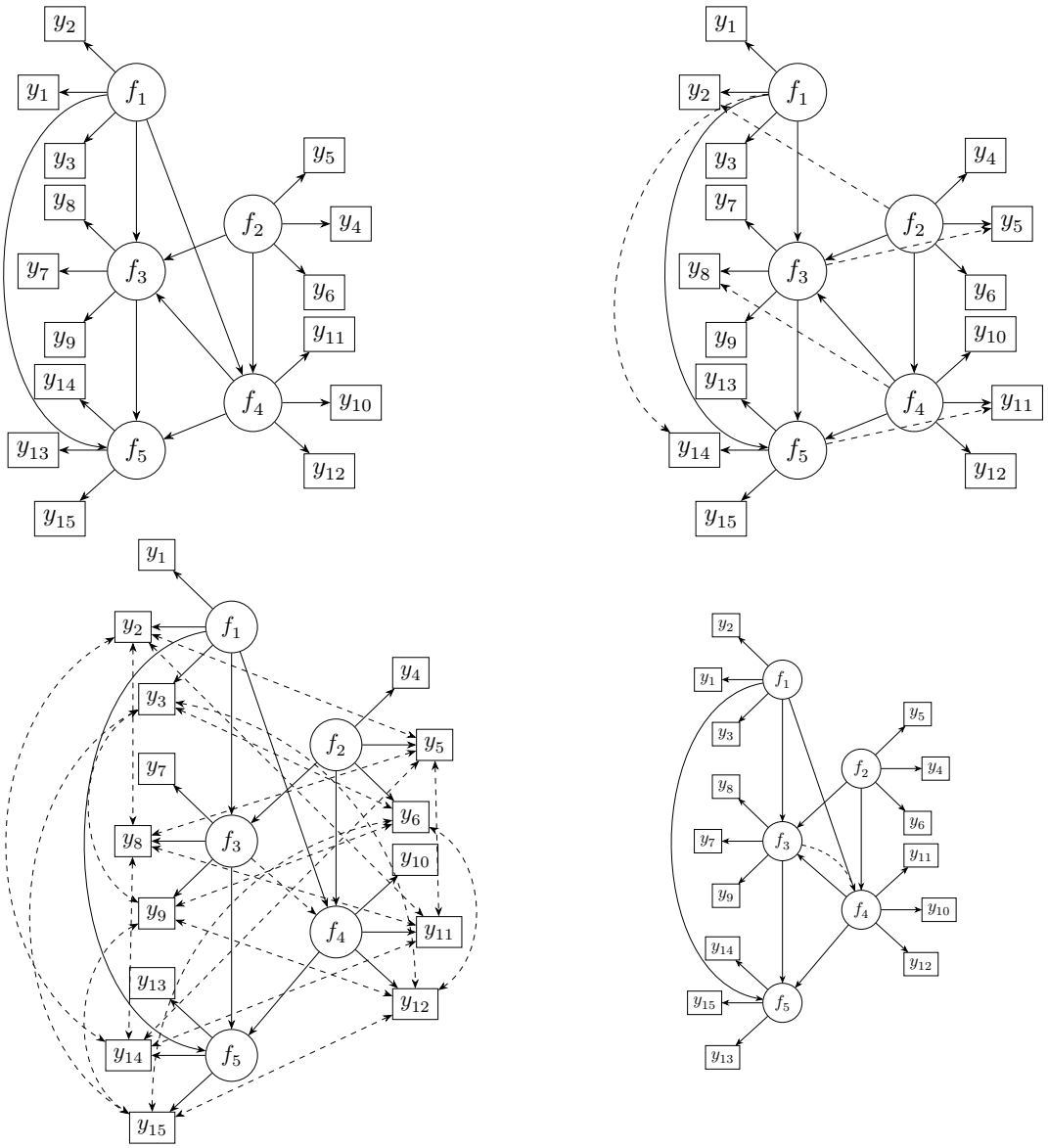
Factor loadings were fixed across all reliability conditions, with the first indicator of each factor serving as the scaling indicator ($\lambda = 1.0$), and the other two indicators having loadings of 0.7. Indicator reliability levels were manipulated by adjusting the measurement error variances in the Θ matrix. Specifically, the a reliability value was set at different levels (low = 0.3, moderate = 0.5 or high = 0.7) to compute the respective error variances on the diagonal of Θ: $\Theta^* = \text{Var}(\eta)\Lambda^T \times \frac{1}{r-1}$.

Deviation from Rosseel & Loh (2022):

To investigate additioanl possible and realisitic scenarios beyond the ones studied by Rosseel & Loh (2022) model 1.3 included a combination of measuremnt and structural misspecifications as opposed to only measurement misspecifications to introduce an even more severly misspecified model under which SAM methods might perform even better than traditional SEM. Further, model 1.4 included a (not estimated) bidirectional structural relation between factors 3 and 4 as opposed to the unidirectional reversed one. For all models, the population-level values of the structural parameters were set to 0.1.

Figure 1.

Population Model Variations of Study 1



Note. Error terms are not explicitly shown in the figure. Dashed lines represent relations omitted in the estimation model present in the population model."

Study 2:

Data were generated based on a 5-factor population structural model with 3 indicators for each factor with loadings set to 1, 0.9 and 0.8 for each factor and reliability modulated like in study 1. Regression weights were set to either 0.183 and 0.224 (low) or 0.365 and 0.447 (medium). This should represent varying variance explained (R^2) by the endogenous factors set at low ($R^2 = 0.1$) or medium ($R^2 = 0.4$). Note however that the computation of this was a simplification and does not accurately result in said R^2 values. The aim here was only to generally modulate between lower and higher regression weights. The population models resulted in the following model types with varying misspecification in the estimation model:

- Model 2.1: structural misspecifcation with falsely specified paths in the estimation model absent in the population model (Figure 5)
- Model 2.2: correlated residuals and a factor cross-loading in either the exogenous (Model 2.2-exo), endogenous (Model 2.2-endo) part of the model or both (Model 2.2-both) with falsely specified paths in the estimation model absent in the population model (see figure 5-6).

Deviation from Dhaene & Rosseel (2023):

To enable the analysis of the impact of falsely specified paths in the estiamtion model that are not present in the population model and how well the different methods recover these non-existing relations both population models included several such misspecifications in addtion to the measurement misspecifications evaluated by Dhaene & Rosseel (2023).

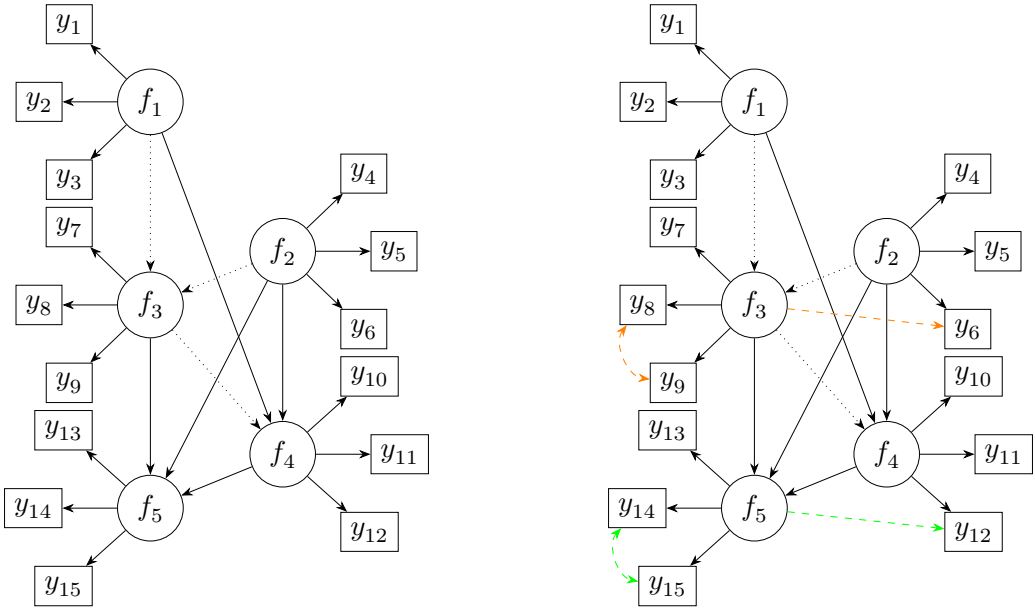
Experimental Design of simulation procedures

Study 1

Study 1 varied three main conditions: (1) sample sizes of small ($N = 100$), moderate ($N = 400$), and large ($N = 6400$); (2) Indicator reliability of low (= 0.3), moderate (0.5), high (= 0.7); (3) Model specifications: correctly specified model and misspecified with not specified cross loadings in the population model (see figure 2), misspecified with not-specified correlated residuals and a reversed structural path between the the third and

Figure 2.

Population Model Variations of Study 2



Note. Error terms are not explicitly shown in the figure. Dotted paths represent relations specified in the estimation model not present in the population model. For Model 2.2, orange lines represent misspecifications in the exogenous part of the model, and green lines represent misspecifications in the endogenous part of the model. These types of misspecifications result in different realizations of model 2.2 when they are modulated as factors in study 2 but are subsumed under one model here.

the fourth latent factor in the population model (see figure 3) and a recursive structural relation between factor 3 and 4 in the population specified as only one directional (see figure 4).

Study 2

Study 2 varied five conditions: (1) sample sizes: small ($N = 100$), medium ($N = 400$), and large ($N = 6400$). (2) Variance explained by endogenous factors: low ($R^2 = 0.1$) and medium ($R^2 = 0.4$). (3) Indicator reliability: low (0.3), moderate (0.5), and high (0.7). (4) Model misspecifications: varying the population model by omitting a residual covariance and a factor cross-loading in different parts of the model. (5) Number of measurement blocks: separate measurement model per latent variable ($b = 5$) and joint measurement model for all exogenous variables ($b = 3$) for the local SAM condition (lSAM-ML).

Method Selection

Both studies compared the performance of four estimation methods: Vanilla SEM with maximum likelihood (ML), Global SAM with maximum likelihood (gSAM), Local SAM with maximum likelihood (lSAM-ML), Local SAM with unweighted least squares (lSAM-ULS).

Performance Measures

For both studies convergence rates were tracked via lavaan's built-in function that indicates convergence. Further, improper solutions, converged models that showed negative variances (as the only type of improper solution present), were tracked via lavaan warning messages. Next of all converged and propper solutions bias ($\bar{T} - \theta$), and RMSE ($\sqrt{\frac{1}{K}\sum_{k=1}^{K}(T_k - \theta)^2}$) where T_k is the estimated parameter, $\bar{T}$ the mean of the estimated parameters and θ the true parameter value, and K is the number of replications computed. For comparability across varying regression weights for study 2, relative bias ($\frac{\bar{T}-\theta}{\theta}$) and relative RMSE ($\sqrt{\frac{(\bar{T}-\theta)^2+S_T^2}{\theta^2}}$) were computed. Monte Carlo standard errors (MCSE) were computed for bias and RMSE as well as relative bias and relative RMSE:

$\sqrt{\frac{S_T^2}{K}}$ and $\sqrt{\frac{S_T^2}{K\theta^2}}$ for bias and relative bias, and $\sqrt{\frac{K-1}{K}\sum_{j=1}^{K}\left(\text{RMSE}_{(j)}-\text{RMSE}\right)^2}$ and $\sqrt{\frac{K-1}{K}\sum_{j=1}^{K}\left(rRMSE_{(j)}-rRMSE\right)^2}$ for RMSE and relative RMSE.

Software

All analyses were conducted in R Core Team (2023). Simulation and estimation was done using Rosseel (2012). To ensure reproducability and avoid synchronization in parallelized a pre-generated list of seeds was used for all replications. For further details and a complete list of libraries and dependencies, visit https://github.com/valentinkm/AdversarialSimulation.

Analysis and Interpretation plan

Similar to the studies by Rosseel & Loh (2022) and Dhaene & Rosseel (2023) results were interpreted by descriptively comparing the performance measures of the different estimation methods under varying sample sizes, indicator reliability levels, and model misspecifications without predetermined cut-off values or critical distances. Performance metric values were aggregated across all parameters excluding the misspecified parameters (present in the population but not in the estimation model).

Studies by Kosanke

```
Current working directory:  /home/rstudio/VK/thesis
```

```
Does LK/thesis.qmd exist?  TRUE
```

Methods

The structure of this section closely aligns to our agreed upon structure of simulation studies in Table 1.

In a first step, I published a simulation protocol containing all the planned analysis to be replicated from the original paper by Robitzsch (2022). This protocol can be accessed

here: https://github.com/lkosanke/AdversarialSimulation/blob/main/LK/simulation_protocol.pdf.

Aims, objectives and research questions

For my individual study, I replicated parts of Robitzsch (2022) that were relevant to our two substantive research questions. Overall, I conducted 6 simulation studies.

Population Models and Data Generation Mechanisms

The most important details with regards to the population models and data-generating mechanisms are visible in Table 7. With regards to the population models, all factors in all studies loaded onto 3 indicators each. I chose the population values to align with the original paper by Robitzsch (2022). The multivariate normally distributed data was generated parametrically, based on a specified population model. All simulations were conducted using seeds to allow for the reproducibility of results.

For more details on the exact values of each study, see the simulation scripts in the Github repository.

Study	Model	Correct model included?	Unmodelled RC	Unmodelled CL	N Sizes	φ/ β	λ
Study 1	2-factor-CFA	Yes	1 and 2, both pos. and neg.	x	7	φ = 0.6	Fixed
Study 1b	2-factor-CFA	Yes	x	x	2	φ = 0,2 - 0.8	Varied
Study 2	2-factor-CFA	x	x	1 and 2, both pos. and neg.	7	φ = 0.6	Fixed
Study 3	2-factor-CFA	x	1, pos.	1, pos.	7	φ = 0.6	Fixed
Study 4	5-factors	Yes	20, all pos.	5, all pos.	7	β = 0.1	Fixed
Study 4a	5-factors	x	20, all pos.	5, all pos.	7	β = 0.1 - 0.4	Fixed

Note. Φ: factor correlation, N: sample size, λ: factor loading, σ: residual variance, τ: factor variance, RC: residual correlations, CL: cross-loadings, CFA: confirmatory factor analysis, β: regression coefficient between factors.

Overview of Simulation Studies conducted by Kosanke

Experimental Design of simulation procedures

Overall, 3 different types of factors were varied that can be deduced from Table 7 and are detailed again in the simulation scripts provided.

Firstly, I varied the sample size in all studies, ranging from N = 50 to 100.000. I included a smaller sample size N=50 for all studies, to be able to answer our substantive research questions in more detail. Study 1b explicitly investigated the small sample bias of LSAM estimation in low sample sizes. Thus, only N=50 and N=100 were present in this study.

Additionally, I varied the amount of misspecification in all studies, either via different numbers of unmodelled residual correlations, cross-loadings, or both.

Thirdly, in Studies 1b and 4a, I varied the population values for three model parameters (phi, beta and/ or lambda).

Besides studies 1 and 2, I implemented full factorial designs. In Studies 1 and 2 I omitted conditions were both one positive and one negative value would be present. I hypothesize that this was done in Robitzsch (2022) to avoid cancellation of biases, but the authors did not give reasoning for this decision themselves.

In Studies 4 and 4a I investigated the differential performance of the estimators in a model that included a non-saturated structural model (i.e. regressions between some of the factors). These studies were replications not only of the paper by Robitzsch (2022), but of the first paper on the SAM approach by Rosseel & Loh (2022). In contrast to the other studies, studies 4 and 4a differed in the way the misspecification variation was labelled in Robitzsch (2022). Instead of varying a factor misspecification as in the previous study, they varied 3 different data-generating mechanisms (DGM's) as a whole. Thus the conditions are labelled differently: DGM 1 contained no misspecification. DGM 2 contained 5 cross-loadings in the data-generating model, that were not modelled in the estimated models. DGM 3 contained 20 residual correlations that were not modelled in the models. I extended them to investigate the interaction of beta and

N for the 5-factor regression model, as this again was of interest four our substantial research questions. Additionally, I omitted the inclusion of DGM 1 in Study 4a, as it neither contained misspecification (which is central to our research question), nor did it lead to interesting results in the original study.

Method Selection

In terms of estimation methods, I used constrained SEM maximum-likelihood (SEM-ML) and unweighted-least-squares estimation (SEM-ULS), so that loadings and variance parameters were given the constraints that they had to be positive and larger than 0.01. Additionally, I implemented local-SAM (LSAM) and global-SAM (GSAM) estimation, in both maximum-likelihood (LSAM-ML/ GSAM-ML), and unweighted-least-squares estimation (GSAM-ML/ GSAM-ULS) contexts. Exceptions were studies 1b, 4 and 4a, where only LSAM was investigated, as results did not really differ between the two different SAM-methods (Robitzsch, 2022).

Performance Measures

I calculated the bias and RMSE of the estimated factor correlations in all studies, as well as the standard deviation of the one factor correlation present in Studies 1,2 and 3. For the type of bias calculated, I oriented on Robitzsch (2022), besides in Study 1b. Thus, I calculated average relative bias in Studies 1, 2 and 3, and average absolute bias in Studies 1b, 4 and 4a. In Study 1b, I took the absolute value to see if negative and positive biases canceled each other out in the original study for conditions with lower phi values. In addition to what was done in Robitzsch (2022), I calculated confidence intervals for the bias estimates, but omitted them in the results tables for presentation purposes. The exact computation of the performance measures is detailed in the simulation scripts and results.pdf file in my sub-folder of the Github repository.

I did not include a detailed mechanism to capture model convergence as detailed in the first substantive research question. As Robitzsch (2022) argued in their paper, and was shown already in other simulations, using constrained maximum likelihood estimation should resolve convergence issues of classical maximum likelihood estimation in smaller samples (Lüdtke et al., 2021; Ulitzsch et al., 2023). I did include, however, a mechanism

to track the total number of warnings for each estimation and compare it to the total number of estimations as a sanity check.

Software

All analyses were conducted in R (R Core Team, 2023). I used the packages lavaan, purrr, tidyverse, furrr to conduct the simulations, as well as knitr and kableExtra for presenting the results (Rosseel, 2012; Vaughan & Dancho, 2022; Wickham et al., 2019; Wickham & Henry, 2023; Xie, 2024; Zhu et al., 2024) .

Analysis and Interpretation plan

For the interpretation of results, I oriented on cut-offs that were used in the original paper by Robitzsch (2022). For bias, I interpreted differences of 0.05 or higher as substantial. For SD, I explicitly mentioned percentage reductions of more or equal to 5%. For RMSE, the same interpretation was used for differences of 0.03 or higher. The simulation was repeated 1500 times for each Study.

Methods of "Joint" Simulation Study

After collaborating based on the individually conducted studies and the respective results, we did not jointly arrive at the conclusion that conducting a collaborative simulation study as planned was warrented.

However I identified several reasons for setting up another simulation. Firstly, to test and evaluate the viability and technical fesability of AC for simulation studies, setting up a study based on the individual studies, their results and with Kosanke can provide valuable…

Aims, objectives and research questions

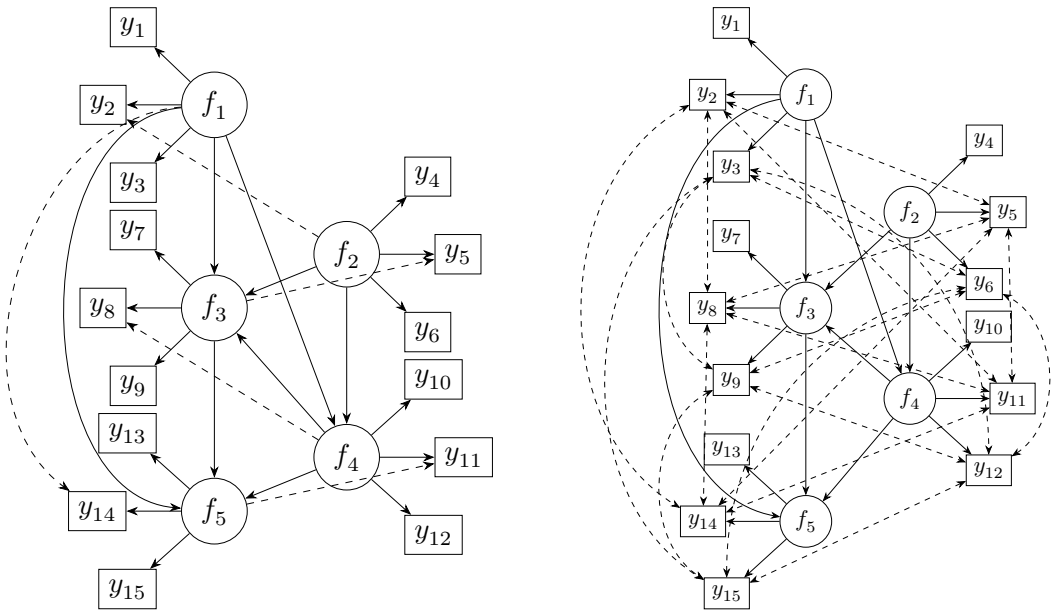
Following our framework for collaboration the research questions for the joint study remains the same as specified prior to the individual studies.

Population Models and Data Generation Mechanisms

As in study 1 and 2 data for study 3 was generated based on a 5-factor population structural model with 3 indicators for each factor. Factor loadings and indicator reliability was computed in the same way as in study 1. Two different population models were simulated that resulted in misspecifications of either omitted crossloadings (model 3.1) or omitted correlated residuals (model 3.2). The population-level values of the structural parameters were set to 0.1. Reliability levels were manipulated as in Study 1. The omitted crossloadings (see figure 7) could either be all positive or negative and were set to be 10% lower in absolute values than the factor loadings. Correlated residuals were also either all positive or all negative and were set to not exceed a factor of 0.6 of the residual variances of the indicators.

Figure 3.

Population Model Variations for Study 3



Note. Note. Error terms are not explicitly shown in the figure. Dashed lines represent relations omitted in the estimation model present in the population model. Unspecified crossloadings and correlated residuals could be either positive or negative resulting in 2 modulations of model 3.1 and 3.2 in the study.

Experimental Design of simulation procedures**

The joint study varied three conditions: (1) sample sizes of very small ($N = 50$), small ($N = 100$) or moderate ($N = 400$). (2) Indicator reliability of low ($= 0.3$), moderate (0.5) or high ($= 0.7$); (3) Model misspecifications with not-specified cross loadings in the population model that were positive or negative (see figure) or not-specified correlated residuals in the population model that were postive or negative (see figure 8).

Method Selection

To address the question ...

Performance Measures

Software

To fully evaluate the effect of bound SEM on convergence convergence rate and rate of proper solutions were tracked condition wise (Kriegmair's individual studies).

Analysis and Interpretation plan

The analysis was conducted largely in the same way as in the individual studies

Results

Results of Individual Simulation Studies

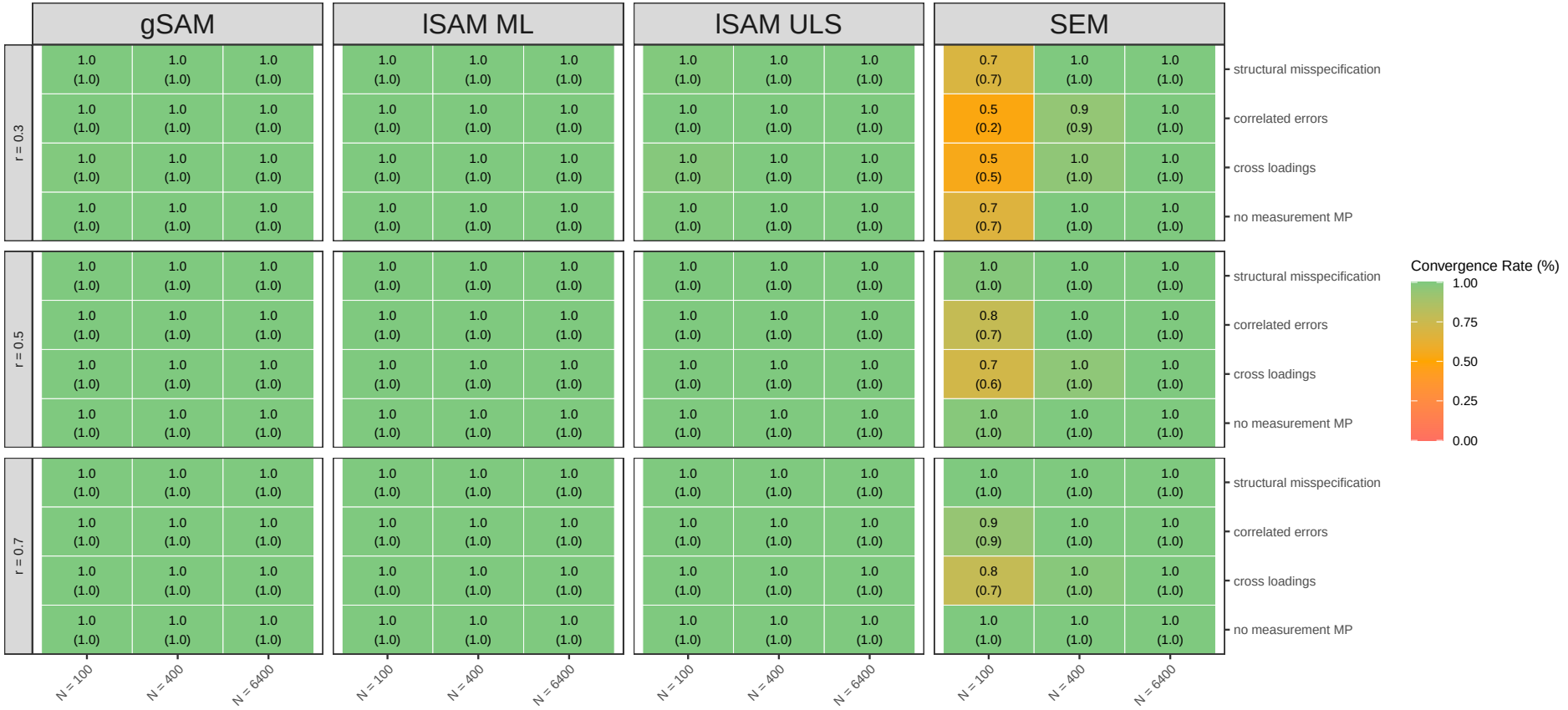
Results of Kriegmair's Simulation Studies

As shown in Figure 4 there were no convergence issues for all SAM methods (gSAM, lSAM ML and ULS) with a convergence rate of 100% and no improper solutions across all conditions even in small samples with low reliability. Standard SEM however showed severe convergence issues in small samples with low to moderate reliability with a

convergence rate of as low as 50% and 50% improper solutions in the cross loading misspecification condition as the most challenging condition.

Figure 4.

Convergence Rate and Rate of Proper Solutions in Study 1



Note. Convergence and proper solutions (in parentheses) rates across sample sizes (N), reliability (r), and model misspecifications for global SAM (gSAM), local SAM with Maximum Likelihood (lSAM-ML), Unweighted Least Squares (lSAM-ULS), and SEM.

Convergence rates in study 2 were consistent with this with 100% convergence rates for all SAM methods and as low as 60% for standard SEM with exogenous measurement misspecifications posing more challenges than endogenous misspecifications (see Figure A1 in Appendix B).

Results of Kosanke's Simulation Studies

Results of the "Joint" Simulation Study

Results of the Adversarial Collaboration

Discussion

Discussing the substanital results

Disucssing the Adversarial Collaboration

Idea: living simulations

References

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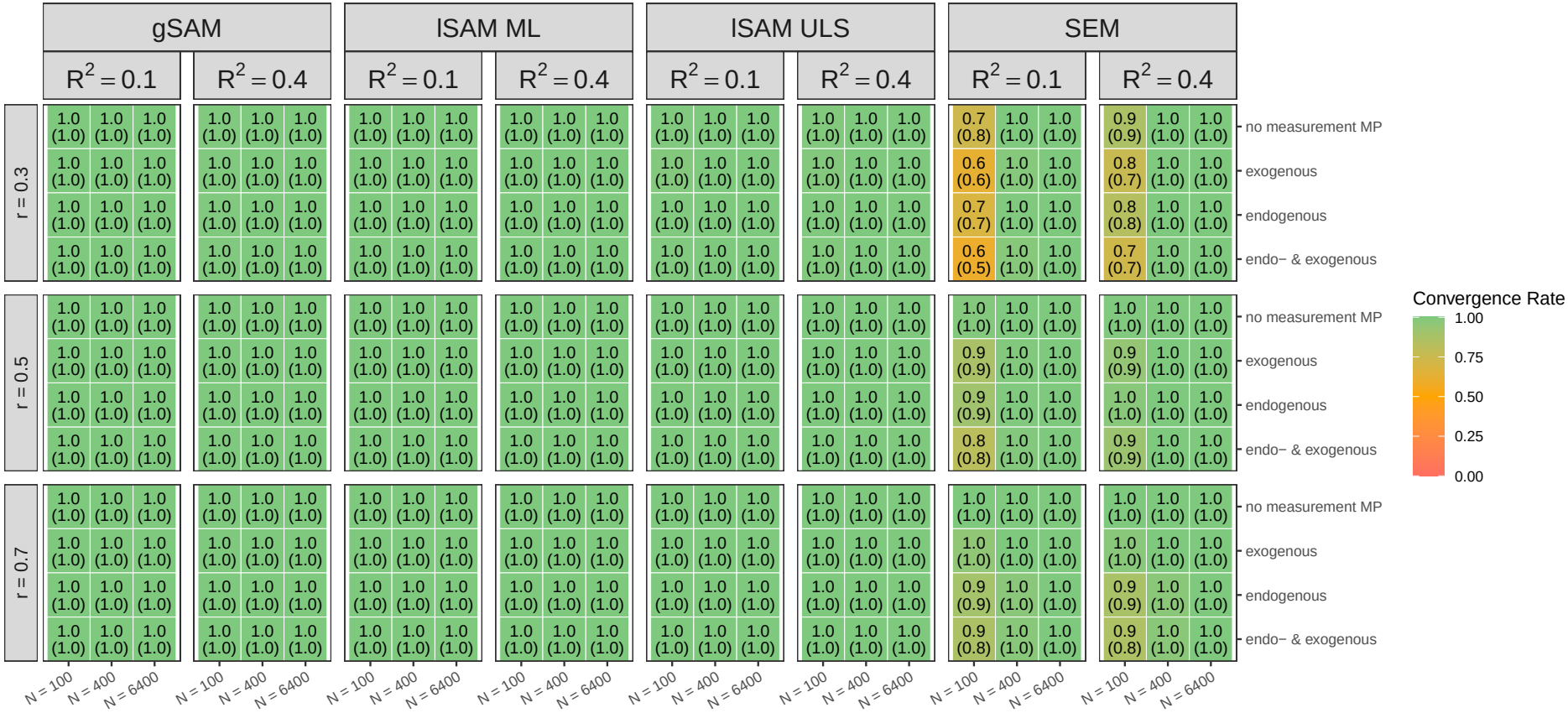
Appendix A: Simulation Protocol

Appendix B: Supplementary Figures

Figure A1.

Convergence Rate and Rate of Proper Solutions in Study 2



Note. Convergence and proper solutions (in parentheses) rates across sample sizes (N), reliability (r), and model misspecification location for global SAM (gSAM), local SAM with Maximum Likelihood (lSAM-ML), Unweighted Least Squares (lSAM-ULS), and SEM.