Abstract

Lorem Ipsum is simply dummy text of the printing and typesetting industry. Lorem Ipsum has been the industry's standard dummy text ever since the 1500s, when an unknown printer took a galley of type and scrambled it to make a type specimen book. It has survived not only five centuries, but also the leap into electronic typesetting, remaining essentially unchanged. It was popularised in the 1960s with the release of Letraset sheets containing Lorem Ipsum passages, and more recently with desktop publishing software like Aldus PageMaker including versions of Lorem Ipsum.

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Table of contents

Introduction

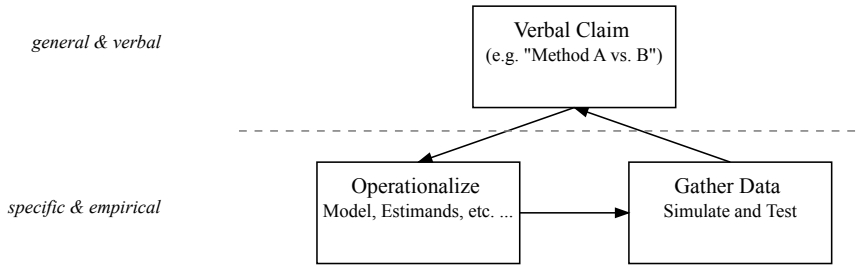
The Challenge of Generalizability within the Research Cycle of Simulation Studies

Karl Popper once described science "as the art of systematic over-simplification — the art of discerning what we may with advantage omit" (Popper, 1988). This pointedly encapsulates the fundamental cycle of empirical research. Researchers formulate general claims about the world, translate them into specific, measurable constructs, select appropriate methods to collect data from specific populations, and finally update their beliefs about these general claims based on the gathered data (Supino, 2012). A core challenge in every research endeavour is this mapping from the general to the specific when designing and conducting a study and, conversely, from the specific and empirical back to the general when interpreting the results. This traversing between layers of abstraction is the crux of most research, and it is where many, if not all, of a researcher's degrees of freedom lie (Carrillo & Martínez, 2023; Dellsén & Baghramian, 2021; Martínez & Huang, 2011). If there is ambiguity or lack of transparency in these mappings, irreproducible and ungeneralizable results (Camerer et al., 2018; Earp & Trafimow, 2015; Nosek et al., 2022) as well as persistent and seemingly unresolvable disagreements on the general and verbal level can emerge (Cleeremans, 2022; Dellsén & Baghramian, 2021).

This challenge of generalizability manifests uniquely in Monte Carlo simulation studies. These are widely utilized tools to assess the reliability and validity of statistical methods by testing their performance against controlled, simulated data, where the true population parameter values (of the data generating mechanism) are known. This approach allows researchers to investigate biases, variances, and other properties of estimators or models under various conditions, often informing best practices and model improvements Morris et al. (2019). These simulations, constrained by their specific settings, heavily depend on inductive reasoning to draw general conclusions, as it is impossible to simulate and test every conceivable combination of population and analysis model (Feinberg & Rubright, 2016; Gilbert & Miratrix, 2024). Consequently, researchers face numerous degrees of freedom in deciding which prototypical models and settings to examine when assessing a method's general applicability and performance Kulinskaya et al. (2020). Hence, it becomes clear that simulation studies follow the same general research cycle as empirical studies, with similar challenges of generalizability ambiguity (see Figure 1).

Figure 1

The research cycle of simulation studies



Note. Arrows represent the progression from each stage of the research cycle to the next, involving various decision-making elements when moving from the general to the specific and back to the general.

To address these challenges, just like for empirical research, open science practices such as preregistration, transparency, and reproducibility have been proposed for simulation studies (O'Kelly et al., 2017; Pawel et al., 2023). These practices are pivotal for increasing rigour and transparency in simulations and beyond. However, in the basic cyclical process of research, as outlined above, they mainly address the issue of generalizability at the point of moving from operationalization to data simulation, e.g. by enforcing transparency and reproducibility of the simulation (Luijken et al., 2023), or at the point of verbally interpreting gathered data through adherence to preregistration protocols. Crucially, however, these practices do not address the transition from the verbal claim to its operationalization (in empirical research, referred to as *translational validity(Slife et al. (2016))). Decisions about operationalizing, for example, which models and settings to choose and how to design the study, remain subject to researchers' degrees of freedom and their (often implicit) biases (Buchka et al., 2021). Furthermore, even rigorous and transparent studies may produce conflicting verbal claims from ambiguities in operationalizations and specific simulation setups. Such disagreements may not be readily resolvable, or only inefficiently so, by independently conducting and publishing simulation studies. Researchers' biases toward specific methods they have developed themselves may further amplify these divergences, affecting not only the interpretation of results but also choices in the design of simulation studies (Buchka et al., 2021).

Adversarial Collaboration

For empirical research, Adversarial Collaboration (AC) has been proposed to address ambiguity and improve generalizability throughout the research cycle, mainly when entrenched

disagreements between researchers and theories have emerged. Pioneered by Ralph Hertwig and Daniel Kahneman and in their attempt to resolve a debate on frequency representation involving Barbara Mellers as a neutral arbiter (Mellers et al., 2001), it has since been recognized for its potential within the open science movement (C. J. Clark et al., 2022; C. Clark & Tetlock, 2021; Rakow, 2022). Unlike standard open science practices, which may not account for researchers' degrees of freedom in hypothesis generation and operationalization, AC allows for detecting and reducing biased methodological decisions. In AC, opposing researchers first identify general verbal theoretical disputes, agree on a shared research question that could settle the debate, and collaboratively design studies they agree to have the potential to change their minds and jointly publish the results regardless of the outcome (Melloni et al., 2021). This process aims to unveil and concretize even subtle discrepancies in methodological assumptions and decisions as well as framing of conclusions (C. J. Clark et al., 2022), thus tracing back general and verbal disagreements of conflicting theories to their specific and empirical roots, reducing ambiguity and increasing generalizability by generating shared language of assumptions and operationalizations. Hence, it promises to enhance rigour and transparency and, importantly, reduce ambiguity and bias at the stage of operationalization and design of studies (C. Clark & Tetlock, 2021).

SAM vs. SEM - A Case Study for *Adversarial Simulation*

In this project, we aimed to adapt this concept of AC from empirical research to Monte Carlo simulation studies, examining the feasibility and viability of such an *Adversarial Simulation* (AS). As a substantive test case, we focused on recent conflicting findings regarding the performance of Structural After Measurement (SAM) — a method for Structural Equation Model (SEM) estimation recently reintroduced by Rosseel & Loh (2022).

Structural equation modelling (SEM) encompasses various statistical techniques frequently applied in the social and behavioural sciences (Bollen, 2014; Hoyle, 2012). SEM is most commonly employed to study models incorporating measurement and structural components. The measurement model describes the relationships between latent variables and their observed indicators, while the structural model specifies the relationships among the latent variables themselves, often reflecting substantive theoretical constructs of interest (Hair Jr et al., 2021). Traditional SEM estimation methods, like maximum likelihood estimation, optimize all parameters of a model simultaneously (under the assumption of multivariate normality) by minimizing a discrepancy function $F(\theta)$, where θ represents all parameters of both the measurement and structural models (Kline, 2023). While powerful, this system-wide estimation suffers from several shortcomings, such as non-convergence, improper solutions (with solutions including parameters out of their definitional range, such as negative variances (Van Driel, 1978)),

poor model fit, and estimation biases arising from local measurement misspecifications that can affect the entire model. They also typically require large sample sizes for adequate performance, especially in complex models with many parameters(Rosseel, 2020). SAM - as proposed by Rosseel & Loh (2022) - addresses these issues and separates the estimation process into two distinct stages. First, the measurement model parameters are estimated independently to capture the relationships between latent variables (η) and their observed indicators (y), represented by:

$$y = \mu + \Lambda\eta + \epsilon,$$

where μ is a vector of intercepts, Λ is the factor loading matrix, and ϵ denotes measurement errors. In the second stage, structural model parameters are estimated using the latent variable estimates from the first stage, modelled as:

$$\eta = \alpha + B\eta + \zeta,$$

with α as a vector of intercepts, B as the matrix of structural coefficients, and ζ as structural disturbances. Rosseel & Loh (2022) proposes two distinct approaches to SAM estimation: (1) Local SAM constructs estimators for latent variable means and covariances from first-stage estimates and applies them directly in second-stage analyses (e.g., linear regression). Expected values $E(\eta)$ and covariance $\text{Var}(\eta)$ are derived as:

$$E(\eta) = M(y - \mu),$$

$$\text{Var}(\eta) = M(S - \Theta)M^T,$$

where M is derived from factor loadings and measurement error covariances, S is the sample covariance matrix of y, and Θ is the covariance matrix of ϵ. (2) Global SAM keeps first-stage measurement model parameters fixed while estimating structural model parameters using standard SEM techniques.

Recent studies by Rosseel & Loh (2022) and Dhaene & Rosseel (2023) have shown that SAM can outperform traditional SEM estimation in the presence of model misspecifications, especially in small to moderate sample sizes. However, Robitzsch (2022) has challenged these findings, arguing that SAM may systematically underestimate parameters in the presence of negative misspecifications. This disagreement highlights the need for a systematic evaluation of SAM's performance in the presence of model misspecifications in small to moderate sample sizes.

These diverging claims served as the starting point for an adversarial collaboration

between a fellow student researcher (Collaborator B, Kosanke) and me (Collaborator A, Kriegmair), each representing one of the above sides of the differing findings.

We developed a basic framework to tailor the concept of AC to simulation studies and facilitate a structured and systematic conduct and evaluation of the AC process in which a conceptual replication of respective findings by each collaborator marks the starting point representing a suitable testing ground for *Adversarial Simulation*. The framework, outlined in detail in the following section, consisted of two rounds: In the first round, each collaborator would independently conduct a separate simulation study. In the second round the adversarail collaboration would take place and we planned to collaboratively design and conduct a study based on the first round. This two-stage approach was designed to systematically highlight differences between the individual approaches and establish a virtual foundation for collaboration before engaging in a joint effort in our case study. As the first step of this process, we jointly formulated two *specific* research questions based on the above-mentioned conflicting claims:

1. How do SAM and traditional SEM methods (including ML and ULS) compare regarding bias, 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?

Finally, by conducting this case study, we thus aimed to answer our *general* meta-research question: Is adversarial collaboration a viable and practical applicable tool to resolve disagreeing research claims and enhance generalizability and rigour in the context of simulation studies?

Methods

A Framework for Adversarial Collaboration

We developed a specific adversarial simulation framework and structured the collaboration into two rounds. In the first round, each collaborator independently conducts a separate simulation study. In the second round, they come together to work on a joint study, building on the findings from the first round. This two-step approach is designed to highlight differences in a systematic way and to establish a virtual foundation for collaboration before engaging in a joint effort in our case study. Further, we aimed to adhere the individual studies to a protocol of core steps of a simulation study adapted from Paxton et al. (2001) where critical and distinctive decisions by the researchers occur (see Figure 2). Thus we aimed to facilitate a structured and systematic comparision of the individual studies and enable stepwise retracing of collaborative decisions.

Figure 2

Framework for Simulation Studies

Step	Description
1. Aims & Research Questions	Agreed upon before any adversarial collaboration (e.g., examine model fit under misspecification)
2. Population Model Specification	Optional: Define structure (e.g., CFA, SEM), size (number of latent variables and indicators) and complexity (e.g., cross-loadings) of population models.
3. Data Generating Mechanism	Choose resampling vs. parametric draw and set the random data generation method.
4. Experimental Design	Define varying factors (e.g., sample size and distribution).
5. Method Selection	Select estimation methods based on the research question.
6. Defining Estimands	Reflect applied values, e.g., R^2, statistical significance, power considerations.
7. Performance Measures	Choose performance metrics (e.g., bias, sensitivity, accuracy); set simulation number for adequate Monte Carlo standard error.
8. Software Selection	Select software, libraries, and functions for simulation.
9. Analysis	Decide on descriptive vs. inferential analysis and performance criteria

Individual Simulation Studies

Studies by Collaborator A (Kriegmair)

The methodological setup of my individual simulation studies follows the structure we established for our *adversarial simulation* framework to facilitate stepwise collaboration. It is based on a preregistered protocol but includes some deviations from the preregistration (See Appendix A for the full protocol and all deviations from the preregistration). 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 traditional 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 Generating Mechanism

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). 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

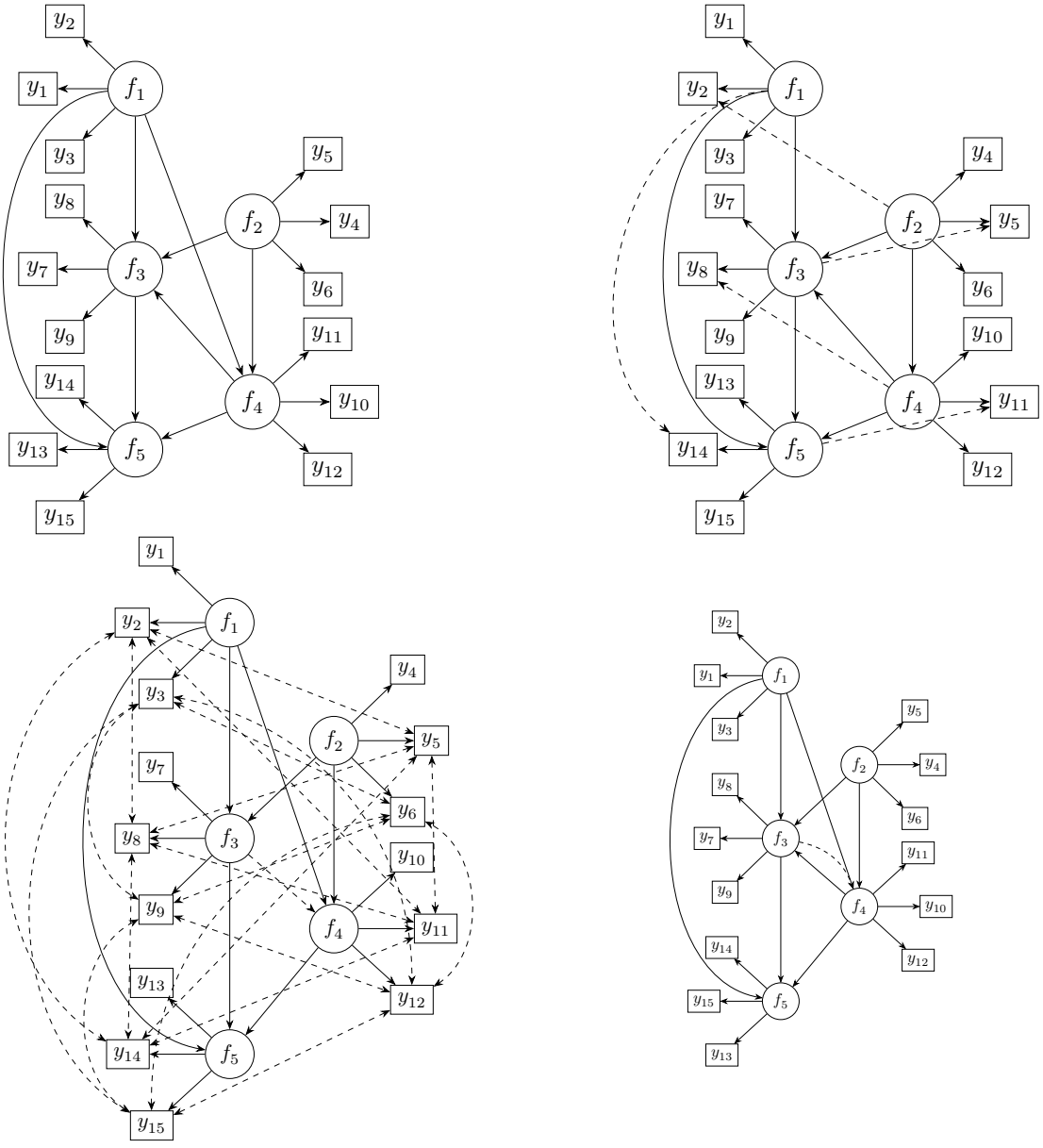
Factor loadings were fixed across all reliability conditions, with the first indicator of each factor serving as the scaling indicator ($\lambda = 1.0$), and the other two indicators having loadings of 0.7. Indicator reliability levels were manipulated by adjusting the measurement error variances in 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: $\Theta^* = \text{Var}(\eta)\Lambda^T \times \frac{1}{r-1}$.

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.

Study 2 Data were generated based on a 5-factor population structural model with three 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

Figure 3

Population Model Variations of Study 1

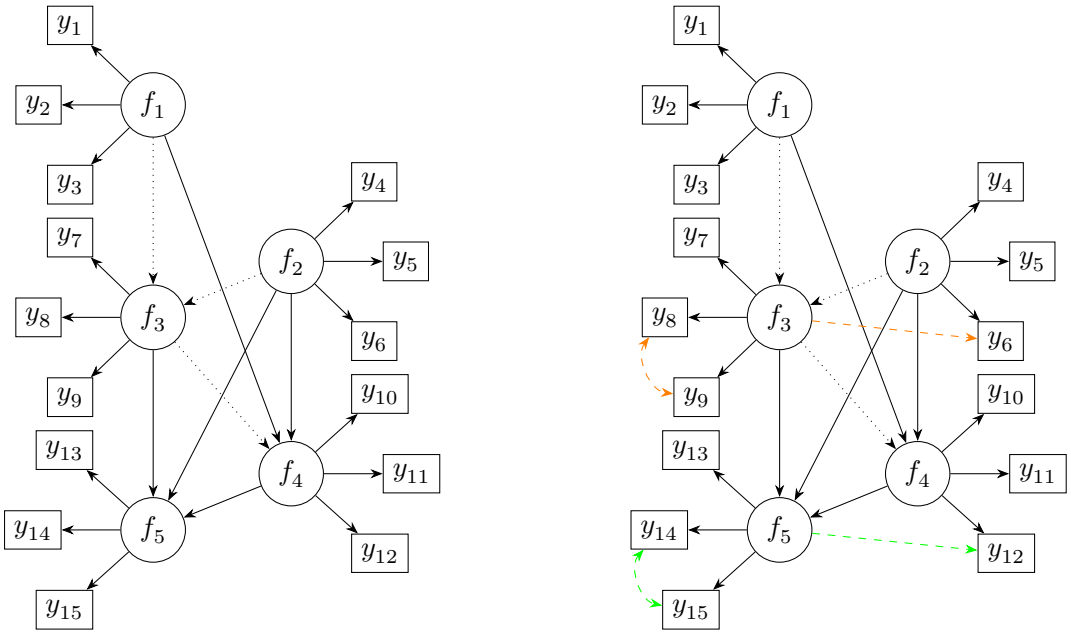


Note. Error terms are not explicitly shown in the figure. Dashed lines represent relations omitted in the estimation model present in the population model."

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: (1) Structural misspecifcation with falsely specified paths in the estimation model absent in the population model (See Figure 2). (2) correlated residuals and a factor cross-loading in either the exogenous, endogenous part of the model or both with falsely specified paths in the estimation model absent in the population model (see Figure 2). 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).

Figure 4

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 the model on the right, orange lines represent misspecifications in the exogenous part of the model, and green lines represent misspecifications in the endogenous part. These types of misspecifications result in different realizations of the model when they are modulated as factors of misspecification (endogenous, exogenous or endo- and exogenous) in study 2 but are subsumed under one model here.

Experimental Design

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 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: Traditional 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 The simulations were executed on the high-performance computing cluster of the Max Planck Institute for Human Development Berlin (MPIB). All analyses were conducted in R (version 4.4). (R Core Team, 2023). Main libraries includeded `lavaan` (Rosseel, 2012) for estimation and data generation, `furrr` (**davis_furrr_2022?**) for parallelization and `tidyverse`(Wickham et al., 2019a), `ggplot2` as well as `kableExtra` (Zhu, 2024) for results

analysis and display. To ensure reproducability and avoid seed synchronization in parallelized execution a pre-generated list of seeds was used for all replications and the simulations were dockerized (Merkel, 2014). Further details and a complete list of libraries and dependencies, are available on GitHub

Analysis and Interpretation 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. Performance metric values were aggregated across all parameters excluding the misspecified parameters (present in the population but not in the estimation model).

Studies by Collaborator B (Kosanke)

Here Kosanke's studies are presented verbatim from his report (Git commit SHA 3e7f706):
The structure of this section closely aligns to our agreed upon structure of simulation studies […]. 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.*

Figure 5

Overview of Simulation Studies Conducted by Kosanke

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.

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., 2019b; 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.*

Joint Simulation Study

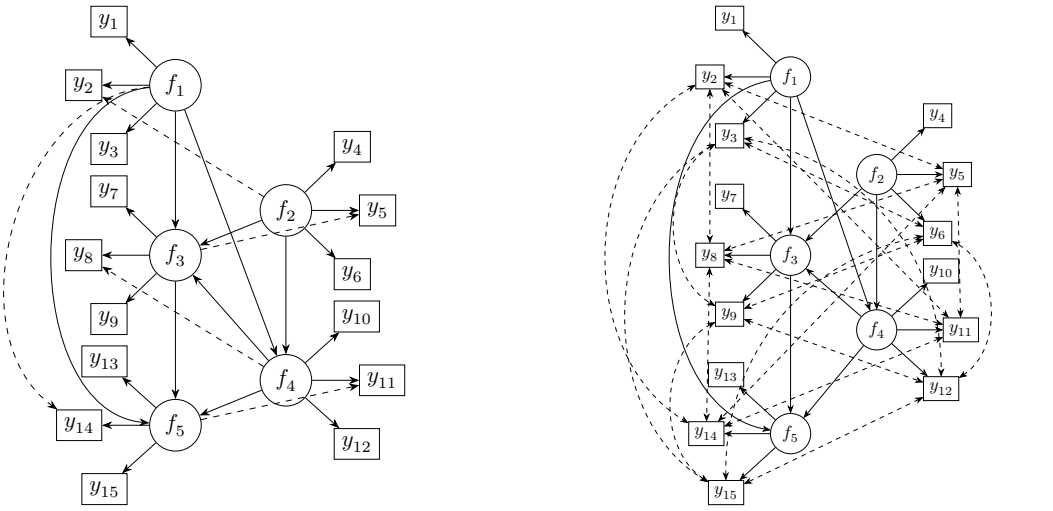
Aims, objectives and research questions Following our framework for collaboration the research questions for the joint study remains the same as specified prior to the individual studies.

Population Models and Data Generation Mechanisms As in my individually conducted studies 1 and 2 (Collaborator A, Kriegmair) data for this *joint* study 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 my first study. Two different population models were simulated, which 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 my first study by adjusting the measurement error variances (instead of Kosanke's approach of factor loadings modulation) to achieve a more valid representation of item reliability as the amount of indicator variance explained by the latent factor. The omitted crossloadings (see Figure 4) 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. Thus, this represents a sufficiently complex model with directed structural paths of interest as a prototypical scenario for which SAM promises to be advantageous, including negative misspecified measurement parameters to test the robustness of SAM to such misspecifications. No CFA models, as in Kosanke's (Collaborator B) studies, were included as SAM is intended to be applied to models with a directed structural part of interest in the presence of misspecifications Dhaene & Rosseel (2023).

Experimental Design of simulation procedures The joint study varied three conditions: (1) sample sizes of very small ($N = 50$), small ($N = 100$), moderate ($N = 400$) and large ($N = 6400$). (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 positive or negative (see Figure 4). Thus, negative misspecifications were here included in a more

Figure 6

Population Model Variations for Study 3



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 cross-loadings and correlated residuals could be either positive or negative, resulting in two modulations of models 3.1 and 3.2 in the study.

complex model with directed structural paths of interest, modulating reliability as before but with a more comprehensive (lower) range of sample sizes as in my studies.

Method Selection Four estimation methods were compared in this study: bound SEM-ML (with factor and residual variances constrained to be positive), unbound SEM-ML, gSAM (also with ML estimation of the structural model) and lSAM-ML. The choice of these methods was based on the results of the individual studies to (1) observe the effect of constraining the analysis model for standard SEM and (2) directly compare this to unbound standard SEM estimation and the SAM methods. To limit the computational scope and narrow down the comparison, SAM-ULS and SEM-ULS were not included as ULS estimation is mainly aimed to provide robust estimates in conditions of non-normal data distribution, which were not simulated in this study, and it was, based on our previous results, not expected to outperform SAM-ML in this study.

Performance Measures The bias and RMSE of the estimated factor correlations were calculated as in the individual studies and averaged (using absolute values) over all parameters in one model for each condition. Further, to better investigate a potential negative bias that Kosanke (based on Robitzsch (2022)) was assuming for SAM in the presence of negative measurement misspecifications, bias values were analyzed parameterwise to investigate negative bias values without cancellation due to averaging.

Software As in the individual studies by both collaborators, the simulation was conducted in R version 4.4 (R Core Team, 2023). The same (parallelizable and dockerized) setup as in my studies was used with a pre-generated set of seeds for reproducibility. The simulation scripts are available on GitHub.

Analysis and Interpretation The analysis was conducted largely in the same way as in the individual studies with the adddition of a display of parameter-wise bias values and a direct difference between metrics of SEM and SAM.

Results

Individual Simulation Studies

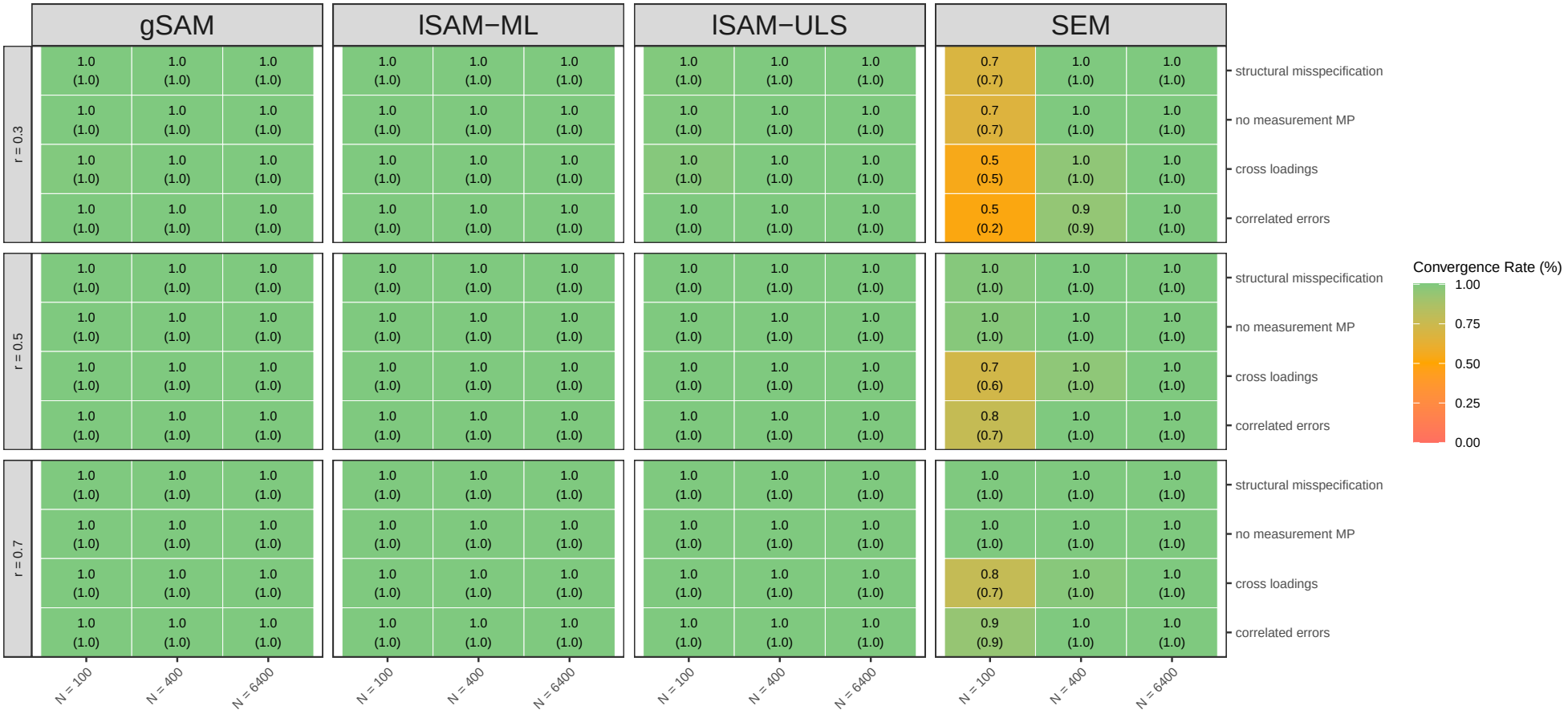
Results of Collaborator A (Kriegmair)

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 demonstrated severe convergence issues, particularly in small samples with low to moderate reliability. The convergence rate was as low as 50%, with 50% of the solutions being improper, especially under the challenging condition of cross-loading misspecification (see Figure 7). Next, the bias of the path coefficient estimates averaged across each model in absolute values showed that in small to medium sample sizes with low to moderate reliability, SAM methods were mostly closer to the true parameters than standard SEM. This difference was especially pronounced under omitted cross-loadings in the analysis model. However under correlated residuals standard SEM was slightly less biased. Large sample sizes and high reliability conditions showed the least bias overall, with no differences observed between the methods (see Figure 8). Further, among the different SAM methods, there was no difference between gSAM and lSAM-ML, while lSAM-ULS performed slightly worse. This pattern was mostly consistent with the RMSE of the path coefficients: SAM methods showed lower values than standard SEM in small to medium sample sizes with low to moderate reliability, indicating higher overall accuracy for SAM methods in challenging conditions. This was notably also the case under correlated residuals where SEM was less biased, which highlights SAM's advantage here as well in light of a trade-off between (slightly higher) bias and precision (see Figure B2). In contrast to the bias, the RMSE showed that lSAM-ML performed better than gSAM and lSAM-ULS under cross-loading and structural misspecifications. However, SAM methods, even though outperforming standard SEM under omitted cross-loadings, still showed substantial deviations in this condition (with bias values between 69% and 77% of the true value for SAM-ML) and inaccuracy (with RMSE values between 86% and 277% of the true value for

SAM-ML). Additionally, while increased sample size led to lower RMSE values for all methods, bias only decreased for standard SEM in larger samples. In contrast, SAM methods showed a slight increase in bias with larger samples with measurement misspecifications in low and moderate reliability.

Figure 7

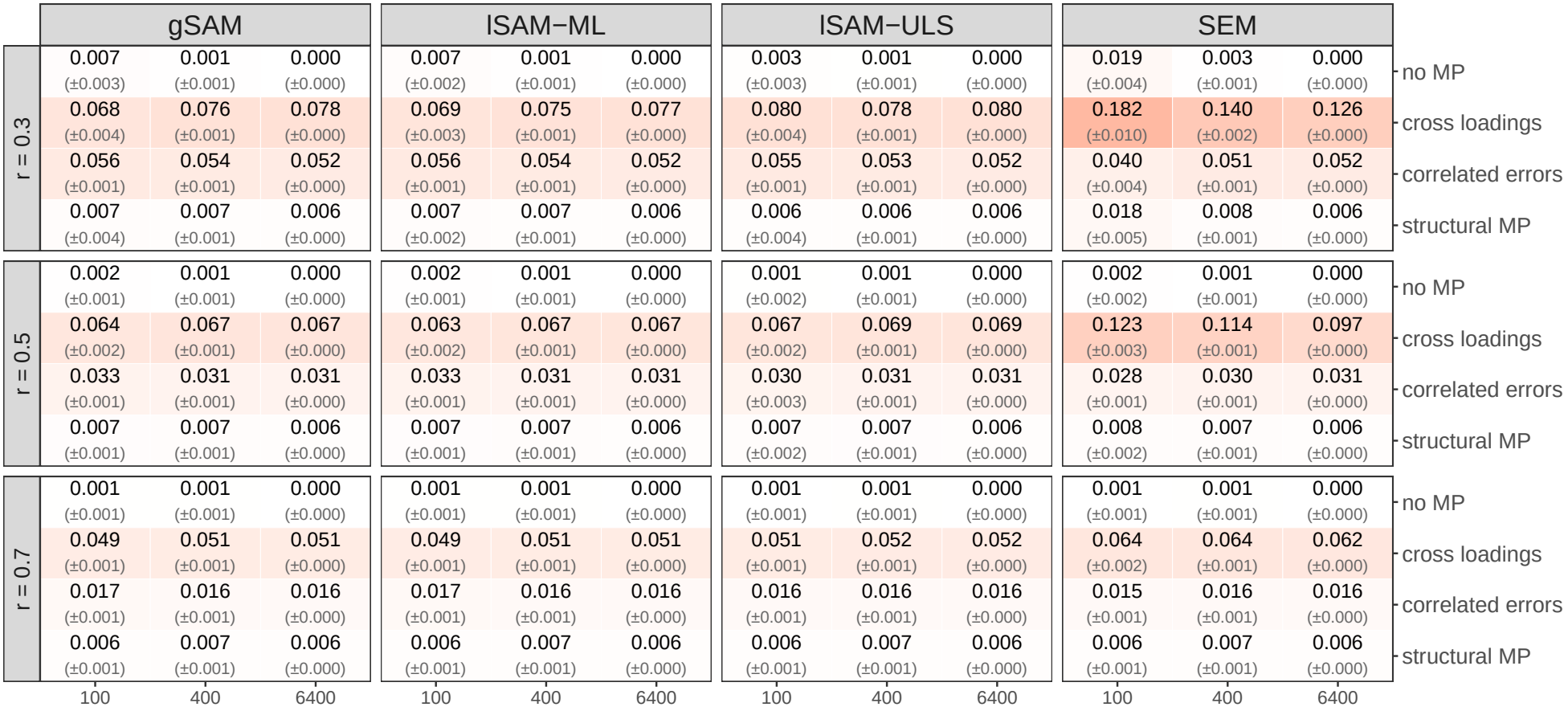
Convergence Rate and Rate of Proper Solutions in Study 1



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.

Figure 8

Mean Average Bias of Regression Parameters in Study 1



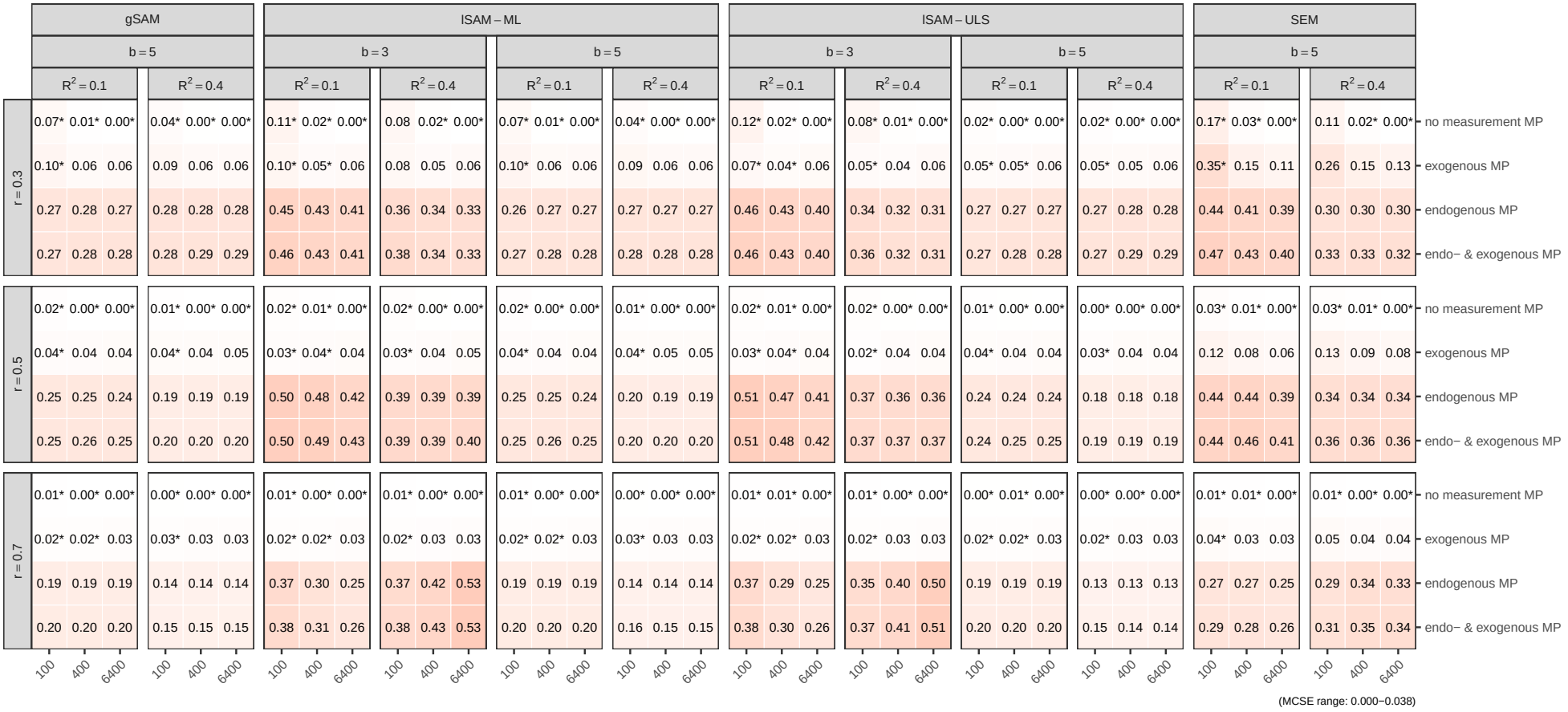
Note. Mean absolute bias averaged (in absolute values) over all parameters with true value of 0.1 in one model for sample sizes (N), reliability (r), and misspecifications for global SAM (gSAM), local SAM with Maximum Likelihood (lSAM-ML), Unweighted Least Squares (lSAM-ULS) and SEM. Monte Carlos Standard Errors (MCSE) are shown in parentheses for each value.

The pattern of results from study 1 was consistent with the findings of study 2, with some additional insights regarding the study-specific conditions. Firstly, as in study 1, there was a 100% convergence rate and rate of proper solutions for all SAM methods across all conditions, even in small samples with low reliability. Standard SEM, in contrast, showed severe convergence issues and frequent improper solutions in small samples with low reliability, with exogenous misspecifications being more challenging than endogenous misspecifications (see Figure B3).

Further, in study 2 the relative bias (to account for modulated path coefficients) of the correctly specified path coefficient estimates averaged across each model in absolute values showed again that in small to medium sample sizes with low to moderate reliability, all SAM estimations were closer to the true parameters than standard SEM. This increased performance of SAM was present only for gSAM and lSAM across all item reliability levels with separate measurement blocks for each factor (b = 5), indicating that joining measurement models in lSAM for exo- and endogenous factors (b = 3) was disadvantageous. All methods performed worse for lower variance explained by the structural model in low and moderate reliability and measurement missepcifcations except SAM methods (with b = 5 and gSAM). The average relative RMSE values of the path coefficients paint a similar picture. Here, too, lower R^2 values were more challenging. Other than for the bias, exogenous misspecifications were more challenging than endogenous misspecifications. Further, gSAM and lSAM-ML with five measurement blocks (here not ULS) produced notably lower RMSE values than standard SEM; however, only in small and medium samples with low item reliability present. As all population models included structural misspecifications in study 2, there was also a slight advantage visible in low sample size and low reliability without measurement misspecification, indicating that SAM methods are also more robust to the impact of falsely specified paths not present in the population on the estimation of the remaining correctly specified parameters. Figure B6 shows the absolute bias of the parameters misspecified (excluded from the results presented above to avoid distortion of relative metric values by parameters with a true value of 0), indicating that also such parameters are recovered more accurately by SAM methods than standard SEM but only if measurement misspecifications are present.

Figure 9

Mean Average Relative Bias of Regression Parameters in Study 2



Note. Mean relative bias averaged (in absolute values) over all parameters in one model for sample sizes (N), reliability (r), and misspecifications for global SAM (gSAM), local SAM with Maximum Likelihood (lSAM-ML), Unweighted Least Squares (lSAM-ULS) and SEM.

Overall, the results indicate that SAM methods (gSAM, lSAM-ML, and lSAM-ULS) outperformed standard SEM under challenging conditions. SAM methods achieved a 100% convergence rate with no improper solutions, even in small samples with low reliability, whereas standard SEM exhibited severe convergence issues and high rates of improper solutions, particularly with cross-loading misspecification. SAM methods provided less biased and more accurate path coefficient estimates, especially in small to medium samples with low to moderate reliability and measurement misspecifications like omitted cross-loadings. Among the SAM variants, gSAM and lSAM-ML generally performed better than lSAM-ULS, with lSAM-ML showing superior accuracy under cross-loading and structural misspecifications. Further, separate compared to joint measurement models in lSAM for latent variables was advantageous. Additionally, SAM methods in Study 2 were more robust to structural misspecifications, providing more accurate estimates of correctly specified parameters even when incorrect paths were included in the model.

Results of Collaborator B (Kosanke)

The results of Kosanke's individual simulation studies are presented verbatim from his report (Git commit SHA 4d0e95e):

The full result analysis for my individual study is available here: https://github.com/lkosanke/AdversarialSimulation/blob/main/LK/results.pdf. The repository readme.md contains a detailed explanation of how the analyses were implemented and how they can be reproduced. In this section, I will focus on the most important results only. For the most part, results from Robitzsch (2022) have been successfully replicated: I did not observe substantial convergence issues in any study. Across studies, as in the original paper, SAM did not generally outperform SEM in small to moderate samples. SAM exhibited a negative small sample bias that made SAM appear superior in conditions with unmodelled positive cross-loadings and residual correlations. This bias was especially strong for lower lambda and higher phi or beta values. Going ahead of what was investigated in Robitzsch (2022), I found that this bias is also present in models with lower phi or beta values. Thus, it cannot be concluded that SAM is more robust in models with non-saturated structural parameters. If there was no misspecification or unmodelled negative cross-loadings and residual correlations, SAM tended to perform worse than traditional SEM, as far as can be concluded from my results.

Convergence *As Robitzsch (2022) argued in their paper, I did not expect convergence issues due to constrained ML estimation that only allows for positive variances and loadings. Nevertheless, I captured all messages, warnings and errors that occurred during the simulations. No messages and errors were present in any of the studies. Multiple warnings were observed in the first 4*

simulations, some of them referring to potential problems with convergence. Overall, the number of these warnings was very small compared to the total number of estimations performed. They amounted to between 0.5-1.8%. In studies 4 and 4a, an even smaller number of warnings was present, amounting to problems in 0.02% of estimations in study 4 and 0.1% in study 4a. These warnings referred to potential problems with positive definite matrices and model identification. In total, these numbers are negligible in size and align with the report of Robitzsch (2022), that convergence issues were not substantial for my estimations. Additionally, a larger number of warnings was present with regards to the computation of fit indices in these final two studies. As we were not interest in fit indices in our research question, they were not relevant for our purposes. A detailed analysis of all the warnings was conducted in the results.pdf* document in my sub-folder of the Github repository.*

Conditions without misspecification *Tables 8 and 9 show the most relevant results of Studies 1 and 4 where I investigated the comparative performance of SAM vs. traditional SEM estimation under correctly specified models. Here it became apparent, that in absence of misspecification, none of the two estimation methods clearly outperformed the other. In Study 4a, only slight differences could be observed in terms of bias and RMSE between LSAM- and classical ML-estimation. In Study 1, both SEM outperformed all SAM estimators in samples of N=50-500. This was true for both relative bias and RMSE, and visible for the former in Table 9. Here, SAM's negative small sample bias is already visible as well.*

Table 1

Study 4 (Kosanke): RMSE for DGM 1 (without misspecification).

	Sample Size						
Method/Metric	**50**	**100**	**250**	**500**	**1000**	**2500**	**100000**
SEM ML	0.188	0.123	0.075	0.051	0.037	0.023	0.004
SEM ULS	1.062	0.128	0.077	0.053	0.037	0.023	0.004
LSAM ML	0.165	0.115	0.072	0.050	0.036	0.023	0.004

Note. SEM ML = Maximum-likelihood estimation, SEM ULS = Unweighted-least-squares estimation, LSAM ML = Local-SAM-maximum-likelihood estimation.

Table 2

Study 1 (Kosanke): Relative bias in conditions without misspecification.

	Sample Size						
Method/Metric	**50**	**100**	**250**	**500**	**1000**	**2500**	**100000**
SEM ML rel bias	-0.045	-0.011	0.001	-0.003	0.003	-0.002	-0.000
SEM ULS rel bias	0.024	0.022	0.012	0.002	0.006	-0.001	-0.000
LSAM ML rel bias	-0.394	-0.270	-0.111	-0.056	-0.022	-0.011	-0.000
LSAM ULS rel bias	-0.393	-0.270	-0.111	-0.056	-0.022	-0.011	-0.000
GSAM ML rel bias	-0.394	-0.270	-0.111	-0.056	-0.022	-0.011	-0.000
GSAM ULS rel bias	-0.393	-0.270	-0.111	-0.056	-0.022	-0.011	-0.000

Note. SEM ML = Maximum-likelihood estimation, SEM ULS = Unweighted-least-squares estimation, LSAM ML = Local-SAM-maximum-likelihood estimation, LSAM ULS = Local-SAM-unweighted-least-squares estimation, GSAM ML = Global-SAM-maximum-likelihood estimation, GSAM ULS = Global-SAM-unweighted-least-squares estimation.

Conditions with negatively valenced unmodelled parameters *Studies 1 and 2 explicitly investigated negatively valenced unmodelled parameters in the generating model. In these studies, it became apparent that traditional SEM outperformed SAM estimation. As can be seen in Table 10, both SEM estimators outperformed all four SAM estimators in terms of relative bias with two negative residual correlations present. The same was true in Study 2, in the presence of two negative cross-loadings. In both these cases, bias values overall remained high but substantially less so in the traditional SEM methods. when comparing them in small to moderate sample sizes. Additionally, slight differences between the two approaches arose in these two examples in terms of RMSE, as can be seen in Table 11 for the negative cross-loadings in study 2.*

Conditions with positively valenced unmodelled parameters *In terms of performance for positively valenced cross-loadings and residual correlations, SAM appeared to outperform traditional SEM estimation, but not in all scenarios of interest. Table 12 shows this finding in Study 3, in conditions with both one unmodelled residual correlation and one cross-loading. Only from N=100-1000 did SAM outperform SEM.*

Table 3

Study 1 (Kosanke): Relative bias in conditions with two negative unmodelled residual correlations.

	Sample Size						
Method/Metric	**50**	**100**	**250**	**500**	**1000**	**2500**	**100000**
SEM ML rel bias	-0.205	-0.175	-0.166	-0.168	-0.161	-0.166	-0.164
SEM ULS rel bias	-0.139	-0.145	-0.159	-0.167	-0.163	-0.170	-0.169
LSAM ML rel bias	-0.498	-0.385	-0.272	-0.225	-0.196	-0.189	-0.180
LSAM ULS rel bias	-0.497	-0.385	-0.272	-0.225	-0.196	-0.189	-0.180
GSAM ML rel bias	-0.497	-0.385	-0.272	-0.225	-0.196	-0.189	-0.180
GSAM ULS rel bias	-0.496	-0.385	-0.272	-0.225	-0.196	-0.189	-0.180

Note. SEM ML = Maximum-likelihood estimation, SEM ULS = Unweighted-least-squares estimation, LSAM ML = Local-SAM-maximum-likelihood estimation, LSAM ULS = Local-SAM-unweighted-least-squares estimation, GSAM ML = Global-SAM-maximum-likelihood estimation, GSAM ULS = Global-SAM-unweighted-least-squares estimation.

Table 4

Study 2 (Kosanke): RMSE in conditions with two negative unmodelled cross-loadings.

	Sample Size						
Method/Metric	**50**	**100**	**250**	**500**	**1000**	**2500**	**100000**
SEM ML	0.48	0.382	0.257	0.211	0.182	0.172	0.161
SEM ULS	0.477	0.367	0.241	0.205	0.182	0.175	0.166
LSAM ML	0.486	0.421	0.323	0.269	0.232	0.216	0.201
LSAM ULS	0.487	0.421	0.323	0.269	0.232	0.216	0.201
GSAM ML	0.49	0.422	0.323	0.269	0.232	0.216	0.201
GSAM ULS	0.49	0.421	0.323	0.269	0.232	0.216	0.201

Note. SEM ML = Maximum-likelihood estimation, SEM ULS = Unweighted-least-squares estimation, LSAM ML = Local-SAM-maximum-likelihood estimation, LSAM ULS = Local-SAM-unweighted-least-squares estimation, GSAM ML = Global-SAM-maximum-likelihood estimation, GSAM ULS = Global-SAM-unweighted-least-squares estimation.

Table 5

Study 3 (Kosanke): Relative bias in conditions with each one positive unmodelled cross-loading and residual correlation.

	Sample Size						
Method/Metric	**50**	**100**	**250**	**500**	**1000**	**2500**	**100000**
SEM ML rel bias	0.209	0.270	0.283	0.289	0.289	0.282	0.284
SEM ULS rel bias	0.250	0.284	0.277	0.280	0.279	0.271	0.272
LSAM ML rel bias	-0.232	-0.061	0.127	0.211	0.246	0.261	0.276
LSAM ULS rel bias	-0.229	-0.060	0.127	0.211	0.246	0.261	0.276
GSAM ML rel bias	-0.230	-0.060	0.127	0.211	0.246	0.261	0.276
GSAM ULS rel bias	-0.228	-0.060	0.127	0.211	0.246	0.261	0.276

Note. SEM ML = Maximum-likelihood estimation, SEM ULS = Unweighted-least-squares estimation, LSAM ML = Local-SAM-maximum-likelihood estimation, LSAM ULS = Local-SAM-unweighted-least-squares estimation, GSAM ML = Global-SAM-maximum-likelihood estimation, GSAM ULS = Global-SAM-unweighted-least-squares estimation.

In Study 4, a comparative advantage of LSAM compared to SEM-ML was present, but only for smaller samples. With regards to RMSE, results were mixed as well. LSAM appeared to outperform in Table 13 for DGM 2 of Study 4. In other conditions, however, no substantial

differences arose in terms of RMSE.

Small sample bias in LSAM estimation *The small sample bias of LSAM estimation in Study 1b revealed that in smaller samples ranging from N=50 to N=100, both LSAM-ML and LSAM-ULS estimation were biased. Table 14 shows this was especially apparent in a sample size of 50.*

Table 6

Study 4 (Kosanke): RMSE in DGM 2 (conditions with five positive unmodelled cross-loadings).

	Sample Size						
Method/Metric	**50**	**100**	**250**	**500**	**1000**	**2500**	**100000**
SEM ML	0.373	0.257	0.166	0.124	0.107	0.100	0.095
SEM ULS	2.070	0.373	0.320	0.306	0.300	0.298	0.296
LSAM ML	0.188	0.141	0.103	0.089	0.080	0.075	0.071

Note. SEM ML = Maximum-likelihood estimation, SEM ULS = Unweighted-least-squares estimation, LSAM ML = Local-SAM-maximum-likelihood estimation.

Table 7

Study 1b (Kosanke): Absolute bias of LSAM-ML for N=50.

	Phi Levels				
Lambda	**0**	**0.2**	**0.4**	**0.6**	**0.8**
0.4	0.202	0.202	0.258	0.346	0.444
0.5	0.187	0.179	0.203	0.245	0.305
0.6	0.176	0.165	0.166	0.170	0.190
0.7	0.164	0.150	0.139	0.122	0.116
0.8	0.150	0.135	0.119	0.098	0.074

Note. LSAM ML = Local-SAM-maximum-likelihood estimation.

Note that the absolute values of bias were calculated in this study. Consequently, the values of the bias should be interpreted as negative, as follows from the results of the original paper (Robitzsch, 2022). The bias persisted, but to a lesser degree in samples of 100. Thus, as expected, a clear effect of sample size was present. Overall, comparing LSAM-ML and -ULS estimation, results were very similar. Importantly, differential effects due to lambda and phi were present in Study 1b. The small sample bias was especially strong for lower lambda and higher phi values, thus in contexts of low reliability and high factor correlations. Also, a new insight is that

the bias remained relevant for low values of phi, unlike in the original paper by Robitzsch (2022). In consequence, there seemed to be no conditions were SAM's small sample bias was negligible. Another new insight lied in the presence of what could be called a reversal effect: For higher values of lambda, the bias did not increase for higher values of phi. On the contrary, absolute bias values decreased for higher phi values, when looking at the conditions with lambda = 0.7-0.8. As an additional investigation of the small sample bias, I included Study 4a to see its effect come to play in a 5-factor-model with regressions. Table 15 shows the performance of SEM-ML, whereas Table 16 shows the performance of LSAM-ML in DGM 2 (in presence of unmodelled cross-loadings). Aligning with the findings of Study 1b, the results suggested an even better relative performance of LSAM- over traditional SEM-ML estimation for smaller N and higher beta. Thus, the negative small sample bias came into play in this study as well. Results looked very similar with regards to RMSE. Note that this trend was less strong, but still present in the conditions of DGM 3 when looking at residual correlations.

Table 8

Study 4a (Kosanke): Absolute bias of SEM-ML for DGM 2 (conditions with five positive unmodelled cross-loadings).

	Sample Size						
Beta	**50**	**100**	**250**	**500**	**1000**	**2500**	**100000**
0.1	0.253	0.172	0.115	0.095	0.085	0.080	0.075
0.2	0.327	0.220	0.162	0.139	0.122	0.114	0.109
0.3	0.545	0.270	0.218	0.206	0.195	0.190	0.180
0.4	0.981	0.336	0.270	0.257	0.252	0.251	0.254

Note. SEM ML = Maximum-likelihood estimation, SEM ULS = Unweighted-least-squares estimation, LSAM ML = Local-SAM-maximum-likelihood estimation, LSAM ULS = Local-SAM-unweighted-least-squares estimation, GSAM ML = Global-SAM-maximum-likelihood estimation, GSAM ULS = Global-SAM-unweighted-least-squares estimation.

Table 9

Study 4a (Kosanke): Absolute bias of LSAM-ML for DGM 2 (conditions with five positive unmodelled cross-loadings).

	Sample Size						
Beta	**50**	**100**	**250**	**500**	**1000**	**2500**	**100000**
0.1	0.150	0.112	0.083	0.072	0.065	0.061	0.057
0.2	0.145	0.108	0.077	0.066	0.059	0.056	0.053

Table 9

Study 4a (Kosanke): Absolute bias of LSAM-ML for DGM 2 (conditions with five positive unmodelled cross-loadings). (continued)

Beta	50	100	250	500	1000	2500	100000
0.3	0.141	0.104	0.073	0.060	0.052	0.047	0.043
0.4	0.151	0.115	0.088	0.076	0.070	0.067	0.065

One aspect to mention is that lambda values were quite high in study 4a (lambda=0.7). Matching the results from Study 1b, SAM's bias did not increase for higher values of beta, unlike SEM's. This effect could hint at a stronger robustness of SAM in contexts of higher correlations with misspecifications present. But, as the effect could not be observed in other conditions (e.g. in DGM 3 with residual correlations), I did not deem it substantial.

Summary of results *For the most part, I succesfully replicated the results from Robitzsch (2022): I did not observe substantial convergence issues in any study. Across studies, as in the original paper, SAM did not generally outperform SEM in small to moderate samples. SAM exhibited a negative small sample bias that made SAM appear superior in conditions with unmodelled positive cross-loadings and residual correlations. This bias was especially strong for lower lambda and higher phi or beta values. Going ahead of what was investigated in Robitzsch (2022), I found that this bias is also present in models with lower phi or beta values. Thus, it cannot be concluded that SAM is more robust in models with non-saturated structural parameters. If there was no misspecification or unmodelled negative cross-loadings and residual correlations, SAM tended to perform worse than traditional SEM, as far as can be concluded from my results.*

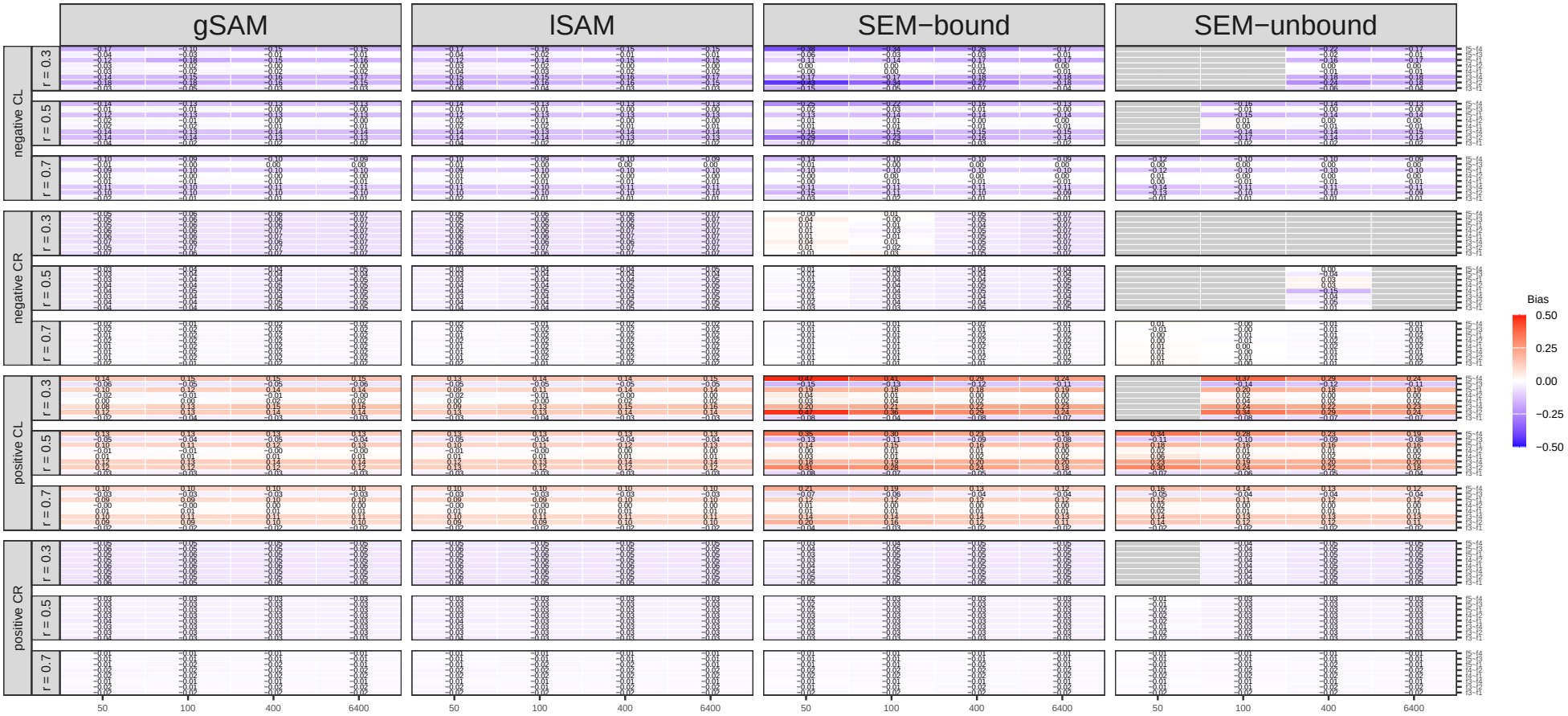
Joint Simulation Study

The joint study showed that using bound maximum likelihood estimation for standard SEM as proposed by Kosanke did infact eliminate the low convergence rate as well as improper solutions in all conditions (see B1). Next, the parameterwise signed mean bias values of the single regression weight estimates showed that omitting positive cross-loadings results in an overall positive bias, whereas omitting negative cross-loadings results in a negative bias. As in previous studies, the positive bias was less pronounced for SAM (gSAM and lSAM) than for SEM, especially with lower sample sizes and reliability. However, contrary to the findings by Kosanke and Robitzsch (2022), in this study the negative bias was also less pronounced for both SAM methods. Conditions with omitted correltated residual correlations resulted in predominantly negative bias values for all methods irrespective of the sign of the misspecification with standard

SEM being slightly less biased than SAM methods (see Figure 10). A direct comparision of standard SEM with SAM for bias and RMSE showed that SAM methods were less biased for cross loadings and when accounting for variance via RMSE more accurate especially in lower samples sizes and indicator reliability levels (see Figure 11). Further, there were little to no differences between gSAM and lSAM with lSAM being overall slightly more accurate in terms of RMSE. Overall these findings suggest that the explanation for SAM's lower bias under positive misspecifications being due to a general negative bias that would lead to overly negative bias in case of negative measurement misspecifications (proposed by Kosanke and Robitzsch (2022)) does not hold in a more complex (and realistic) model that SAM could be favorable choice of SEM estimation especially challenging conditions.

Figure 10

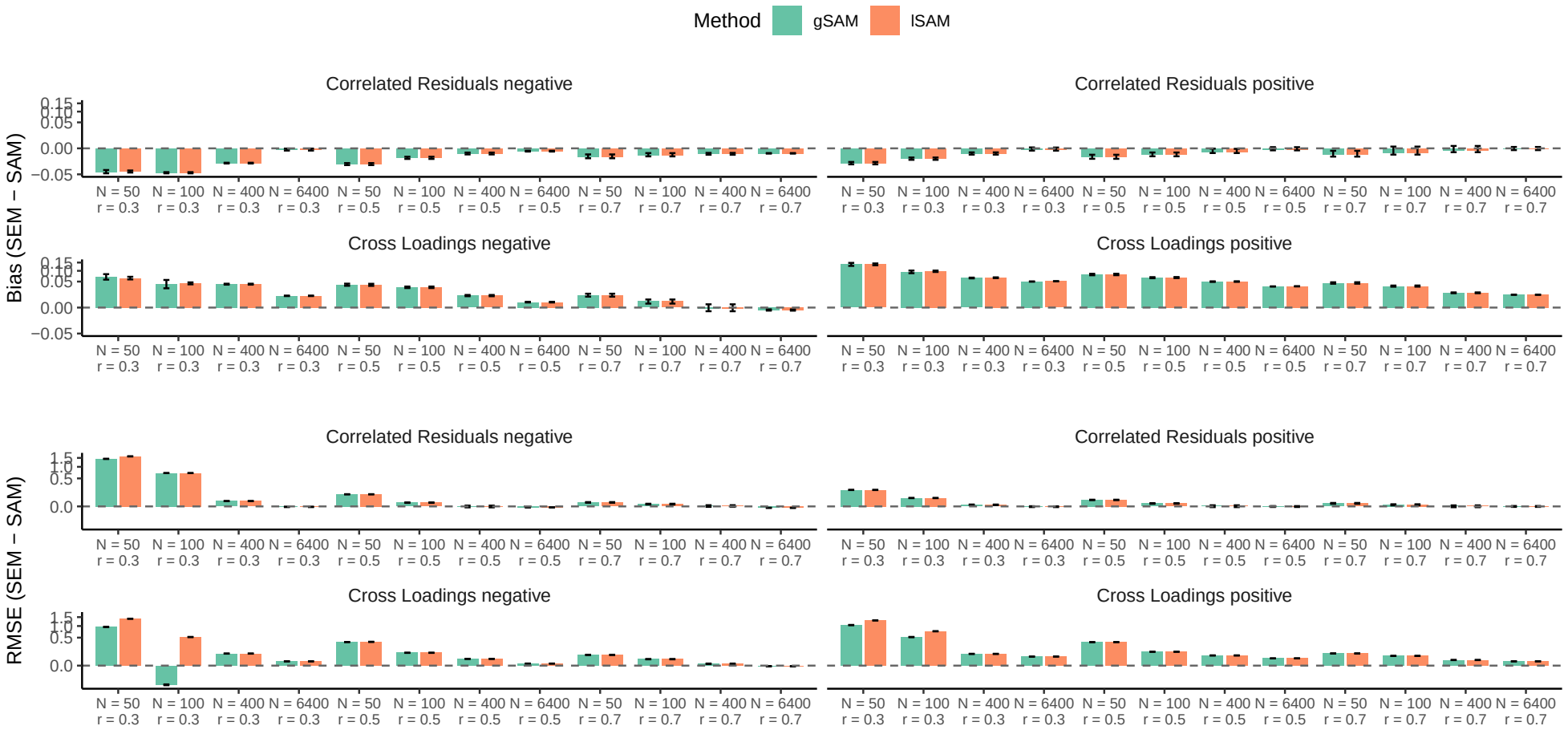
Mean Bias of Regression Parameters in Joint *Study*



Note. Mean absolute bias for each parameter with true value of 0.1 in one model for sample sizes (N), reliability (r), and misspecifications for global SAM (gSAM), local SAM with Maximum Likelihood (lSAM-ML), Unweighted Least Squares (lSAM-ULS) and SEM.

Figure 11

Aggregated Mean Difference between Bound Standard SEM and SAM Estimation in Bias and RMSE of regression coefficients estimates in Joint *Study*



Note. Bias (top) and RMSE (bottom) differences between SEM and gloabal and local SAM (gSAM and lSAM) , averaged across estimates of true regression coefficients (0.1) over varying N, r, and misspecifications. Error bars show Monte Carlo SEs.

Adversarial Collaboration

Although we did not jointly arrive at the conclusion to conduct a collaborative unified simulation study as planned, the individual studies provided a comprehensive basis for a joint study. As outlined in the next section, I decided to conduct a "joint" study on my own formally completing the adversarial collaboration process. The joint study, based on the individual studies, constituted a stepwise integration of settings from the individual studies with the goal of resolving the conflicting verbal claims. A 5-factor population structural model with 3 indicators per factor, as used in Collaborator A's (Kriegmair) approach, was selected to provide a complex model suitable for testing the advantages of SAM. To assess the robustness of SAM, particularly in response to negative misspecifications highlighted by Collaborator B (Kosanke), both positive and negative omitted cross-loadings and correlated residuals were included in the model misspecifications. Indicator reliability was manipulated by adjusting measurement error variances, following Collaborator A's implementation, to achieve a valid representation of item reliability. CFA models from Collaborator B's studies were excluded since SAM is designed for models with directed structural paths. The experimental design extended sample size variation to very small ($N = 50$) for a more extensive range than in Collaborator A's studies. Both positive and negative misspecifications were included to assess a potential negative bias in SAM. In the selection of estimation methods, bound SEM-ML, unbound SEM-ML, gSAM, and lSAM-ML were compared, to address the convergence issues of standard SEM as proposed by Collaborator B. SAM-ULS and SEM-ULS were excluded to focus on the most relevant methods and manage computational demands. Bias and RMSE of the estimated factor correlations were calculated, and parameter-wise bias analysis was performed to identify any potential negative bias in SAM without the averaging effects. The analysis was largely consistent with the individual studies, with the addition of parameter-wise bias displays to gain deeper insights into the biases and a direct computation of metric-differences between SEM and SAM.

Discussion

The goal of this study was twofold: first, to test the viability and practical applicability of adversarial collaboration (AC) as a tool to resolve disagreeing research claims and enhance generalizability and rigor in the context of simulation studies. Second, serving as a case study for this first aim, to evaluate the performance of traditional Structural Equation Modeling (SEM) compared to Structural After Measurement (SAM), and resolve conflicting claims of previous studies regarding whether SAM consistently outperforms traditional SEM in the presence of model misspecifications in small to moderate sample sizes (Dhaene & Rosseel, 2023; Robitzsch, 2022; Rosseel & Loh, 2022).

We successfully agreed on a joint starting point and translated conflicting verbal claims from prior studies into shared research questions. Based on these research questions, we independently conducted simulation studies largely based on the simulations by Rosseel & Loh (2022), Dhaene & Rosseel (2023), and Robitzsch (2022), thereby successfully translating the verbal dispute back to empirical grounds. It is important to note that this constituted only an emulated process of adversarial collaboration, including the additional layer of replicating previously published research findings in *Round 1* of our framework. In a practical application of AC to simulation studies as proposed here, this intermediary step could be bypassed. Instead, collaborators could design two original studies or choose to work directly together on a unified research study, contingent upon their identification of a specific verbal disagreement. After assessing our individual studies and their results, we did not jointly conclude that conducting a collaborative unified simulation study as planned was warranted. Kosanke decided to terminate the AC at this point. He argued that while in most cases the Structural After Measurement (SAM) approach showed less bias and root mean square error (RMSE), in some settings—especially in cases of negative unmodeled residuals and cross-loadings—the advantages of traditional Structural Equation Modeling (SEM) countered those of SAM. This indicated that neither method consistently outperformed the other in broader applications. However, I identified several reasons for conducting another simulation based on this first round of replicated studies and, based on this, set up a joint study. Kosanke's conclusion about SAM's inconsistent outperformance of SEM in the presence of negative misspecifications was applied to a very specific type of confirmatory factor analysis (CFA) model and was not tested in a more complex model with directed structural paths of interest. These represent scenarios for which Rosseel & Loh (2022) proposed SAM to be advantageous. In addition, to thoroughly investigate this assumed systematic underestimation of SAM, a parameter-wise analysis of bias was warranted. Aggregation of bias values across model parameters could lead to canceling out negative and positive values or not showing them at all when using absolute values. Furthermore, a joint study allowed for unifying simulation choices, such as extending the sample range to very small sizes (N = 50) to examine more extreme settings. Also, collaborator-specific choices of tracking convergence rates and computing modulated indicator reliability levels could be identified as another potential source of diverging results, which was resolved in the joint study. Even if conducted only by myself, such a joint study served as a demonstrative proof of concept for the application of adversarial collaboration to simulation studies addressing the question of technical feasability of Adverarial Simulation.

Evaluation of the Substantive Research Questions

Evaluation of Adversarial Collaboration in Simulation Studies

All in all the current study demonstrates that adversarial collaboration is a technically feasible and viable approach in the context of simulation studies. By successfully translating a general conflict in conclusions about the performance of SAM and standard SEM in a joint research question and based on this directly juxtaposing our different simulation setups, we were able to trace back general diverging conclusions to specific methodological operationalizations and technical decisions. This effectively enhanced transparency and reduced ambiguity of the conflicting claims allowing for a more precise identification of the sources of disagreement in a similar way as its was previously demonstrated in empirical research (Mellers et al. (2001); (**mell?**)).

In particular, this approach enforced direct engagement with each adversary's specific arguments for their conclusions, transparently linking each argument to its operationalized source and integrating it into a joint study that respects both viewpoints. This led to more targeted and arguably generalizable results by adjusting multiple aspects of the simulation setup, such as model type, misspecifications, reliability computation, sample size, and analysis. However, it is important to note that due to the specific circumstances of this case study, which included a prior replication of previous results, these results explicitly impacted the collaboration and the joint study. If this step were omitted in a practical application of adversarial collaboration, the joint study would potentially need to be more comprehensive, covering a broader range of settings, as prior results would not be available to inform it. For preexisting disagreements, nevertheless, this initial independent replication phase has the advantage of isolating initial discrepancies in results, which can clarify the specific origins of divergence in methodological setups, as observed in this case. Similarly, as demonstrated in an empirical project by Melloni et al. (2023) involving cross-lab replications, this step can help identify key factors that contribute to conflicting claims, allowing collaborators to design a more streamlined and focused joint study.

Despite the above, several challenges for Adversarial Simulation emerged. First, even after collaboration, the simulation studies remained limited to specific settings. While we attempted to create prototypical models representative of practical applications, the generalizability of our findings is constrained by the scope of the simulations. Without additional empirical data or broader simulation conditions, it is difficult to make comprehensive claims about the methods' performance in all possible scenarios.

Second, adversarial collaboration demands increased resources in terms of time and coordination. The process requires careful planning, open communication, and a willingness to

reconcile differing viewpoints. In our case, the termination of the collaboration by one party underscores the potential difficulties in sustaining such efforts. The additional time and effort required may pose practical constraints, especially in academic environments with tight schedules and resource limitations.

Third, the applicability of adversarial collaboration may be limited to specific settings where there are clear, conflicting viewpoints on particular methods or theories. It may not be as effective in areas where disagreements are less defined or more complex. The focus on specific methodological disputes means that broader issues or more subtle disagreements might not be as amenable to this approach.

Despite these challenges, adversarial collaboration has the potential to increase generalizability and rigor in simulation studies by promoting transparency, reducing biases, and fostering a more comprehensive exploration of methodological issues. By bringing together researchers with opposing views, it encourages a more thorough examination of assumptions and methodological choices, potentially leading to more robust and reliable conclusions.

Outlook

An alternative promising avenue to address the generalizability challange specifically at the point of operationalization and simulation design more head on is the to ground simulation studies in empirical data by incorporating actual models and parameters used in practice (Bollmann et al., 2015). By sampling model data from the literature and directly using it in simulation setups, researchers can enhance the relevance and applicability of their findings. This approach would bridge the gap between protoypical models and practical applications, providing insights that are more directly transferable to real-world scenarios. An alternative approach to address the the generalizability challange specifically at the point of operationalization and simulation design more head on is to ground simulations in empirical data, incorporating actual models and parameters from practice (Bollmann et al., 2015) by sampling model and parameters from the literature to effectively bridge the gap between prototypical simulations and real-world applications.

Another avenue for future research stimulated by the current study is the development of collaborative simulation platforms that could facilitate ongoing contributions from multiple researchers. By leveraging open-source tools and platforms such as GitHub similar to the current project but more elaborate and refined, simulations can be made “living” projects that are continuously updated and refined. Collaborators could open pull requests to add new conditions or settings to existing simulations, allowing for dynamic testing and integration of new results. For example, a research team interested in assessing the performance of SAM in a specific type of

model or data relevant to their work could contribute to an existing simulation repository. With minimal coding effort, they could add their model conditions, request a rerun of the simulation, and obtain updated results that inform both their specific research and the general understanding of the method's performance. This collaborative approach could effectively enhance generalizability of simulation studies, making them more accessible and responsive to the needs of the research community, better capturing the complexities across different contexts. Implementing such collaborative simulation platforms would require computational infrastructure and a system for regulating when simulations are rerun to manage computational costs. Streamlined pipelines, involving containerization technologies like Docker or Singularity, could facilitate a dynamic deployment of simulations on high-performance computing resources. Additionally, establishing guidelines and open peer review mechanisms for contributions would ensure the quality and integrity of the simulations.

The first part of the disagreement concerned convergence rate and improper solutions: In my studies SEM showed a low convergence rate, particularly in small samples with low reliability. In contrast, Kosanke reported minimal convergence issues. This issue could be traced back to differences in *method selection*. Kosanke (as Robitzsch (2022)) applied bounded ML SEM, which constrains variances and loadings within theoretical limits, potentially improving convergence and preventing improper solutions compared to unconstrained ML in studies by me (and Rosseel & Loh (2022) and Dhaene & Rosseel (2023)). Additionally Kosanke only indirectly tracked non-convergence while the other studies provided condition wise direct tracking of improper solutions and convergence rate. Thus in the joint study we decided to include bounded ML SEM as a method to compare to SAM and unbounded ML SEM

Idea: living simulations..

References

Banack, H. R., Hayes-Larson, E., & Mayeda, E. R. (2021). Monte carlo simulation approaches for quantitative bias analysis: A tutorial. *Epidemiologic Reviews*, *43*(1), 106–117. https://doi.org/10.1093/epirev/mxab012

Bartlett, M. S. (1937). The Statistical Conception of Mental Factors. *British Journal of Psychology. General Section*, *28*(1), 97–104. https://www.proquest.com/docview/1293463650/citation/9FE530638F5041E0PQ/1

Bartlett, M. S. (1938). Methods of estimating mental factors. *Nature*.

Bollen, K. A. (2014). *Structural equations with latent variables*. John Wiley & Sons.

Bollmann, S., Heene, M., Küchenhoff, H., & Bühner, M. (2015). *What can the Real World do for simulation studies? A comparison of exploratory methods*.

https://doi.org/10.5282/UBM/EPUB.24518

Buchka, S., Hapfelmeier, A., Gardner, P. P., Wilson, R., & Boulesteix, A.-L. (2021). On the optimistic performance evaluation of newly introduced bioinformatic methods. *Genome Biology*, *22*(1), 152. https://doi.org/10.1186/s13059-021-02365-4

Camerer, C. F., Dreber, A., Holzmeister, F., Ho, T.-H., Huber, J., Johannesson, M., Kirchler, M., Nave, G., Nosek, B. A., Pfeiffer, T., et al. (2018). Evaluating the replicability of social science experiments in nature and science between 2010 and 2015. *Nature Human Behaviour*, *2*(9), 637–644.

Carrillo, N., & Martínez, S. (2023). Scientific inquiry: From metaphors to abstraction. *Perspectives on Science*, *31*(2), 233–261. https://doi.org/10.1162/posc_a_00571

Clark, C. J., Costello, T., Mitchell, G., & Tetlock, P. E. (2022). Keep your enemies close: Adversarial collaborations will improve behavioral science. *Journal of Applied Research in Memory and Cognition*, *11*(1), 1–18. https://doi.org/10.1037/mac0000004

Clark, C., & Tetlock, P. (2021). *Adversarial collaboration: The next science reform*. https://doi.org/10.1007/978-3-031-29148-7_32

Cleeremans, A. (2022). Theory as adversarial collaboration. *Nature Human Behaviour*, *6*(4), 485–486.

Dellsén, F., & Baghramian, M. (2021). Disagreement in science: Introduction to the special issue. *Synthese*, *198*(Suppl 25), 6011–6021.

Dhaene, S., & Rosseel, Y. (2023). An Evaluation of Non-Iterative Estimators in the Structural after Measurement (SAM) Approach to Structural Equation Modeling (SEM). *Structural Equation Modeling: A Multidisciplinary Journal*, *30*(6), 926–940. https://doi.org/10.1080/10705511.2023.2220135

Earp, B. D., & Trafimow, D. (2015). Replication, falsification, and the crisis of confidence in social psychology. *Frontiers in Psychology*, *6*. https://doi.org/10.3389/fpsyg.2015.00621

Feinberg, R. A., & Rubright, J. D. (2016). Conducting Simulation Studies in Psychometrics. *Educational Measurement: Issues and Practice*, *35*(2), 36–49. https://doi.org/10.1111/emip.12111

Gilbert, J., & Miratrix, L. (2024). Multilevel metamodels: A novel approach to enhance efficiency and generalizability in monte carlo simulation studies. *arXiv Preprint arXiv:2401.07294*.

Hair Jr, J. F., Hult, G. T. M., Ringle, C. M., Sarstedt, M., Danks, N. P., Ray, S., Hair, J. F., Hult, G. T. M., Ringle, C. M., Sarstedt, M., et al. (2021). An introduction to structural equation modeling. *Partial Least Squares Structural Equation Modeling (PLS-SEM) Using R: A Workbook*, 1–29.

Hoyle, R. H. (2012). *Handbook of structural equation modeling*. Guilford press.

Kline, R. B. (2023). *Principles and practice of structural equation modeling*. Guilford publications.

Kriegmair, V. (2024). *Preregistration: Comparing a structural after measurement (SAM) approach to standard structural equation model (SEM) estimation.* Zenodo. https://doi.org/10.5281/zenodo.11459378

Kulinskaya, E., Hoaglin, D. C., & Bakbergenuly, I. (2020). *Exploring Consequences of Simulation Design for Apparent Performance of Statistical Methods. 1: Results from simulations with constant sample sizes.* arXiv. http://arxiv.org/abs/2006.16638

Lüdtke, O., Ulitzsch, E., & Robitzsch, A. (2021). A Comparison of Penalized Maximum Likelihood Estimation and Markov Chain Monte Carlo Techniques for Estimating Confirmatory Factor Analysis Models With Small Sample Sizes. *Frontiers in Psychology*, *12*. https://doi.org/10.3389/fpsyg.2021.615162

Luijken, K., Lohmann, A., Alter, U., Gonzalez, J. C., Clouth, F. J., Fossum, J. L., Hesen, L., Huizing, A. H. J., Ketelaar, J., Montoya, A. K., Nab, L., Nijman, R. C. C., Vries, B. B. L. P. de, Tibbe, T. D., Wang, Y. A., & Groenwold, R. H. H. (2023). *Replicability of Simulation Studies for the Investigation of Statistical Methods: The RepliSims Project.* https://doi.org/10.48550/ARXIV.2307.02052

Martínez, S. F., & Huang, X. (2011). Epistemic groundings of abstraction and their cognitive dimension. *Philosophy of Science*, *78*(3), 490–511.

Mellers, B., Hertwig, R., & Kahneman, D. (2001). Do Frequency Representations Eliminate Conjunction Effects? An Exercise in Adversarial Collaboration. *Psychological Science*, *12*(4), 269–275. https://doi.org/10.1111/1467-9280.00350

Melloni, L., Mudrik, L., Pitts, M., Bendtz, K., Ferrante, O., Gorska, U., Hirschhorn, R., Khalaf, A., Kozma, C., Lepauvre, A., Liu, L., Mazumder, D., Richter, D., Zhou, H., Blumenfeld, H., Boly, M., Chalmers, D. J., Devore, S., Fallon, F., … Tononi, G. (2023). An adversarial collaboration protocol for testing contrasting predictions of global neuronal workspace and integrated information theory. *PloS One*, *18*(2), e0268577. https://doi.org/10.1371/journal.pone.0268577

Melloni, L., Mudrik, L., Pitts, M., & Koch, C. (2021). Making the hard problem of consciousness easier. *Science*, *372*(6545), 911–912. https://doi.org/10.1126/science.abj3259

Merkel, D. (2014). Docker: Lightweight linux containers for consistent development and deployment. *Linux Journal*, *2014*(239), 2.

Morris, T. P., White, I. R., & Crowther, M. J. (2019). Using simulation studies to evaluate statistical methods. *Statistics in Medicine*, *38*(11), 2074–2102. https://doi.org/10.1002/sim.8086

Nosek, B. A., Hardwicke, T. E., Moshontz, H., Allard, A., Corker, K. S., Dreber, A., Fidler, F., Hilgard, J., Kline Struhl, M., Nuijten, M. B., et al. (2022). Replicability, robustness, and reproducibility in psychological science. *Annual Review of Psychology*, *73*(1), 719–748.

O'Kelly, M., Anisimov, V., Campbell, C., & Hamilton, S. (2017). Proposed best practice for projects that involve modelling and simulation: Proposed Best Practice for Modelling and Simulation. *Pharmaceutical Statistics*, *16*(2), 107–113. https://doi.org/10.1002/pst.1789

Pawel, S., Kook, L., & Reeve, K. (2023). Pitfalls and potentials in simulation studies: Questionable research practices in comparative simulation studies allow for spurious claims of superiority of any method. *Biometrical Journal*, *66*(1). https://doi.org/10.1002/bimj.202200091

Paxton, P., Curran, P. J., Bollen, K. A., Kirby, J., & Chen, F. (2001). Monte Carlo Experiments: Design and Implementation. *Structural Equation Modeling: A Multidisciplinary Journal*, *8*(2), 287–312. https://doi.org/10.1207/S15328007SEM0802_7

Popper, K. R. (1988). *The open universe: An argument for indeterminism* (Vol. 2). Psychology Press.

R Core Team. (2023). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing. https://www.R-project.org/

Rakow, T. (2022). Adversarial Collaboration. In W. O'Donohue, A. Masuda, & S. Lilienfeld (Eds.), *Avoiding Questionable Research Practices in Applied Psychology* (pp. 359–377). Springer International Publishing. https://doi.org/10.1007/978-3-031-04968-2_16

Robitzsch, A. (2022). Comparing the Robustness of the Structural after Measurement (SAM) Approach to Structural Equation Modeling (SEM) against Local Model Misspecifications with Alternative Estimation Approaches. *Stats*, *5*(3), 631–672. https://doi.org/10.3390/stats5030039

Rosseel, Y. (2012). Lavaan: An R Package for Structural Equation Modeling. *Journal of Statistical Software*, *48*, 1–36. https://doi.org/10.18637/jss.v048.i02

Rosseel, Y. (2020). Small sample solutions for structural equation modeling. In *Small sample size solutions* (pp. 226–238). Routledge.

Rosseel, Y., & Loh, W. W. (2022). A structural after measurement approach to structural equation modeling. *Psychological Methods*. https://doi.org/10.1037/met0000503

Slife, B. D., Wright, C. D., & Yanchar, S. C. (2016). Using operational definitions in research: A best-practices approach. *The Journal of Mind and Behavior*, 119–139.

Supino, P. G. (2012). Overview of the research process. In P. G. Supino & J. S. Borer (Eds.), *Principles of research methodology: A guide for clinical investigators* (pp. 1–14). Springer New York. https://doi.org/10.1007/978-1-4614-3360-6_1

Thomopoulos, N. T. (2012). *Essentials of monte carlo simulation: Statistical methods for building simulation models*. Springer Science & Business Media.

Ulitzsch, E., Lüdtke, O., & Robitzsch, A. (2023). Alleviating estimation problems in small sample structural equation modeling—A comparison of constrained maximum likelihood, Bayesian

estimation, and fixed reliability approaches. *Psychological Methods*, *28*(3), 527–557. https://doi.org/10.1037/met0000435

Van Driel, O. P. (1978). On various causes of improper solutions in maximum likelihood factor analysis. *Psychometrika*, *43*, 225–243.

Vaughan, D., & Dancho, M. (2022). *Furrr: Apply mapping functions in parallel using futures*. https://furrr.futureverse.org/

Wickham, H., Averick, M., Bryan, J., Chang, W., McGowan, L. D., François, R., Grolemund, G., Hayes, A., Henry, L., Hester, J., Kuhn, M., Pedersen, T. L., Miller, E., Bache, S. M., Müller, K., Ooms, J., Robinson, D., Seidel, D. P., Spinu, V., … Yutani, H. (2019a). Welcome to the tidyverse. *Journal of Open Source Software*, *4*(43), 1686. https://doi.org/10.21105/joss.01686

Wickham, H., Averick, M., Bryan, J., Chang, W., McGowan, L. D., François, R., Grolemund, G., Hayes, A., Henry, L., Hester, J., Kuhn, M., Pedersen, T. L., Miller, E., Bache, S. M., Müller, K., Ooms, J., Robinson, D., Seidel, D. P., Spinu, V., … Yutani, H. (2019b). Welcome to the tidyverse. *Journal of Open Source Software*, *4*(43), 1686. https://doi.org/10.21105/joss.01686

Wickham, H., & Henry, L. (2023). *Purrr: Functional programming tools*. https://purrr.tidyverse.org/

Xie, Y. (2024). *Knitr: A general-purpose package for dynamic report generation in r*. https://yihui.org/knitr/

Zhu, H. (2024). *kableExtra: Construct complex table with 'kable' and pipe syntax*. http://haozhu233.github.io/kableExtra/

Zhu, H., Travison, T., Tsai, T., Beasley, W., Xie, Y., Yu, G., Laurent, S., Shepherd, R., Sidi, Y., Salzer, B., Gui, G., Fan, Y., Murdoch, D., Arel-Bundock, V., & Evans, B. (2024). *kableExtra: Construct Complex Table with 'kable' and Pipe Syntax*. https://cran.r-project.org/web/packages/kableExtra/index.html

Appendix

Appendix A: Simulation Protocol

Here the full simulation protocol of my simulation studies conducted individually prior to collaboration as well as the follow up study I conducted in light of the collaboration with Kosanke after the first round of conducting and evaluating our individual studies is presented. It is based on the preregistration of my individual studies (Kriegmair, 2024) and outlines all deviations from it.

Preregistration template designed by: Björn S. Siepe, František Bartoš, Tim P. Morris, Anne-Laure Boulesteix, Daniel W. Heck, and Samuel Pawel

1. General Information

1.1 What is the title of the project?

Comparing a Structural After Measurement (SAM) Approach to Standard Structural Equation Model (SEM) Estimation

1.2 Who are the current and future project contributors?

Valentin Kriegmair

1.3 Provide a description of the project.

The studies registered were part of an adversarial collaboration project. The aim was to conceptually (only in part) replicate the results obtained by Dhaene & Rosseel (2023) and Rosseel & Loh (2022). I set out to evaluate the performance of a Structural After Measurement (SAM) approach for estimating structural equation models (SEM) in comparison to standard SEM estimation methods. This served as the basis for the adversarial collaboration with another researcher who evaluated the same research question from the perspective of a conceptual replication of the (in part contradicting) results obtained by Robitzsch (2022). However, the following only describes the first (conceptual) replication.

1.4 Did any of the contributors already conduct related simulation studies on this specific question?

No prior related simulation studies have been conducted by the contributors.

2. Aims

Structural After Measurement (SAM) is an estimation method for structural equation models that consists of a stepwise estimation of the measurement and structural parts of a model. The research questions of the current simulation were:

1. How do SAM and traditional SEM methods (including ML and ULS) compare in terms of bias, 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?

3. Data-Generating Mechanism

3.1 Study 1

In study 1 (conceptually replicating Rosseel & Loh (2022)) data was generated parametrically. Four different population structural equation models (SEM) with five latent variables and three continuous indicators per facotr based on the following matrices were simulated:

- B as $M \times M$ matrix representing latent regression coefficients with all $b = 0.1$.
  - Model 1.1 and 1.2:

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0.1 & 0.1 & 0 & 0.1 & 0 \\ 0.1 & 0.1 & 0 & 0 & 0 \\ 0.1 & 0 & 0.1 & 0.1 & 0 \end{bmatrix}$$

  - Model 1.3 in deviation from the preregistration with a reversed effect between latent factors f3 and f4 to introduce another realistic and more severe misspecification to show the potential of SAM in most challenging conditions:

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0.1 & 0.1 & 0 & 0 & 0 \\ 0.1 & 0.1 & 0.1 & 0 & 0 \\ 0.1 & 0 & 0.1 & 0.1 & 0 \end{bmatrix}$$

  - Model 1.4 in deviation from the preregistration with a bidirectional structural relation between f3 and f4 specified as only one directional instead of just reversing the effect to investigate a different type of misspecification:

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0.1 & 0.1 & 0 & 0.1 & 0 \\ 0.1 & 0.1 & 0.1 & 0 & 0 \\ 0.1 & 0 & 0.1 & 0.1 & 0 \end{bmatrix}$$

- Ψ as $M \times M$ as diagonal matrix representing the residual variances in deviation from the preregistration not adjusted for the varying structural relations. This was only updated in the joint study (study 3) to adjust residual variances of all endogenous factors to accurately

reflect the number of regressors

- Model 1.1, 1.2, 1.3, and 1.4:

$$\Psi = \begin{bmatrix} 1.0 & 0 & 0 & 0 & 0 \\ 0 & 1.0 & 0 & 0 & 0 \\ 0 & 0 & 1.0 & 0 & 0 \\ 0 & 0 & 0 & 1.0 & 0 \\ 0 & 0 & 0 & 0 & 1.0 \end{bmatrix}$$

- Λ as $P \times M$ matrix representing factor loadings.
  - Model 1.1, 1.3 and 1.4:

$$\Lambda = \begin{bmatrix} 1.0 & 0 & 0 & 0 & 0 \\ 0.7 & 0 & 0 & 0 & 0 \\ 0.7 & 0 & 0 & 0 & 0 \\ 0 & 1.0 & 0 & 0 & 0 \\ 0 & 0.7 & 0 & 0 & 0 \\ 0 & 0.7 & 0 & 0 & 0 \\ 0 & 0 & 1.0 & 0 & 0 \\ 0 & 0 & 0.7 & 0 & 0 \\ 0 & 0 & 0.7 & 0 & 0 \\ 0 & 0 & 0 & 1.0 & 0 \\ 0 & 0 & 0 & 0.7 & 0 \\ 0 & 0 & 0 & 0.7 & 0 \\ 0 & 0 & 0 & 0 & 1.0 \\ 0 & 0 & 0 & 0 & 0.7 \\ 0 & 0 & 0 & 0 & 0.7 \end{bmatrix}$$

  - Model 1.2: cross loadings will be set to be 10% lower than the factor loadings: $\Lambda_{ik,jk} = 0.63 = 0.9 \times 0.7$. They will be generated by the following elements in Λ: (2, 2), (5, 3), (8, 4), (11, 5), (14, 1).

- Θ as a $P \times P$ matrix representing the residual variances and covariances of the indicators.
  - Model 1.1, 1.2 and 1.4: The diagonal generated as:

$$\Theta^* = \text{Var}(\eta)\Lambda^T \times \frac{1}{r-1}$$

    (where r is the reliability of the indicators) and 0 on all off-diagonal elements
  - Model 1.3:

- Θ^* on the diagonal.
- Correlated residuals generated between specific indicator pairs: for $i = (2, 5, 8, 11, 14)$ and $i' = (3, 6, 9, 12, 15)$, and for each $k = 1, \dots, 4$ and $l = k + 1, \dots, 5$, the entries (i_k, i'_l) and (i'_l, i_k) in Θ are set to $0.6 \times \min \Theta^*$, ensuring correlated errors among selected indicator pairs without exceeding a 0.6 correlation coefficient.

3.1.2 Study 2

For study 2, again, different five-factor population models with three continious indicators per facotr were generated parametrically . Further, the different models of study 2 were used for different simulation settings resulting in two sub-studies 2.1 and 2.2 (see simulation settings).

- B as $M \times M$ matrix representing latent regression coefficients with varying parameter size defined by two conditions of endogenous factor variance explained by the exogenous factors (low: $R^2 = 0.1$ or medium: $R^2 = 0.4$ see below under factor):
  - Model 2.1 and 2.2:

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \beta_{\eta_4,\eta_1} & \beta_{\eta_4,\eta_2} & 0 & 0 & 0 \\ 0 & \beta_{\eta_5,\eta_2} & \beta_{\eta_5,\eta_3} & \beta_{\eta_5,\eta_4} & 0 \end{bmatrix}$$

- Λ as $P \times M$ matrix representing factor loadings of indicators on the latent factors.

– Model 2.1:

$$\Lambda = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0.9 & 0 & 0 & 0 & 0 \\ 0.8 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0.9 & 0 & 0 & 0 \\ 0 & 0.8 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0.9 & 0 & 0 \\ 0 & 0 & 0.8 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0.9 & 0 \\ 0 & 0 & 0 & 0.8 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0.9 \\ 0 & 0 & 0 & 0 & 0.8 \end{bmatrix}$$

– Model 2.2 with cross-loadings either in the exogenous ($\lambda_{6,3}$), endogenous ($\lambda_{12,5}$) or both parts of the model. Which cross loading was present depended on the misspecification simulation factor. The specific magnitude of the endogenous ($\lambda_{12,5}$) loading depended on R^2 (see under 3.2.2):

$$\Lambda = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0.9 & 0 & 0 & 0 & 0 \\ 0.8 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0.9 & 0 & 0 & 0 \\ 0 & 0.8 & \lambda_{6,3} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0.9 & 0 & 0 \\ 0 & 0 & 0.8 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0.9 & 0 \\ 0 & 0 & 0 & 0.8 & \lambda_{12,5} \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0.9 \\ 0 & 0 & 0 & 0 & 0.8 \end{bmatrix}$$

- Θ as a $P \times P$ matrix representing the residual variances and covariances of the indicators. This was computed as the portion of the indicator's total variance that is not explained by the latent factors, after accounting for the strength and reliability of its relationship to these factors (factor loadings), as well as the effects of regressions between the latent factors themselves.

  - Model 2.1: The diagonal of Θ generated as:

$$\Theta^* = \text{Var}(\eta)\Lambda^T \times \frac{1}{r-1}$$

    (where r is the reliability of the indicators) and 0 on all off-diagonal elements

  - Model 2.2:

    * Θ^* on the diagonal.
    * Correlated residuals generated between specific indicator pairs in either the endogenous, exogenous or both parts of the model.

    Thus depending on the simulation setting either:

    * $\Theta_{8,9}$, $\Theta_{9,8}$ (exogenous part)
    * $\Theta_{14,15}$ and $\Theta_{15,14}$ (endogenous part)
    * $\Theta_{8,9}$, $\Theta_{9,8}$, $\Theta_{14,15}$ and $\Theta_{15,14}$ (both parts)

    were set $0.6 \times \min \Theta^*$, ensuring correlated errors among selected indicator pairs without exceeding a 0.6 correlation coefficient:

3.1.3 Study 3

For study 3, again, four different five-factor population models with three indicators per factor were generated parametrically with B as $M \times M$ matrix representing latent regression coefficients with all $b = 0.1$ for all models in study 3:

$$\Psi = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0.1 & 0.1 & 0 & 0.1 & 0 \\ 0.1 & 0.1 & 0 & 0 & 0 \\ 0.1 & 0 & 0.1 & 0.1 & 0 \end{bmatrix}$$

and Ψ as $M \times M$ as diagonal matrix (0 on the off diagonal) representing variances of the factors with $1 - kb^2$ on the diagonal where k is the number of latent regressor per factor and b the regression coefficients (0.1) for all models in study 3. Each model in study 3 included either cross

loadings or correlated residual errors in the measurement model based on Λ and Θ (constructed as in study 1) but these modifications in the measurement models could be either positive or negative.

3.2 Factors of the Data-Generating Mechanism

3.2.1 Study 1 The first study modulated the following factors:

- Different misspecifications of the population model where the population model varies between the different models (1.1, 1.2, 1.3, 1.4) as described above, while the analysis model remains specified as model 1.1.
- Sample sizes of small (N = 100), medium (N = 400), or large (N = 6400)
- Indicator reliability of low (.3), moderate (.5), or high (.7)

3.2.2 Study 2 The second study modulated the following factors of the data generating process across both studies:

- Sample sizes of small (N = 100), medium (N = 400), or large (N = 6400)
- Variance explained (R^2) of the endogenous factor variance explained by the exogenous factors: low ($R^2 = 0.1$) or medium ($R^2 = 0.4$)
- Indicator reliability of three indicators per factor: *all high* (.8), *all low* (.5), *average low* (.5) varying between .7 to .3 with the highest reliability for the scaling indicator.
- Sample sizes of small (N = 100), medium (N = 400), or large (N = 6400)
- Deviating from the preregistration distribution (normal vs. non-normal) was not considered in the simulation settings to limit the scope of the study.
- Measurement misspecifications of a residual covariance and a factor loading either in the exogenous, endogoneous or both parts of the model (in deviation from the preregistration without additional structural misspecifications and only three modulations to limit the scope of the study):
- Number of measurement blocks (how many separate measurement models are fitted in the first step of SAM) of either a separate measurement model per latent variable (b = k = 5) or one joint measurement model for all exogenous variables (b = 3)

In deviation from the preregistration, additionally all models in study 2 were estimated including stuructral specifications that were not present in the population model to investigate the performance of the methods on recovering falsely specified absent structural relations.

3.2.3 Study 3 The third study modulated the following factors of the data generating process:

- Sample sizes of N = 50, N = 100, N = 250 and N = 400.
- Indicator reliability of low (.3), moderate (.5), or high (.7)

3.3 Simulation Conditions

- Study 1: in deviation from the preregistration only one estimattion model was considered to limit the scope of the study resulting in 36 conditions (4 population models x 3 sample sizes x 3 reliabilities)
- Study 2.1 (4 population models x 3 sample sizes x 2 R^2 x 3 reliabilities x 2 measurement blocks = 144 conditions) (in dviation from the preregistration the misspecifications were reduced and counted here as differnet population odels as well)

4. Estimands and Targets

Estimated structural model parameters (path coefficients) represented the estimands of interest.

5. Methods

Both studies will compare four different estimation methods for SEMs:

- Traditional SEM: (structural and measurement model estimated simultaneously) (rationale: the current standard approach in SEM estimation serving as a baseline with maximum likelihood (ML)):
- SAM: (separating the estimation of the measurement and structural model to alleviate the potential for propagation of bias from (e.g. misspecified) measurement part to the structural part of the model)
  - Local SAM (Uses summary statistics from the measurement model to derive the model-implied mean vector and variance-covariance matrix of latent variables. These statistics are then utilized to estimate the structural parameters. A mapping matrix (M) is used to transform the observed data into the latent variable space. It can be estimated using different methods.)
    - With ML mapping matrix (Akin to a factor score approach Bartlett (1938))
    - With ULS mapping matrix (Uses the Moore-Penrose pseudoinverse, suitable for scenarios with complex or underdetermined systems, where the K matrix is rank-deficient but requires adjustments for structural constraints.)
  - Global SAM (rationale: Fixing the parameters obtained from the measurement model in the first step, and then using them as constants in the full SEM during the second step. Suitable for models where local SAM is impractical due to higher-order latent variables or rank deficiencies in λ.)

Traditional SEM as well as both steps in the SAM approach will be estimated using Maximum Likelihood (ML) using `lavaan` (Rosseel, 2012) in R 4.4 (R Core Team, 2023).

6. Performance Measures

Across both studies the following performance measures were captured:

- Convergence rates: Proportions of observed data sets that successfully converged for each estimation method detected using `lavaan`.
- In deviation from the preregistration also impropper solutions of converged models showing negative variances as the only type of improper solution present were computed.
- Rrelative biases: Average difference between an estimate and its true value, normalized by the true value, assessed across all path coefficients: $\frac{\bar{T}-\theta}{\theta}$
- Absolute biases: (in deviation from the preregistration this measure as it might be more intuitive and applicable for study 1 and 3 with invariant regression weights): $(\bar{T}-\theta)$
- Root Mean Squared Errors (RMSE): Calculated as the square root of the average squared difference between an estimate and its true value, evaluated under conditions of model misspecification: $(\sqrt{\frac{1}{K}\sum_{k=1}^{K}(T_k-\theta)^2})$ 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.
- Relative Root Mean Squared Errors (RRMSE) in deviation from preregistration for better comparability in study 2 under varying regression weights:$\sqrt{\frac{(\bar{T}-\theta)^2+S_T^2}{\theta^2}}$
- Empirical coverage levels of 95% confidence intervals (CIs): Proportion of observed data sets where the constructed CIs included the true value. (Not reported to limit the scope)

7. Monte Carlo Uncertainty of the Estimated Performance Measures

Monte Carlo uncertainty was calculated (manually in deviation from the preregistration) for the absolute and relative metrics: $\sqrt{\frac{S_T^2}{K}}$ 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.

8. Simulation Repetitions

- Replicating Rosseel & Loh (2022) study 1 consisted of 5000 repetitions per condition.
- Replicating Dhaene & Rosseel (2023) study 2 will consisted of 10000 repetitions per condition.

- Study 3 entailed 5000 repitiions as this resulted in sufficiently small Monte Carlo standard errors for the performance measures.

9. Missing Values due to non-convergence or other reasons

As mentioned above convergence rates were captured and only converged propper solutions were used for performance measure computation.

10. Software and Libraries

The simulation was set up and conducted in R Core Team (2023) using `lavaan` (Rosseel, 2012) for generating data and estimation. The `furrr` (**davis_furrr_2022?**) package for parallel simulation execution. A full list of libraries and dependencies can be found on GitHub

11. Computational Environment

The simulations were conducted using the TARDIS high-performance computing cluster at the Max Planck Institute for Human Development. The computational environment was set up in R, utilizing a suite of packages for analysis and parallel computing. Key libraries included:

- Analysis and Data Manipulation Packages: `MASS`, `dplyr`, `tidyr`, `lavaan`, `purrr`, and `Matrix`.
- Parallel Computing Packages: `future`, `furrr`, `parallel`, `future` and `batchtools`.

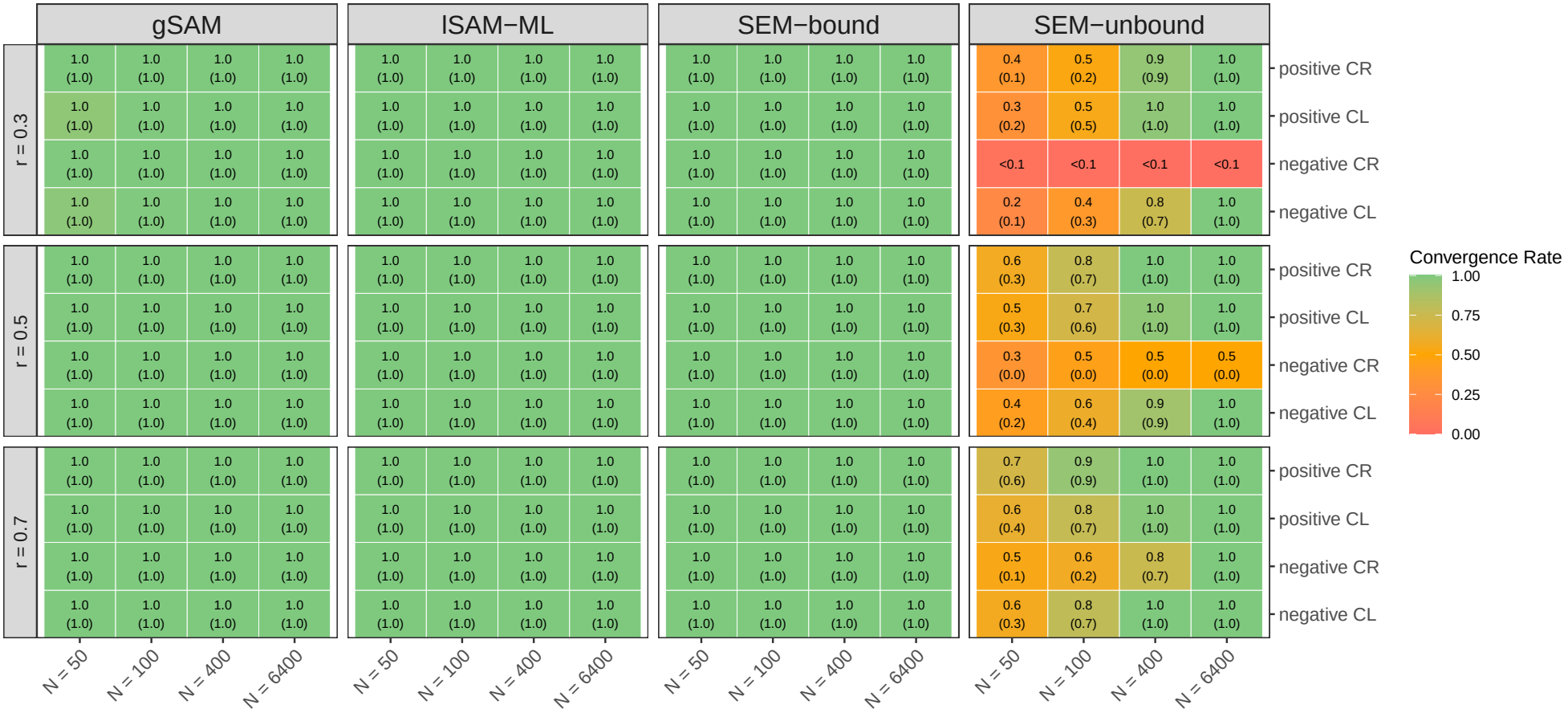
12. Reproducibility

The code of the simulation was made available on [GitHub] (https://github.com/valentinkm/AdversarialSimulation). A pre-generated list of seeds was used for all replications to ensure reproducibility and avoid synchronization in parallelized computations. As a examplary replication the simulation can be reproduced in this GitHub action here.

Appendix B: Supplementary Figures

Figure B1

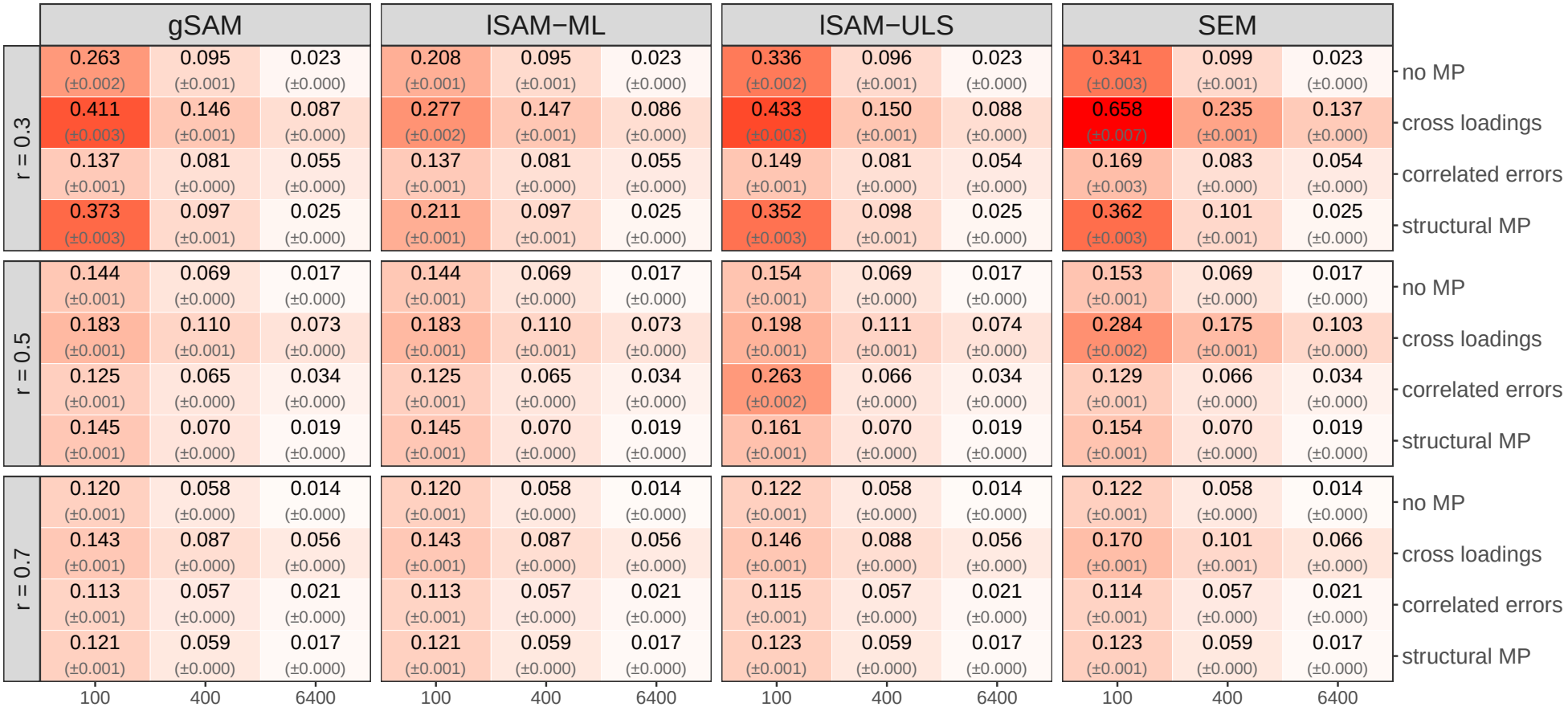
Convergence Rate and Rate of Proper Solutions in Study 3



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.

Figure B2

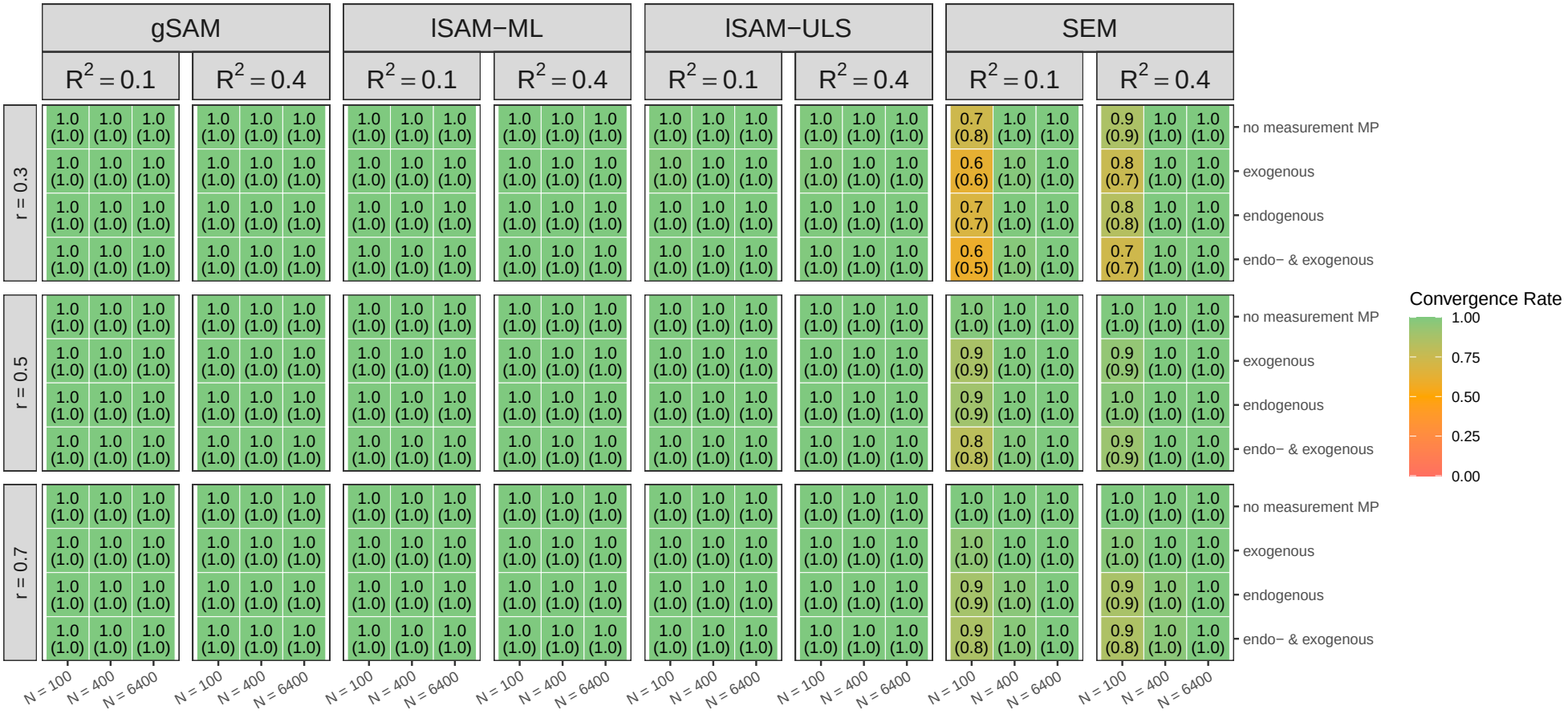
Mean Average Root Mean Squared Error (RMSE) of Regression Parameters in Study 1



Note. Mean RMSE averaged (in absolute values) over all parameters in one model for sample sizes (N), reliability (r), and misspecifications for global SAM (gSAM), local SAM with Maximum Likelihood (lSAM-ML), Unweighted Least Squares (lSAM-ULS) and SEM.

Figure B3

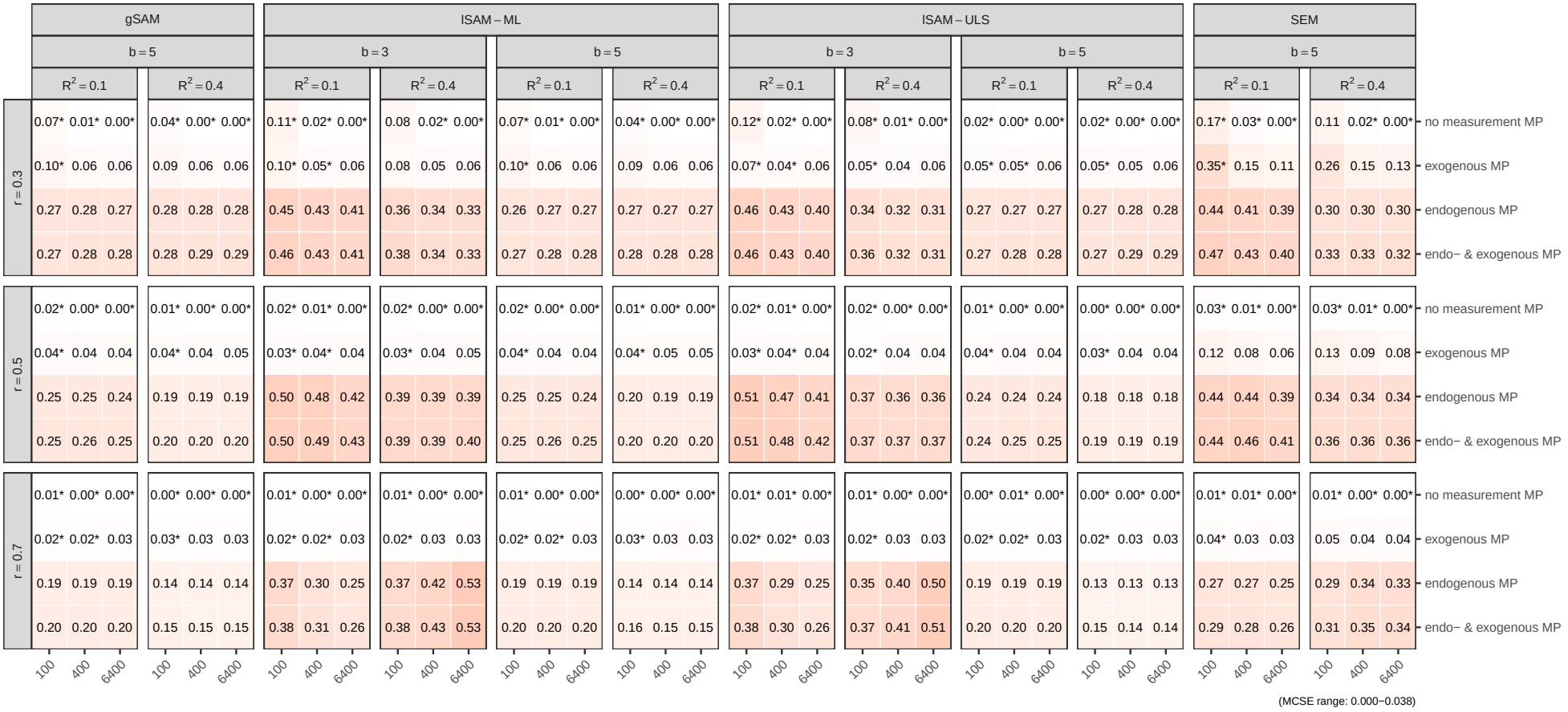
Convergence Rate and Rate of Proper Solutions in Study 2



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.

Figure B4

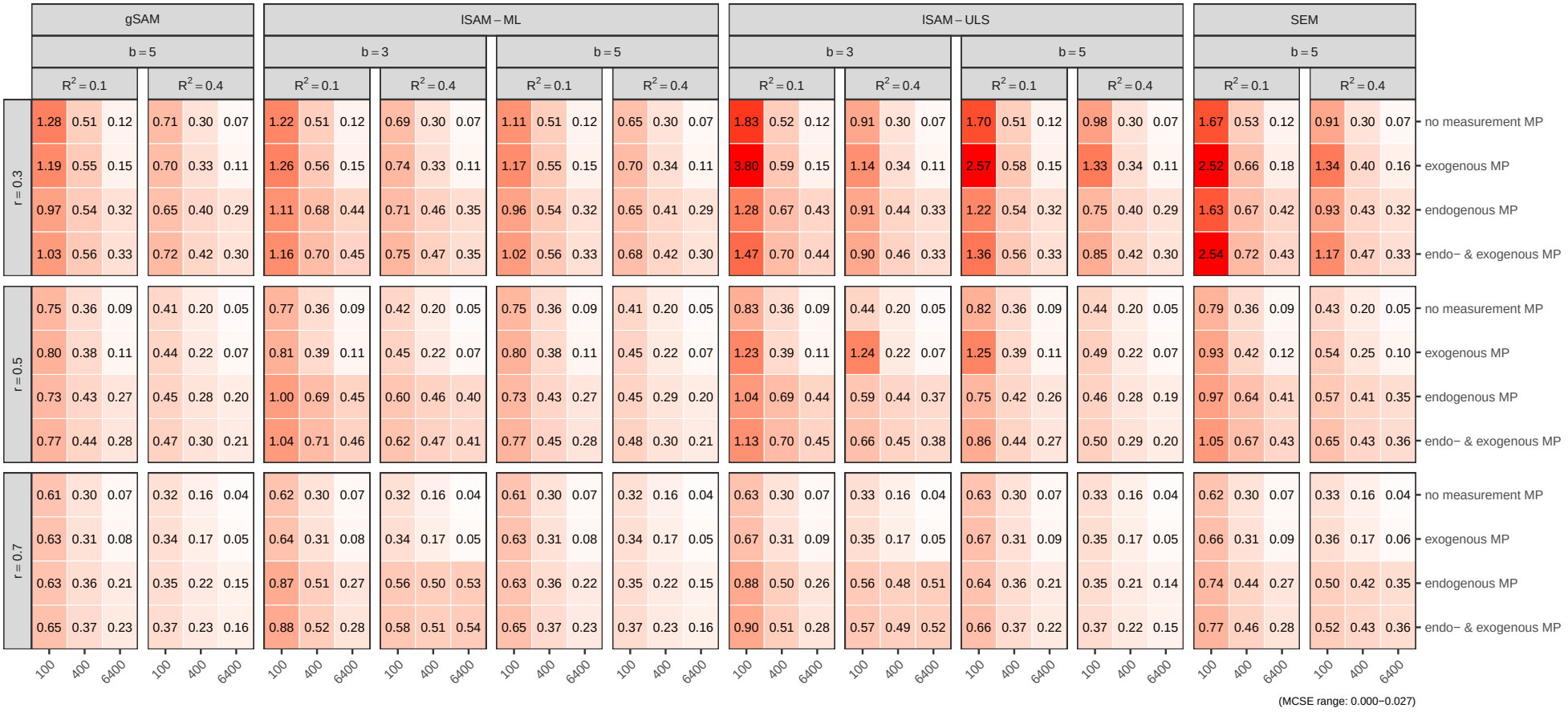
Relative Bias of Regression Parameters in Study 2



Note. Mean relative bias averaged (in absolute values) over all parameters in one model for sample sizes (N), reliability (r), and misspecifications for global SAM (gSAM), local SAM with Maximum Likelihood (lSAM-ML), Unweighted Least Squares (lSAM-ULS) and SEM. * indicating Monte-Carlos Standard Error (MCSE) above 10% of the estimate.

Figure B5

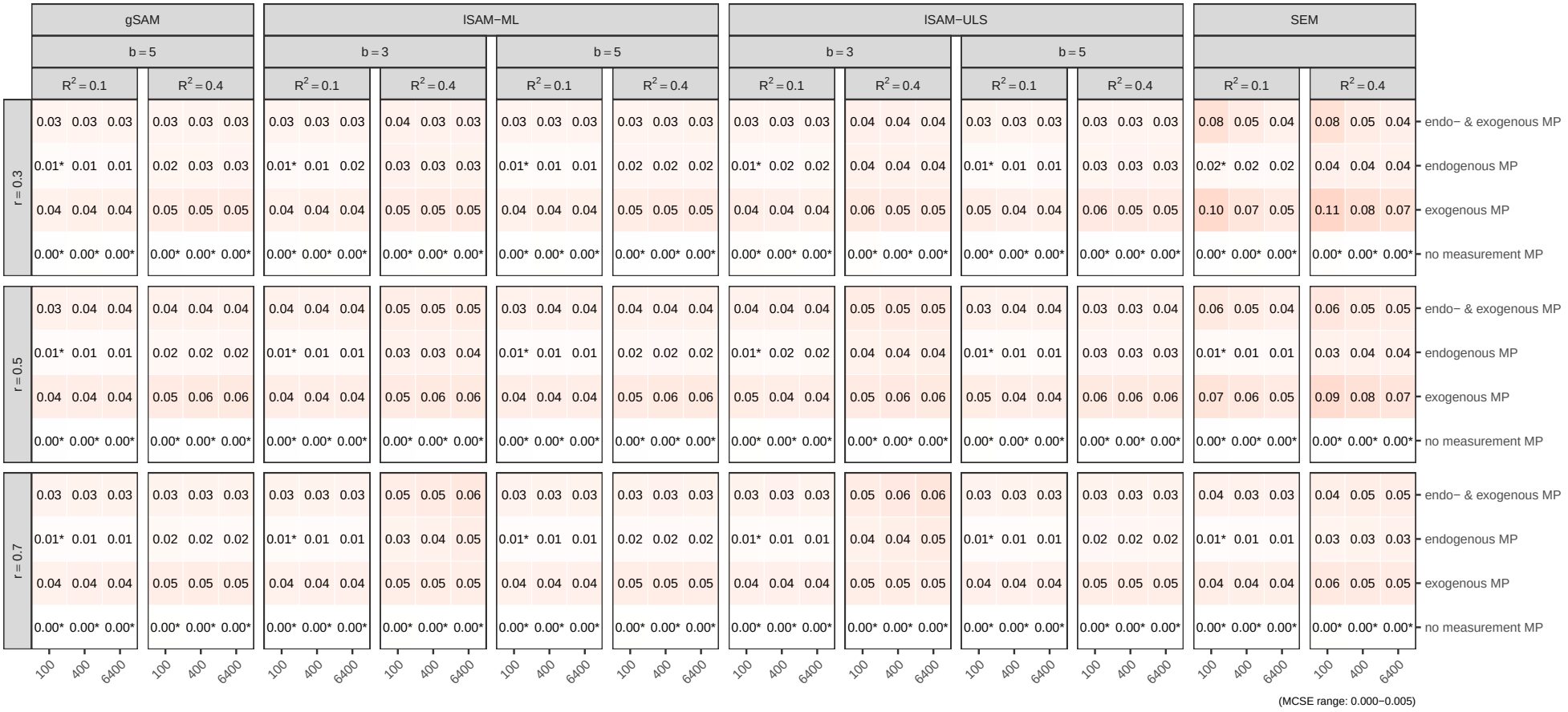
Relative RMSE of Regression Parameters in Study 2



Note. Mean relative RMSE averaged (in absolute values) over all parameters in one model for sample sizes (N), reliability (r), and misspecifications for global SAM (gSAM), local SAM with Maximum Likelihood (lSAM-ML), Unweighted Least Squares (lSAM-ULS) and SEM. * indicating Monte-Carlos Standard Error (MCSE) above 10% of the estimate.

Figure B6

Bias of Misspecified Regression Parameters in Study 2



Note. Mean bias of parameters absent in the population and misspecified in the analysis model for sample sizes (N), reliability (r), and misspecifications for global SAM (gSAM), local SAM with Maximum Likelihood (lSAM-ML), Unweighted Least Squares (lSAM-ULS) and SEM. * indicating Monte-Carlos Standard Error (MCSE) above 10% of the estimate.

Appendix C: Detailed Error and Warning Messages

In the following, all different warning and error messages raised during the studies are listed (see Table C1) and shown how often they occurred under various fitting conditions (see Table C2).

Table C1

List of Unique Warnings and Errors

ID	Message
1	lavaan WARNING: some estimated ov variances are negative
2	lavaan WARNING: the optimizer warns that a solution has NOT been found!
3	lavaan WARNING: the optimizer (NLMINB) claimed the model converged, but not all elements of the gradient are (near) zero; the optimizer may not have found a local solution use check.gradient = FALSE to skip this check.
4	lavaan WARNING: some estimated lv variances are negative
5	lavaan WARNING: some estimated ov variances are negative, lavaan WARNING: some estimated lv variances are negative
6	number of items to replace is not a multiple of replacement length
7	lavaan WARNING: Could not compute standard errors! The information matrix could not be inverted. This may be a symptom that the model is not identified., lavaan WARNING: some estimated ov variances are negative
8	lavaan WARNING: covariance matrix of latent variables is not positive definite; use lavInspect(fit, ”cov.lv”) to investigate.
9	lavaan WARNING: The variance-covariance matrix of the estimated parameters (vcov) does not appear to be positive definite! The smallest eigenvalue is smaller than or close to zero. This may be a symptom that the model is not identified., lavaan WARNING: some estimated ov variances are negative
10	lavaan WARNING: Could not compute standard errors! The information matrix could not be inverted. This may be a symptom that the model is not identified., lavaan WARNING: some estimated lv variances are negative
11	lavaan WARNING: Could not compute standard errors! The information matrix could not be inverted. This may be a symptom that the model is not identified., lavaan WARNING: some estimated ov variances are negative, lavaan WARNING: some estimated lv variances are negative

Table C1

List of Unique Warnings and Errors (continued)

ID	Message
12	lavaan WARNING: some estimated ov variances are negative, lavaan WARNING: covariance matrix of latent variables is not positive definite; use lavInspect(fit, "cov.lv") to investigate.
13	lavaan WARNING: Could not compute standard errors! The information matrix could not be inverted. This may be a symptom that the model is not identified.
14	lavaan WARNING: The variance-covariance matrix of the estimated parameters (vcov) does not appear to be positive definite! The smallest eigenvalue is smaller than or close to zero. This may be a symptom that the model is not identified., lavaan WARNING: covariance matrix of latent variables is not positive definite; use lavInspect(fit, "cov.lv") to investigate.
15	lavaan WARNING: Could not compute standard errors! The information matrix could not be inverted. This may be a symptom that the model is not identified., lavaan WARNING: covariance matrix of latent variables is not positive definite; use lavInspect(fit, "cov.lv") to investigate.
16	lavaan WARNING: the covariance matrix of the residuals of the observed variables (theta) is not positive definite; use lavInspect(fit, "theta") to investigate.
17	lavaan WARNING: The variance-covariance matrix of the estimated parameters (vcov) does not appear to be positive definite! The smallest eigenvalue is smaller than or close to zero. This may be a symptom that the model is not identified.

Note. This table lists all unique warnings and errors encountered during the simulation studies.

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 1	correlated errors	100	0.3	SEM	Warning	6860	1
Study 1	cross loadings	100	0.5	SEM	Warning	3575	1
Study 1	correlated errors	100	0.5	SEM	Warning	2923	1
Study 1	cross loadings	100	0.7	SEM	Warning	2903	1
Study 1	cross loadings	100	0.3	SEM	Warning	2769	1
Study 1	no measurement MP	100	0.3	SEM	Warning	2700	1
Study 1	structural MP	100	0.3	SEM	Warning	2577	1
Study 1	cross loadings	100	0.3	SEM	Warning	2037	2
Study 1	no measurement MP	100	0.3	SEM	Warning	1258	2

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies (continued)

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 1	structural MP	100	0.3	SEM	Warning	1133	2
Study 1	cross loadings	100	0.3	SEM	Warning	729	3
Study 1	correlated errors	100	0.3	SEM	Warning	692	3
Study 1	correlated errors	100	0.7	SEM	Warning	688	1
Study 1	correlated errors	400	0.3	SEM	Warning	606	1
Study 1	correlated errors	100	0.3	SEM	Warning	507	2
Study 1	cross loadings	400	0.3	SEM	Warning	450	1
Study 1	cross loadings	400	0.5	SEM	Warning	429	1
Study 1	cross loadings	100	0.3	SEM	Warning	417	4
Study 1	cross loadings	400	0.7	SEM	Warning	248	1
Study 1	no measurement MP	100	0.3	SEM	Warning	242	3
Study 1	structural MP	100	0.3	SEM	Warning	223	3
Study 1	cross loadings	100	0.5	SEM	Warning	203	2
Study 1	no measurement MP	100	0.5	SEM	Warning	197	1
Study 1	structural MP	100	0.5	SEM	Warning	183	1
Study 1	cross loadings	100	0.3	lSAM-ULS	Warning	150	1
Study 1	cross loadings	100	0.3	SEM	Warning	146	5
Study 1	structural MP	100	0.3	lSAM-ULS	Warning	62	1
Study 1	no measurement MP	100	0.3	lSAM-ULS	Warning	52	1
Study 1	cross loadings	100	0.3	gSAM	Warning	50	4
Study 1	structural MP	100	0.3	SEM	Warning	50	4
Study 1	cross loadings	100	0.5	SEM	Warning	42	3
Study 1	cross loadings	100	0.3	lSAM-ULS	Error	38	6
Study 1	no measurement MP	100	0.3	SEM	Warning	29	4
Study 1	no measurement MP	100	0.3	lSAM-ULS	Error	25	6
Study 1	structural MP	100	0.3	lSAM-ULS	Error	24	6
Study 1	cross loadings	100	0.3	SEM	Warning	23	7
Study 1	cross loadings	400	0.3	SEM	Warning	15	2

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies (continued)

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 1	no measurement MP	100	0.3	SEM	Warning	14	7
Study 1	cross loadings	100	0.3	gSAM	Error	14	6
Study 1	no measurement MP	100	0.3	SEM	Warning	12	5
Study 1	structural MP	100	0.3	SEM	Warning	11	5
Study 1	structural MP	100	0.3	SEM	Warning	9	7
Study 1	cross loadings	100	0.7	SEM	Warning	7	2
Study 1	structural MP	100	0.7	SEM	Warning	7	1
Study 1	cross loadings	100	0.3	SEM	Warning	5	8
Study 1	no measurement MP	100	0.5	SEM	Warning	4	2
Study 1	correlated errors	100	0.5	SEM	Warning	4	3
Study 1	no measurement MP	100	0.3	SEM	Warning	3	9
Study 1	no measurement MP	100	0.7	SEM	Warning	3	1
Study 1	cross loadings	100	0.3	SEM	Warning	3	10
Study 1	cross loadings	100	0.3	SEM	Warning	3	11
Study 1	no measurement MP	100	0.3	gSAM	Error	2	6
Study 1	no measurement MP	100	0.3	gSAM	Warning	2	4
Study 1	no measurement MP	400	0.3	SEM	Warning	2	1
Study 1	cross loadings	100	0.3	SEM	Warning	2	12
Study 1	cross loadings	100	0.3	lSAM-ULS	Warning	2	3
Study 1	cross loadings	100	0.5	SEM	Warning	2	4
Study 1	cross loadings	400	0.3	SEM	Warning	2	3
Study 1	correlated errors	100	0.5	lSAM-ULS	Error	2	6
Study 1	correlated errors	100	0.5	lSAM-ULS	Warning	2	1
Study 1	structural MP	100	0.3	SEM	Warning	2	9
Study 1	structural MP	100	0.3	gSAM	Error	2	6
Study 1	structural MP	100	0.3	gSAM	Warning	2	4
Study 1	structural MP	100	0.5	lSAM-ULS	Error	2	6
Study 1	no measurement MP	100	0.3	SEM	Warning	1	11
Study 1	no measurement MP	100	0.3	lSAM-ULS	Warning	1	3

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies (continued)

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 1	no measurement MP	100	0.5	lSAM-ULS	Warning	1	1
Study 1	cross loadings	100	0.3	SEM	Warning	1	9
Study 1	cross loadings	100	0.3	gSAM	Warning	1	8
Study 1	cross loadings	100	0.5	lSAM-ULS	Error	1	6
Study 1	cross loadings	100	0.5	lSAM-ULS	Warning	1	1
Study 1	correlated errors	100	0.3	SEM	Warning	1	7
Study 1	correlated errors	100	0.3	lSAM-ULS	Warning	1	1
Study 1	correlated errors	100	0.5	SEM	Warning	1	2
Study 1	correlated errors	400	0.5	SEM	Warning	1	1
Study 1	structural MP	100	0.3	SEM	Warning	1	10
Study 1	structural MP	100	0.3	lSAM-ULS	Warning	1	3
Study 1	structural MP	100	0.3	lSAM-ULS	Warning	1	2
Study 1	structural MP	100	0.5	lSAM-ULS	Warning	1	1
Study 2	endo- & exogenous MP	100	0.3	SEM	Warning	5265	1
Study 2	exogenous MP	100	0.3	SEM	Warning	4622	1
Study 2	endogenous MP	100	0.3	SEM	Warning	3615	1
Study 2	endo- & exogenous MP	100	0.7	SEM	Warning	2904	1
Study 2	endo- & exogenous MP	100	0.5	SEM	Warning	2743	1
Study 2	no measurement MP	100	0.3	SEM	Warning	2701	1
Study 2	endogenous MP	100	0.7	SEM	Warning	2336	1
Study 2	exogenous MP	100	0.5	SEM	Warning	1814	1
Study 2	endo- & exogenous MP	100	0.3	SEM	Warning	1625	2
Study 2	exogenous MP	100	0.3	SEM	Warning	1624	2
Study 2	endogenous MP	100	0.5	SEM	Warning	1252	1
Study 2	endogenous MP	100	0.3	SEM	Warning	1211	2
Study 2	no measurement MP	100	0.3	SEM	Warning	1121	2
Study 2	exogenous MP	100	0.7	SEM	Warning	702	1
Study 2	endo- & exogenous MP	100	0.3	SEM	Warning	675	3

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies (continued)

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 2	endo- & exogenous MP	400	0.7	SEM	Warning	599	1
Study 2	endogenous MP	400	0.7	SEM	Warning	588	1
Study 2	exogenous MP	100	0.3	SEM	Warning	559	3
Study 2	endogenous MP	100	0.3	SEM	Warning	305	3
Study 2	exogenous MP	100	0.3	lSAM-ULS	Warning	286	1
Study 2	endo- & exogenous MP	100	0.3	SEM	Warning	242	4
Study 2	endo- & exogenous MP	400	0.3	SEM	Warning	239	1
Study 2	no measurement MP	100	0.3	SEM	Warning	220	3
Study 2	exogenous MP	400	0.3	SEM	Warning	195	1
Study 2	exogenous MP	100	0.3	SEM	Warning	175	4
Study 2	no measurement MP	100	0.5	SEM	Warning	165	1
Study 2	endogenous MP	100	0.3	SEM	Warning	157	4
Study 2	no measurement MP	100	0.3	lSAM-ULS	Warning	138	1
Study 2	no measurement MP	100	0.3	SEM	Warning	132	4
Study 2	endo- & exogenous MP	400	0.5	SEM	Warning	130	1
Study 2	endo- & exogenous MP	100	0.3	lSAM-ULS	Warning	128	1
Study 2	exogenous MP	100	0.3	lSAM-ULS	Error	121	6
Study 2	endo- & exogenous MP	100	0.5	SEM	Warning	105	2
Study 2	exogenous MP	100	0.5	SEM	Warning	93	2
Study 2	endogenous MP	100	0.3	lSAM-ULS	Warning	78	1
Study 2	exogenous MP	400	0.5	SEM	Warning	77	1
Study 2	endo- & exogenous MP	100	0.3	SEM	Warning	57	5
Study 2	no measurement MP	100	0.3	lSAM-ULS	Error	44	6
Study 2	exogenous MP	100	0.3	SEM	Warning	43	5
Study 2	endo- & exogenous MP	100	0.3	lSAM-ULS	Error	41	6
Study 2	endogenous MP	400	0.5	SEM	Warning	40	1
Study 2	endo- & exogenous MP	100	0.3	gSAM	Warning	31	4

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies (continued)

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 2	endogenous MP	400	0.3	SEM	Warning	29	1
Study 2	endogenous MP	100	0.3	SEM	Warning	26	5
Study 2	endogenous MP	100	0.3	gSAM	Warning	26	4
Study 2	exogenous MP	100	0.3	gSAM	Warning	20	4
Study 2	no measurement MP	100	0.3	gSAM	Warning	18	4
Study 2	endo- & exogenous MP	100	0.5	SEM	Warning	18	3
Study 2	endo- & exogenous MP	100	0.5	lSAM-ULS	Warning	17	1
Study 2	exogenous MP	100	0.5	lSAM-ULS	Warning	16	1
Study 2	no measurement MP	100	0.3	SEM	Warning	15	5
Study 2	no measurement MP	100	0.3	SEM	Warning	14	7
Study 2	exogenous MP	100	0.5	SEM	Warning	14	3
Study 2	endogenous MP	100	0.3	lSAM-ULS	Error	14	6
Study 2	endogenous MP	100	0.5	SEM	Warning	13	2
Study 2	exogenous MP	100	0.3	SEM	Warning	10	7
Study 2	exogenous MP	400	0.3	SEM	Warning	10	2
Study 2	endo- & exogenous MP	100	0.3	SEM	Warning	10	7
Study 2	endo- & exogenous MP	400	0.3	SEM	Warning	8	2
Study 2	exogenous MP	100	0.3	lSAM-ULS	Warning	7	3
Study 2	endo- & exogenous MP	100	0.3	gSAM	Error	7	6
Study 2	exogenous MP	100	0.3	SEM	Warning	6	10
Study 2	exogenous MP	100	0.5	lSAM-ULS	Error	5	6
Study 2	endo- & exogenous MP	100	0.5	lSAM-ULS	Error	5	6
Study 2	exogenous MP	400	0.7	SEM	Warning	4	1
Study 2	endogenous MP	100	0.3	SEM	Warning	4	7
Study 2	no measurement MP	100	0.3	SEM	Warning	3	10
Study 2	no measurement MP	100	0.5	lSAM-ULS	Warning	3	1
Study 2	exogenous MP	100	0.3	SEM	Warning	3	11
Study 2	endo- & exogenous MP	100	0.3	SEM	Warning	3	10

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies (continued)

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 2	endo- & exogenous MP	100	0.3	SEM	Warning	3	11
Study 2	endo- & exogenous MP	100	0.7	SEM	Warning	3	2
Study 2	no measurement MP	100	0.7	SEM	Warning	2	1
Study 2	exogenous MP	100	0.3	gSAM	Error	2	6
Study 2	exogenous MP	100	0.3	lSAM-ULS	Warning	2	2
Study 2	exogenous MP	100	0.7	SEM	Warning	2	2
Study 2	exogenous MP	400	0.3	SEM	Warning	2	3
Study 2	endogenous MP	100	0.5	SEM	Warning	2	3
Study 2	endo- & exogenous MP	100	0.3	gSAM	Warning	2	3
Study 2	endo- & exogenous MP	100	0.5	SEM	Warning	2	4
Study 2	no measurement MP	100	0.3	gSAM	Error	1	6
Study 2	no measurement MP	400	0.3	SEM	Warning	1	1
Study 2	exogenous MP	100	0.3	SEM	Warning	1	13
Study 2	exogenous MP	100	0.3	SEM	Warning	1	12
Study 2	exogenous MP	100	0.5	lSAM-ULS	Warning	1	3
Study 2	exogenous MP	100	0.7	SEM	Warning	1	3
Study 2	exogenous MP	400	0.3	lSAM-ULS	Error	1	6
Study 2	endogenous MP	100	0.3	SEM	Warning	1	9
Study 2	endogenous MP	100	0.3	lSAM-ULS	Warning	1	3
Study 2	endogenous MP	100	0.5	lSAM-ULS	Error	1	6
Study 2	endogenous MP	100	0.5	lSAM-ULS	Warning	1	1
Study 2	endogenous MP	400	0.3	SEM	Warning	1	2
Study 2	endo- & exogenous MP	100	0.3	lSAM-ULS	Warning	1	2
Study 2	endo- & exogenous MP	100	0.3	lSAM ML	Error	1	6
Study 2	endo- & exogenous MP	100	0.5	lSAM-ULS	Warning	1	2

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies (continued)

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 2	endo- & exogenous MP	100	0.7	lSAM-ULS	Warning	1	1
Study 2	endo- & exogenous MP	400	0.3	SEM	Warning	1	3
Study 2	endo- & exogenous MP	400	0.3	SEM	Warning	1	4
Study 3	positive CL	50	0.3	lSAM-ULS	Warning	248	1
Study 3	positive CL	50	0.3	gSAM	Warning	209	4
Study 3	negative CL	50	0.3	lSAM-ULS	Warning	208	1
Study 3	negative CL	50	0.3	gSAM	Warning	164	4
Study 3	positive CR	50	0.3	lSAM-ULS	Warning	82	1
Study 3	negative CR	50	0.3	lSAM-ULS	Warning	82	1
Study 3	negative CL	50	0.3	lSAM-ULS	Error	79	6
Study 3	positive CL	50	0.3	lSAM-ULS	Error	72	6
Study 3	positive CR	50	0.3	SEM	Warning	71	8
Study 3	negative CR	50	0.3	SEM	Warning	71	8
Study 3	positive CL	100	0.3	lSAM-ULS	Warning	62	1
Study 3	negative CL	50	0.3	SEM	Warning	61	8
Study 3	positive CL	50	0.3	SEM	Warning	53	8
Study 3	negative CL	100	0.3	lSAM-ULS	Warning	52	1
Study 3	positive CL	50	0.5	lSAM-ULS	Warning	51	1
Study 3	negative CL	50	0.3	gSAM	Error	47	6
Study 3	negative CL	50	0.5	lSAM-ULS	Warning	37	1
Study 3	positive CL	50	0.3	gSAM	Error	36	6
Study 3	positive CR	50	0.3	SEM	Warning	31	14
Study 3	positive CR	100	0.3	lSAM-ULS	Warning	31	1

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies (continued)

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 3	negative CR	50	0.3	SEM	Warning	31	14
Study 3	negative CR	100	0.3	lSAM-ULS	Warning	31	1
Study 3	positive CL	100	0.3	lSAM-ULS	Error	28	6
Study 3	positive CR	50	0.3	lSAM-ULS	Warning	19	2
Study 3	negative CR	50	0.3	lSAM-ULS	Warning	19	2
Study 3	positive CL	50	0.5	lSAM-ULS	Error	18	6
Study 3	positive CR	50	0.3	lSAM-ULS	Warning	18	3
Study 3	negative CL	100	0.3	lSAM-ULS	Error	18	6
Study 3	negative CR	50	0.3	lSAM-ULS	Warning	18	3
Study 3	positive CL	100	0.3	gSAM	Warning	17	4
Study 3	positive CR	50	0.3	lSAM-ULS	Error	17	6
Study 3	negative CL	50	0.3	SEM	Warning	17	14
Study 3	negative CR	50	0.3	lSAM-ULS	Error	17	6
Study 3	negative CL	50	0.5	lSAM-ULS	Error	13	6
Study 3	negative CL	100	0.3	gSAM	Warning	12	4
Study 3	positive CR	100	0.3	lSAM-ULS	Warning	11	3
Study 3	negative CR	100	0.3	lSAM-ULS	Warning	11	3
Study 3	positive CL	50	0.3	SEM	Warning	10	15
Study 3	positive CL	50	0.3	gSAM	Warning	10	3
Study 3	positive CR	50	0.3	gSAM	Warning	10	4
Study 3	negative CL	100	0.3	SEM	Warning	10	8
Study 3	negative CR	50	0.3	gSAM	Warning	10	4

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies (continued)

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 3	positive CL	50	0.3	gSAM	Warning	9	8
Study 3	positive CR	100	0.3	lSAM-ULS	Error	9	6
Study 3	negative CR	100	0.3	lSAM-ULS	Error	9	6
Study 3	positive CL	50	0.5	gSAM	Warning	8	4
Study 3	positive CL	50	0.7	lSAM-ULS	Warning	7	1
Study 3	positive CR	100	0.3	lSAM-ULS	Warning	7	2
Study 3	negative CR	100	0.3	lSAM-ULS	Warning	7	2
Study 3	positive CL	50	0.3	SEM	Warning	6	14
Study 3	positive CL	100	0.3	SEM	Warning	6	8
Study 3	positive CR	50	0.3	SEM	Warning	6	15
Study 3	negative CL	50	0.3	SEM	Warning	6	15
Study 3	negative CL	50	0.3	gSAM	Warning	6	8
Study 3	negative CL	50	0.7	lSAM-ULS	Warning	6	1
Study 3	negative CR	50	0.3	SEM	Warning	6	15
Study 3	positive CL	50	0.7	lSAM-ULS	Error	5	6
Study 3	positive CR	50	0.5	lSAM-ULS	Warning	5	1
Study 3	negative CL	100	0.3	gSAM	Error	5	6
Study 3	negative CR	50	0.5	lSAM-ULS	Warning	5	1
Study 3	positive CL	50	0.3	lSAM-ULS	Warning	4	2
Study 3	positive CR	50	0.5	lSAM-ULS	Error	4	6
Study 3	positive CR	100	0.3	SEM	Warning	4	8
Study 3	negative CL	50	0.3	lSAM-ULS	Warning	4	2
Study 3	negative CL	50	0.5	SEM	Warning	4	8

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies (continued)

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 3	negative CR	50	0.5	lSAM-ULS	Error	4	6
Study 3	negative CR	100	0.3	SEM	Warning	4	8
Study 3	positive CL	50	0.3	lSAM-ULS	Warning	3	16
Study 3	negative CL	50	0.3	gSAM	Warning	3	3
Study 3	negative CL	100	0.5	lSAM-ULS	Warning	3	1
Study 3	positive CL	50	0.3	lSAM-ULS	Warning	2	3
Study 3	positive CL	50	0.5	SEM	Warning	2	8
Study 3	positive CL	100	0.3	gSAM	Error	2	6
Study 3	positive CL	100	0.5	lSAM-ULS	Error	2	6
Study 3	positive CL	250	0.3	lSAM-ULS	Warning	2	1
Study 3	positive CR	100	0.3	SEM	Warning	2	14
Study 3	negative CL	50	0.3	lSAM-ULS	Warning	2	3
Study 3	negative CL	50	0.3	lSAM-ULS	Warning	2	16
Study 3	negative CL	50	0.5	gSAM	Warning	2	4
Study 3	negative CL	100	0.3	SEM	Warning	2	14
Study 3	negative CL	100	0.3	lSAM-ULS	Warning	2	3
Study 3	negative CR	100	0.3	SEM	Warning	2	14
Study 3	positive CL	50	0.5	gSAM	Error	1	6
Study 3	positive CL	50	0.5	lSAM-ULS	Warning	1	3
Study 3	positive CL	50	0.5	lSAM-ULS	Warning	1	2
Study 3	positive CL	100	0.3	SEM	Warning	1	14
Study 3	positive CL	100	0.3	gSAM	Warning	1	8
Study 3	positive CL	100	0.3	lSAM-ULS	Warning	1	3

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies (continued)

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 3	positive CL	100	0.5	lSAM-ULS	Warning	1	1
Study 3	positive CL	250	0.3	lSAM-ULS	Error	1	6
Study 3	positive CR	50	0.3	gSAM	Error	1	6
Study 3	positive CR	50	0.3	lSAM-ULS	Warning	1	16
Study 3	positive CR	50	0.5	gSAM	Warning	1	4
Study 3	positive CR	50	0.5	lSAM-ULS	Warning	1	3
Study 3	positive CR	50	0.7	lSAM-ULS	Warning	1	1
Study 3	positive CR	250	0.3	lSAM-ULS	Warning	1	3
Study 3	positive CR	250	0.3	lSAM-ULS	Warning	1	2
Study 3	positive CR	250	0.3	lSAM-ULS	Warning	1	1
Study 3	positive CR	400	0.3	lSAM-ULS	Warning	1	1
Study 3	negative CL	50	0.5	gSAM	Error	1	6
Study 3	negative CL	50	0.5	lSAM-ULS	Warning	1	16
Study 3	negative CL	50	0.7	lSAM-ULS	Error	1	6
Study 3	negative CL	50	0.7	lSAM-ULS	Warning	1	3
Study 3	negative CL	100	0.3	SEM	Warning	1	13
Study 3	negative CL	100	0.3	SEM	Warning	1	17
Study 3	negative CL	100	0.3	gSAM	Warning	1	8
Study 3	negative CL	250	0.3	lSAM-ULS	Error	1	6
Study 3	negative CL	250	0.3	lSAM-ULS	Warning	1	1
Study 3	negative CR	50	0.3	gSAM	Error	1	6

Table C2

Summary of Warnings and Errors by Condition with ID for All Studies (continued)

Study	Misspecification	N	Reliability	Method	Type	Count	ID
Study 3	negative CR	50	0.3	lSAM-ULS	Warning	1	16
Study 3	negative CR	50	0.5	gSAM	Warning	1	4
Study 3	negative CR	50	0.5	lSAM-ULS	Warning	1	3
Study 3	negative CR	50	0.7	lSAM-ULS	Warning	1	1
Study 3	negative CR	250	0.3	lSAM-ULS	Warning	1	3
Study 3	negative CR	250	0.3	lSAM-ULS	Warning	1	2
Study 3	negative CR	250	0.3	lSAM-ULS	Warning	1	1
Study 3	negative CR	400	0.3	lSAM-ULS	Warning	1	1

Note. This table summarizes the count of warnings and errors for each condition in all three simulation studies with the respective ID number corresponding to Table 1.