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Mplus

ABSTRACT

In this article, we discuss single and multilevel SEM models with latent variable interactions. We describe the Bayesian estimation for these models and show through simulation studies that the Bayesian method outperforms other methods such as the maximum-likelihood method. We show that multilevel moderation models can easily be estimated with the Bayesian method.

KEYWORDS

Bayesian analysis; latent variable interactions; multilevel moderation; multilevel moderated mediation

Introduction

In this article, we discuss the analysis of single and multilevel structural equation models with latent variable interactions. In the single-level context, the maximum-likelihood (ML) estimation is described in Klein and Moosbrugger (2000). The ML computations are heavier than for models without latent variable interactions because numerical integration is needed. The ML estimation in the two-level context, discussed in Muthén and Asparouhov (2009), is even more difficult to utilize because the dimensions of numerical integration can increase quickly beyond what is computationally feasible. For an overview of the ML approach and various estimators suggested in earlier work, see Marsh et al. (2004). Different estimation methods are also discussed in Klein and Muthén (2007), Cudeck et al. (2009), Mooijart and Bentler (2010), and Brandt et al. (2020), but these estimation methods are also limited in scope. For example, the methods discussed in Brandt et al. (2020) do not extend to multilevel analysis, models with categorical data, incomplete data, or are computationally demanding. Bayesian estimation in the single-level context is discussed in Arminger and Muthén (1998) and Lee et al. (2007). In this article, we describe a new Bayesian estimation method for the single-level latent variable interaction model which appears to be very efficient. We also discuss how the Bayesian estimation can easily be extended to multilevel models, models with categorical dependent variables, as well as modeling with incomplete data. Preacher et al. (2016) and Zyphur et al. (2019) describe several two-level moderation models with interactions among the predictors at the within level, the between level, and across the two levels. For these multilevel moderation models, the interaction terms are necessarily interactions of latent variables because of the within-between decomposition of the variables. In this article, we use simulation studies to illustrate the advantages of the Bayesian estimation of the two-level moderation models.

In the next section, we discuss several basic concepts for models with latent variable interactions. We then discuss the Bayesian estimation and its advantages over the maximum-

likelihood estimation. Simulation studies are presented for single- and two-level models, including two-level moderation models and two-level moderated mediation models. Higher-order interaction terms are discussed as well.

The latent variable interaction model

In this section, we discuss some basic concepts of the latent variable interaction model such as model interpretation, model testing, model implied means, variance and covariances, standardization of model parameters as well as plotting of interaction terms.

Interpretation

As an example, consider the latent variable interaction model depicted in Figure 1. The factor η_3 is regressed on η_1 and η_2 as well as the interaction between η_1 and η_2 , as shown by the structural equation

$$\eta_3 = \beta_1 \eta_1 + \beta_2 \eta_2 + \beta_3 \eta_1 \eta_2 + \zeta_3. \quad (1)$$

The interaction variable $\eta_1 \eta_2$ involves only one parameter, the slope β_3 . The model also contains a second structural equation where η_4 is linearly regressed on η_3 , but there is no direct effect on η_4 from η_1 and η_2 , or their interaction.

For ease of interpretation, the regression Equation (1) can be re-written in the equivalent form

$$\eta_3 = (\beta_1 + \beta_3 \eta_2) \eta_1 + \beta_2 \eta_2 + \zeta_3, \quad (2)$$

where $(\beta_1 + \beta_3 \eta_2)$ is a moderator function (Klein & Moosbrugger, 2000) so that the β_1 strength of influence of η_1 on η_3 is moderated by $\beta_3 \eta_2$. The choice of moderator when translating (1) to (2) is arbitrary from an algebraic point of view and is purely a choice based on ease of substantive interpretation. As an example, Cudeck et al. (2009) consider school achievement (η_3) influenced by general reasoning (η_1), quantitative ability (η_2), and their interaction. In line with (2), the interaction is expressed as quantitative

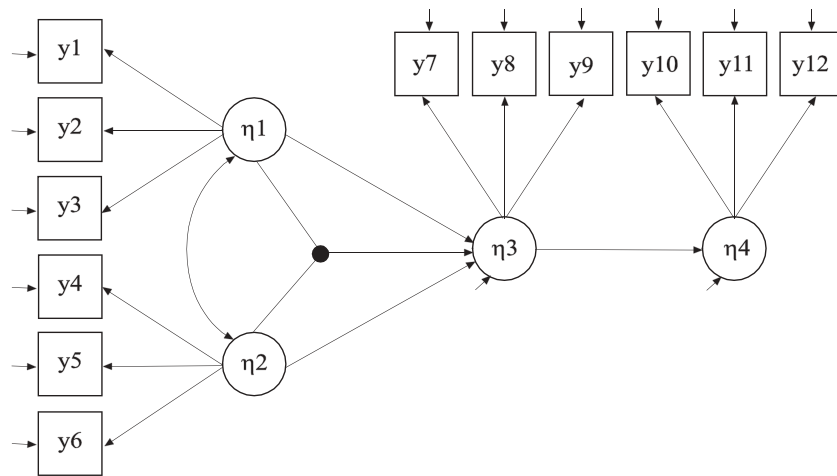


Figure 1. Structural equation model with interaction between latent variables.

ability moderating the influence of general reasoning on school achievement.

Model testing

As pointed out in Mooijaart and Satorra (2009), for some SEM models, the likelihood-ratio χ^2 obtained by ML for models without latent variable interactions is not sensitive to incorrectly leaving out latent variable interactions. For example, the model of Figure 1 without the interaction term $\beta_3 \eta_1 \eta_2$ fits data generated as in (1) perfectly. This is due to general maximum-likelihood results on robustness to non-normality (Satorra, 1990, 2002). Misfit for that model can be detected only by considering higher-order moments than the second-order variances and covariances of the outcomes. For other SEM models (models where interaction terms have a direct effect on the observed variables) omitted interaction terms can be detected by the chi-square test of fit, see further below. In such cases, traditional model modification guidance based on the chi-square test of fit would be incorrect and would lead to linear models that fit the first- and second-order moments approximately but would fail to discover the need for interaction terms. All this suggests that the standard chi-square test of fit has fairly limited capabilities when dealing with interaction modeling.

Without involving higher-order moments, a reasonable modeling strategy is to first fit a model without interactions and then add an interaction term. The significance of the interaction can be tested by either a z-test or a likelihood-ratio χ^2 difference test. Likelihood-ratio or Wald tests can be used to test the joint significance of several interaction terms.

Mean, variance, and R^2

To compute a dependent variable mean, variance, and R^2 for models with latent variable interactions, the following results are needed. The covariance between two variables X_j and X_k is defined as

$$Cov(X_j, X_k) = E(X_j X_k) - E(X_j) E(X_k), \tag{3}$$

so that the variance is obtained as

$$Cov(X_j, X_j) = V(X_j) = E(X_j^2) - [E(X_j)]^2. \tag{4}$$

With $E(X_j) = 0$ or $E(X_k) = 0$, (3) gives the mean of a product

$$E(X_j X_k) = Cov(X_j, X_k). \tag{5}$$

Assuming multivariate normality for four random variables X_i, X_j, X_k, X_l any third-order moment about the mean (μ) is zero (see, e.g., Anderson, 1984),

$$E((X_i - \mu_i)(X_j - \mu_j)(X_k - \mu_k)) = 0, \tag{6}$$

while the fourth-order moment about the mean is a function of covariances,

$$E((X_i - \mu_i)(X_j - \mu_j)(X_k - \mu_k)(X_l - \mu_l)) = \sigma_{ij} \sigma_{kl} + \sigma_{ik} \sigma_{jl} + \sigma_{il} \sigma_{jk}, \tag{7}$$

where, for example, $\sigma_{jk} = Cov(X_j, X_k)$ and $\sigma_{kk} = Var(X_k)$. This gives

$$E(X_j X_k X_j X_k) = V(X_j) V(X_k) + 2 [Cov(X_j, X_k)]^2, \tag{8}$$

so that the variance of a product is obtained as

$$V(X_j X_k) = E(X_j X_k X_j X_k) - [E(X_j X_k)]^2 \tag{9}$$

$$= V(X_j) V(X_k) + 2 [Cov(X_j, X_k)]^2 - [Cov(X_j, X_k)]^2 \tag{10}$$

$$= V(X_j) V(X_k) + [Cov(X_j, X_k)]^2. \tag{11}$$

Consider the application of these results in the mean and variance of the factor η_3 in (1) of Figure 1. Because of zero factor means, using (5) the mean of η_3 in (1) is obtained as

$$E(\eta_3) = \beta_1 0 + \beta_2 0 + \beta_3 E(\eta_1 \eta_2) + 0 \tag{12}$$

$$= \beta_3 Cov(\eta_1, \eta_2). \tag{13}$$

Using (4), the variance of η_3 is

$$V(\eta_3) = E(\eta_3 \eta_3) - [E(\eta_3)]^2, \tag{14}$$

where the second term has already been determined. As for the first term, multiplying the right-hand side of (1) by itself results in products of two, three, and four factors. Expectations for three- and four-factor terms are simplified by the following two results, assuming bivariate normality and zero means for η_1 and η_2 . All third-order moments $E(\eta_i \eta_j \eta_k)$ are zero by (6). The formula (8) is used to obtain the result

$$E(\eta_1 \eta_2 \eta_1 \eta_2) = V(\eta_1) V(\eta_2) + 2 [Cov(\eta_1, \eta_2)]^2. \tag{15}$$

Collecting terms, it follows that the variance of η_3 is obtained as

$$V(\eta_3) = \beta_1^2 V(\eta_1) + \beta_2^2 V(\eta_2) + 2 \beta_1 \beta_2 Cov(\eta_1, \eta_2) + \beta_3^2 V(\eta_1 \eta_2) + V(\zeta_3), \tag{16}$$

whereby (9–11)

$$V(\eta_1 \eta_2) = V(\eta_1) V(\eta_2) + [Cov(\eta_1, \eta_2)]^2. \tag{17}$$

R-square for η_3 can be expressed as usual as

$$[V(\eta_3) - V(\zeta_3)]/V(\eta_3). \tag{18}$$

Using (16), the proportion of $V(\eta_3)$ contributed by the interaction term can be quantified as (cf. Mooijaart & Satorra, 2009, p. 445)

$$\beta_3^2 [V(\eta_1) V(\eta_2) + [Cov(\eta_1, \eta_2)]^2]/V(\eta_3). \tag{19}$$

Consider as a hypothetical example the latent variable interaction model of Figure 2. Here, the latent variable interaction is between an exogenous and an endogenous latent variable. This example is useful to study the details of how to portray the model. The structural equations are

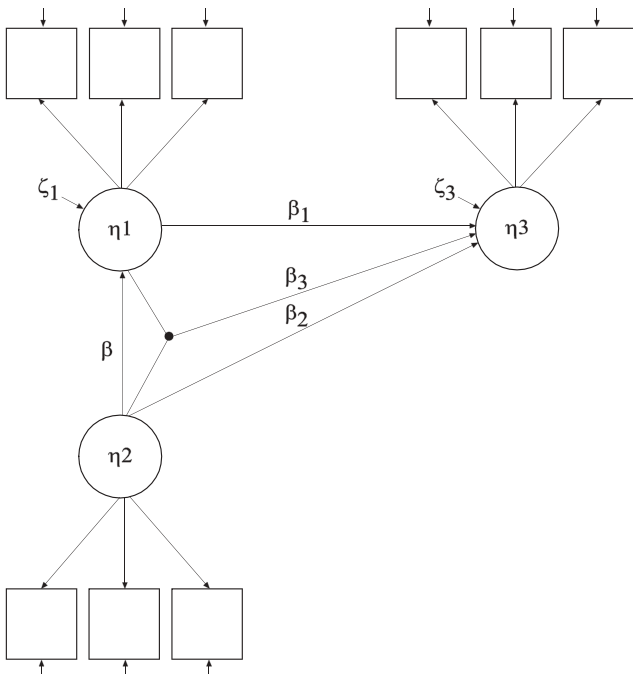


Figure 2. Structural equation model with interaction between an exogenous and an endogenous latent variable.

$$\eta_1 = \beta \eta_2 + \zeta_1, \tag{20}$$

$$\eta_3 = \beta_1 \eta_1 + \beta_2 \eta_2 + \beta_3 \eta_1 \eta_2 + \zeta_3. \tag{21}$$

Let $\beta = 1, \beta_1 = 0.5, \beta_2 = 0.7, \beta_3 = 0.4, V(\eta_2) = 1, V(\zeta_1) = 1,$ and $V(\zeta_3) = 1$. This implies that $V(\eta_1) = \beta^2 V(\eta_2) + V(\zeta_1) = 1^2 \times 1 + 1 = 2$ and $Cov(\eta_1, \eta_2) = \beta V(\eta_2) = 1 \times 1 = 1$. Using (16), $V(\eta_3) = 3.17$. The η_3 R-square is 0.68 and the variance percentage due to the interaction is 15%.

The general computation of the model implied means and variances is given in the Appendix.

Standardization

Because latent variables have arbitrary metrics, it is useful to also present interaction effects in terms of standardized latent variables. Noting that (21) is identical to (1), the model interpretation is aided by considering the moderator function $(\beta_1 + \beta_3 \eta_2) \eta_1$ of (2), so that η_2 moderates the η_1 influence on η_3 .

As usual, standardization is obtained by dividing by the standard deviation of the dependent variable and multiplying by the standard deviation of the independent variable. The standardized β_1 and β_3 coefficients in the term $(\beta_1 + \beta_3 \eta_2) \eta_1$ are obtained by dividing both by $\sqrt{V(\eta_3)} = \sqrt{3.17}$, multiplying β_1 by $\sqrt{V(\eta_1)} = \sqrt{2}$, and multiplying β_3 by $\sqrt{V(\eta_1)} \sqrt{V(\eta_2)} = \sqrt{2}$. This gives a standardized $\beta_1 = 0.397$ and a standardized $\beta_3 = 0.318$. The standardization of β_3 is in line with Equation (10) in Wen et al. (2010). These authors discuss why standardization of β_3 using $\sqrt{V(\eta_1)} \sqrt{V(\eta_2)}$ is preferred over using $\sqrt{V(\eta_1 \times \eta_2)}$.

The standard deviation change in η_3 as a function of a one standard deviation change in η_1 can now be evaluated at different values of η_2 using the moderator function. At the zero mean of η_2 , a standard deviation increase in η_1 leads to a 0.397 standard deviation increase in η_3 . At one standard deviation above the mean of η_2 , a standard deviation increase in η_1 leads to a $0.397 + 0.318 \times 1 = 0.715$ standard deviation increase in η_3 . At one standard deviation below the mean of η_2 , a standard deviation increase in η_1 leads to a $0.397 - 0.318 \times 1 = 0.079$ standard deviation increase in η_3 . In other words, the biggest effect of η_1 on η_3 occurs for subjects with high values on η_2 .

A more general treatment of standardization in matrix terms is given in the Appendix.

Plotting of interactions

The interaction can be plotted as in Figure 3. Using asterisks to denote standardization, consider the rearranged (20),

$$\eta_3^* = (\beta_1^* + \beta_3^* \eta_2^*) \eta_1^* + \beta_2^* \eta_2^* + \zeta_3^*. \tag{22}$$

Using (22), the three lines in the figure are expressed as follows in terms of the conditional expectation function for η_3^* at the three levels of η_2^* ,

$$E(\eta_3^* | \eta_1^*, \eta_2^* = 0) = \beta_1^* \eta_1^*, \tag{23}$$

$$E(\eta_3^* | \eta_1^*, \eta_2^* = 1) = (\beta_1^* + \beta_3^*) \eta_1^* + \beta_2^*, \tag{24}$$

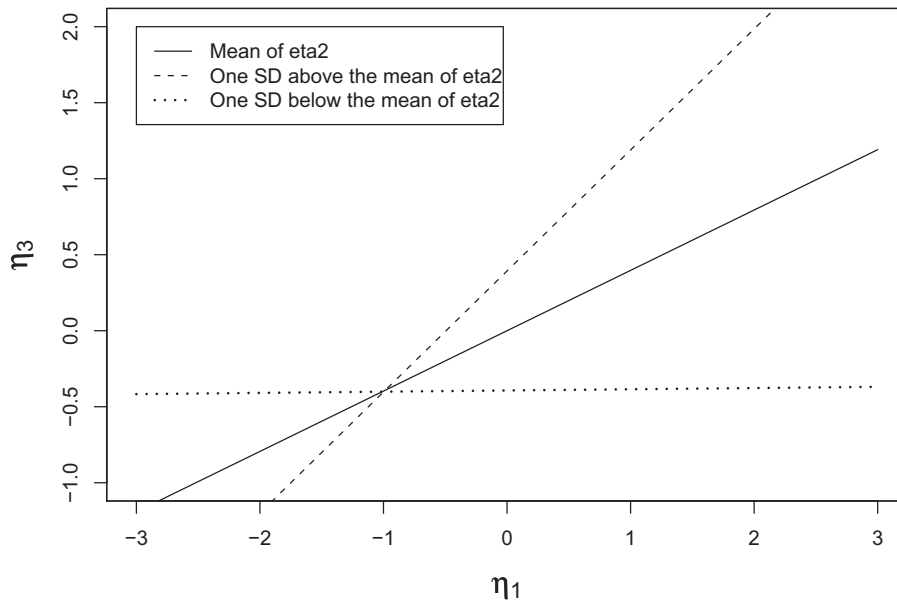


Figure 3. Interaction plot for structural equation model with interaction between an exogenous and an endogenous latent variable.

$$E(\eta_3^* | \eta_1^*, \eta_2^* = -1) = (\beta_1^* - \beta_3^*) \eta_1^* - \beta_2^* \tag{25}$$

$$\tag{26}$$

Here, the standardized value $\beta_2^* = \beta_2 \times \sqrt{V(\eta_2)} / \sqrt{V(\eta_3)} = 0.7 \times 1 / \sqrt{3.17} = 0.393$.

Bayesian estimation

The interactions between a latent variable and an observed variable can be estimated with the maximum-likelihood estimator using a closed-form expression for the likelihood, see Muthén and Asparouhov (2003). Because numerical integration is not used in that case, the estimation is efficient and can accommodate any number of interaction terms. Interactions between two latent variables, however, do not lead to closed form expressions for the likelihood and cannot be estimated with the maximum-likelihood method without numerical integration, see Klein and Moosbrugger (2000). In Mplus, the dimension of numerical integration corresponds to the number of latent variables used in the interaction terms. Numerical integration with more than three dimensions of integration, i.e., with more than three latent variables involved in interactions, is generally computationally intractable. It is possible to estimate models with a larger number of dimensions of integration using Monte Carlo integration in Mplus or using quadrature integration with very few integration points per dimension; however, such estimation often lacks precision and results in non-convergence.

By using the Bayesian estimation, however, we can resolve these limitations of the ML estimator, and estimate models with any number of latent variables and interaction terms. Consider the following single-level SEM model with interactions. Let Y_p denote the observed dependent variables, $p = 1, \dots, P$, η_m denote the latent variables in the model, $m = 1, \dots, M$ and X_q denote the covariates,

$q = 1, \dots, Q$. The general interaction model can be described as follows:

$$Y_p = v_p + \sum_{i=1}^M \lambda_{pi} \eta_i + \sum_{i=1}^M \sum_{j=i}^M \gamma_{pij} \eta_i \eta_j + \varepsilon_p \tag{27}$$

$$\eta_m = \alpha_m + \sum_{i=1}^M \beta_{mi} \eta_i + \sum_{i=1}^M \sum_{j=i}^M \delta_{mij} \eta_i \eta_j + \sum_{q=1}^Q \kappa_{mq} X_q + \xi_m \tag{28}$$

where $v_p, \lambda_{pi}, \gamma_{pij}, \alpha_m, \beta_{mi}, \delta_{mij}, \kappa_{mq}$ are model parameters and ξ_m and ε_p are normally distributed residuals.

To estimate this model with the Bayesian method, we follow the MCMC estimation framework described in Asparouhov and Muthén (2010a) for the estimation of the general SEM model. All aspects of that estimation method remain the same with the exception of one – the Gibbs sampler step for generating the latent variables η_m . In the standard SEM model, the posterior distribution for the latent variables used in the Gibbs sampler is a multivariate normal distribution. Due to the interaction terms, however, the posterior distribution will not be normal for the above model. To resolve this issue, we split the Gibbs sampler for the latent variables so that each latent variable is generated conditional on all other latent variables, i.e., we replace the Gibbs sampler that generates $\eta_1, \eta_2, \dots, \eta_M$ simultaneously with a Gibbs sampler with m steps that generates one latent variable at a time using the posterior distributions:

$$[\eta_1 | \eta_2, \eta_3, \dots, \eta_M, *] \tag{29}$$

$$[\eta_2 | \eta_1, \eta_3, \dots, \eta_M, *] \tag{30}$$

...

$$[\eta_M | \eta_1, \eta_2, \dots, \eta_{M-1}, *] \tag{31}$$

The advantage of this approach is that the above univariate distributions are easier to solve. There are two separate cases. Consider the posterior distribution $[\eta_1|\eta_2, \eta_3, \dots, \eta_M, *]$. The first and the simpler case is the situation when $\gamma_{p11} = \delta_{m11} = 0$ for each p and m . In that case, the quadratic term η_1^2 is not included in the model. The variable η_1 can be included in interaction terms such as $\eta_1\eta_2, \eta_1\eta_3$, but because the variables η_2, η_3, \dots are conditioned on, the model remains linear in terms of η_1 . Therefore, in this case, the posterior $[\eta_1|\eta_2, \eta_3, \dots, \eta_M, *]$ is the normal distribution with closed-form expression that can be computed as in Asparouhov and Muthén (2010a).

The second case is the situation when η_1^2 is included in the model, i.e., some of the parameters γ_{p11} or δ_{m11} are not zero. In that case, the posterior distribution of η_1 is not explicit and does not have a closed-form expression. We utilize the Metropolis–Hastings algorithm. The effectiveness of this algorithm is based on a being able to formulate a good approximation to the needed posterior distribution. The approximate posterior distribution is referred to in the literature as the jumping distribution. Fortunately, in this framework, we are able to provide a very good approximation. We specify the jumping distribution J as follows. If the current value for η_1 is η_1^* we consider the model where the interaction terms η_1^2 are replaced by $\eta_1\eta_1^*$. The posterior distribution of η_1 from that new model is a normal distribution and has a closed-form expression which we choose as the jumping distribution J for drawing a proposal value for η_1 , i.e., we draw a new value η_1^{**} from this distribution. The new value is accepted with probability $\min(1, A)$ where A is

$$A = \frac{p(y, \eta_{-1}, \eta_1^{**}|x)J(\eta_1^*|\eta_1^{**})}{p(y, \eta_{-1}, \eta_1^*|x)J(\eta_1^{**}|\eta_1^*)} \quad (32)$$

where p is the normal densities for that conditional distribution which can be derived from the model for ϵ_p and ξ_m in a sequential way under general regularity conditions (ex. η_1 is not regressed on η_1^2 or more generally – no reciprocal interactions). The vector η_{-1} denotes all η variables except the first. As formulated, the jumping distribution is a good approximation because if the interaction term has a small effect (or zero), the acceptance probability will be near 1 (or exactly 1), which facilitates fast mixing and fast populating of the desired posterior distributions. Note again that this model estimation complexity is needed only when a latent variable multiplies itself. The majority of the latent variable interaction models do not actually include such terms and are primarily focused on interaction terms between different variables, where fast explicit posterior distributions, described in case one above, will guarantee superior MCMC quality.

The above estimation method easily extends to two-level models, models with categorical dependent variables, and models with incomplete data as it is done in Asparouhov and Muthén (2010a). In the two-level model, the dependent variables are split as within and between and each of the two parts follows the SEM model with interactions (27–28), i.e., the within portion of a variable can be predicted by interactions of within-level latent variables, while the between portion of the variable can be predicted by interactions of between-level latent variables. Cross-interactions of within-level latent variables and between-

level latent variables are easily accommodated as well since such terms are essentially random slope coefficients for within-level latent variables. The Bayesian estimation of two-level models with interactions is simply the combination of the Gibbs sampler for two-level models without interactions with the Gibbs sampler for the latent variables described above for the single level. Conditional on the latent variables, the two-level model with interactions is just a standard two-level model. Conditional on the within-between split of the observed variables, the latent variable interaction model is essentially a two-group model. Similar logic allows us to extend the estimation to models with categorical dependent variables and missing data.

The interaction model can also be extended to incorporate interactions between latent variables and observed variables. In Mplus this can be done directly by specifying the interaction effect using the XWITH option between a latent variable and an observed variable. It can also be done by introducing a latent variable "behind" the observed variable (i.e., the observed variable is a perfect indicator for the latent variable) and then using the XWITH option for the two latent variables. The second approach is less efficient as it generally yields MCMC chains with worse mixing quality; however, if the observed variable has missing values it would be the only available approach in Mplus. Another condition that requires the second approach is the situation where the observed variables are in a two-level model and are latent-centered.

The Bayesian estimation described here is fairly close to the one described in Arminger and Muthén (1998). There are two main differences. The first one is that the latent variables are updated one at a time which allows us to use conjugate posterior distributions in most cases instead of the less efficient Metropolis–Hastings algorithm. The second difference is in the proposal distribution used in the Metropolis–Hastings algorithm. The proposal distribution used in Arminger and Muthén (1998) is the same across individuals and is based on the model estimated prior distribution for the latent variables. The proposal distribution used in this algorithm incorporates the entire model, including the quadratic terms where the latent variables are involved, as well as the observed variables. This makes the proposal distribution subject specific and very close to the desired posterior distribution, which leads to a well mixing MCMC estimation. The Bayesian estimation described in Lee et al. (2007) and implemented in WINBUGS is also very similar to the estimation described here. In the absence of square terms η_1^2 , the model updating in WINBUGS will match precisely the MCMC estimation described here. When square terms are present, the detailed jumping distribution we formulated above is likely to outperform the more generic symmetric normal jumping distribution used in WINBUGS. Neither Arminger and Muthén (1998) nor Lee et al. (2007) expand the methodology to multilevel models, which is the most substantial contribution of this work.

In the next sections, we illustrate the methodology with several examples.

Factor analysis with interactions

In this section we consider a factor analysis model where 5 factors are measured by 3 indicator variables each, i.e., we

have a total of 15 observed variables. All loadings are set to 1, intercepts are set to 0, residual and factor variances are set to 1, factor correlations are set to 0.3. We add the following three interaction terms in the model $\eta_1\eta_2$, $\eta_1\eta_5$ and $\eta_3\eta_4$. The effects of these interaction terms on the observed variables are all zero except for the following three effects $\eta_1\eta_2$ on Y_1 is set to $\gamma_{112} = -0.25$, the effect of $\eta_1\eta_5$ on Y_1 is set to $\gamma_{115} = 0.25$, and the effect of $\eta_3\eta_4$ on Y_7 is set to $\gamma_{734} = 0.25$. The model is described by the following equations:

$$Y_1 = v_1 + \lambda_{11}\eta_1 + \gamma_{112}\eta_1\eta_2 + \gamma_{115}\eta_1\eta_5 + \varepsilon_1 \quad (33)$$

$$Y_p = v_p + \lambda_{p1}\eta_1 + \varepsilon_p, p = 2, 3 \quad (34)$$

$$Y_p = v_p + \lambda_{p2}\eta_2 + \varepsilon_p, p = 4, 5, 6 \quad (35)$$

$$Y_7 = v_7 + \lambda_{73}\eta_3 + \gamma_{734}\eta_3\eta_4 + \varepsilon_7 \quad (36)$$

$$Y_p = v_p + \lambda_{p3}\eta_3 + \varepsilon_p, p = 8, 9 \quad (37)$$

$$Y_p = v_p + \lambda_{p4}\eta_4 + \varepsilon_p, p = 10, 11, 12 \quad (38)$$

$$Y_p = v_p + \lambda_{p5}\eta_5 + \varepsilon_p, p = 13, 14, 15. \quad (38)$$

We compare the Bayesian estimation method and the ML – Monte Carlo integration method where the number of integration points is set to 500 and 1000. In this article, our choices for the sample size in the simulation studies are driven by the following. We generally choose the smallest sample size that can clearly illustrate our findings, i.e., in all the simulation studies presented here, choosing larger sample sizes will yield similar conclusions. Choosing smaller sample sizes may not. Smaller sample size situations, particularly when the models are complex, may yield more nuanced conclusions that are less connected to the asymptotic theory. The online materials provided with the article can be used to study further the small sample size behavior, which generally tends to be less predictable and more dependent on the rest of the details in the model. In this simulation study, we use 100 data sets of size 1000 and we estimate the correct interaction model with the two estimators. In all simulation studies presented here, we used the Mplus default convergence criteria as well as the Mplus default non-informative priors, see Muthén and Muthén (1998–2017). The non-informative priors are generally adequate for the models discuss here as long as the sample size is not small. If the sample size is small, fine-tuning of the priors along the lines of Smid et al. (2020) can be beneficial.

The simulation study results for the interaction effects are presented in Table 1. All three estimation methods yield acceptable results; however, the ML method with 500 integration points shows significantly larger MSE for the estimates. The reduced precision in the log-likelihood computation

yields reduced precision in the ML estimates. The convergence rates for the Bayesian method and the ML(1000) are 100% while the convergence for the ML(500) is 98%, i.e., a slight drop in the convergence rates. The computational time for Bayesian method and ML(500) is approximately the same while the computational time for ML(1000) is about twice that. Usually, the computational time with Monte Carlo integration is proportional to the number of integration points. Overall the conclusion from this simulation is that the Bayesian estimator appears to be the best in terms of computational time and precision of the estimates; however, the differences with the ML estimator are not large. Increasing the number of integration points increases the precision of the estimates, although, it is not a priori clear on how to determine the optimal number of integration points. In the above simulation, increasing the number of integration points to 5000 did not improve the precision of the estimates in terms of MSE but increased substantially the computation time per replication. This is a clear advantage of the Bayesian estimation as it removes the uncertainty of the number of integration points. Essentially, it automatically determines the amount of computation that has to be done to obtain precise estimates. Note that the precision here means how close the estimates are as compared to the estimates that can be obtained with infinite MCMC iterations. It does not refer to precision in terms of how far the estimates are from the true parameter values. In fact, because the ML and the Bayesian estimator are asymptotically equivalent, we can expect that the MSE of the estimates as compared to the true parameter values will be asymptotically identical if the Bayesian estimator uses an infinite number of iterations and if the ML estimator uses an infinite number of integration points.

We also consider estimating the modified model where all indicator variables are regressed on the three interaction terms. In a typical application that would be the most likely scenario. The effect of estimating this model with many more parameters on the convergence rate is that the convergence rate for ML(500) dropped to 95% while for the Bayesian estimator it remained at 100%. This is a slightly bigger drop on the convergence rate and most likely bigger convergence problems should be expected for models that have flatter likelihoods where estimation precision is more important. Nevertheless, we can see here that the convergence rates remain high. This is primarily due to the fact that there are only five dimensions of integration. For two-level models, however, the situation is completely different. The Monte Carlo integration method appears to completely fall apart and the Bayesian estimation appears to be the only alternative.

As an example, consider the following two-level factor analysis model with interactions. The within-level model would be identical to the model we considered above, while the between-level model simply consists of random intercepts with variance 1. We generate and analyze 100 data sets which consist of 100 clusters of size 20. The ML method as implemented in Mplus uses 20 dimensions of integration, 5 on the within level and 15 on the between level for each of the 15 random intercept variables, one for each observed variable. Using the ML method with 5000 integration points the convergence rate we obtained is 0%. On the other hand, the

Table 1. Factor Analysis with Interactions: Absolute Bias/Coverage/MSE

Parameter	True Value	Bayes	ML(500)	ML(1000)
Y_{112}	-.25	.01/.99/.002	.01/.95/.006	.00/.99/.002
Y_{115}	.25	.01/.95/.002	.01/.96/.004	.00/.96/.002
Y_{734}	.25	.00/.98/.002	.02/.96/.003	.00/.99/.002

Table 2. Two-level Factor Analysis with Interactions: Absolute Bias/Coverage/MSE

Parameter	True Value	Bayes
γ_{112}	-.25	.010/.95/.002
γ_{115}	.25	.00/.90/.002
γ_{734}	.25	.00/.95/.001

Bayesian method has 100% convergence. The results for the interaction parameters are presented in Table 2. The Bayesian estimation is clearly the only alternative for this model and the method performs well. The estimation time for this model using 4 processors is approximately 15 seconds per iteration. The ML Monte Carlo method with 5000 integration points took approximately 20 minutes per iteration (while no convergence was actually achieved).

One important aspect of interaction modeling is the question regarding which interaction effects should be considered for model inclusion in the absence of any substantive guidance. In our example, there are a total of 225 possible interaction parameters γ_{pji} . These parameters would naturally be in addition to any cross-loading parameters. The total number of parameters can easily become quite large. In such a case, one can include all these parameters within the BSEM framework, see Muthén and Asparouhov (2012), where these additional possible parameters will be included with tiny priors centered at zero. In that exploratory framework, interaction effects that must be included in the main model will "escape" the tiny priors to exhibit significance while at the same time allowing the main factor model to be adjusted accordingly for the effect of the included interaction terms.

Another approach that can be utilized for exploratory purposes is to generate plausible values, see Asparouhov and Muthén (2010b), for the factor analysis model without the interactions. A second step then computes the residuals ε_p and all interaction terms $\eta_i\eta_j$ using these plausible values. As a third step one can compute the sample correlation matrix (using Mplus TYPE = IMPUTATION option) for all of these variables and select for model inclusion the interactions that have substantial correlations with the residual variables ε_p .

The effect of ignoring interaction terms

In this section, we address the important question regarding why we need to incorporate interaction effects in the SEM models. Perhaps ignoring the interaction effects would lead to no essential problems. In principle, SEM models are estimated by fitting the first and the second-order sample statistics. Interaction terms tend to be needed to fit higher-order moments. It is conceivable from that point of view that ignoring interaction terms might have no effect on the SEM model. This, however, is not the case and we will illustrate this point with several CFA and EFA simulation studies.

We generate data using a model similar to the model (33–39) used in the previous section with some small modifications. In this section, we use the same interaction terms as in (33–39) but we include two additional non-zero interaction effects, i.e., a total of five non-zero interaction effects: $\gamma_{112} = -.5$, $\gamma_{115} = .5$, $\gamma_{212} = .5$, $\gamma_{412} = .5$, $\gamma_{734} = .5$. We

generate 100 data sets of size 1000 and we analyze the data using the CFA model without the interaction terms. We utilize the ML and the MLR estimators in Mplus. The MLR estimator is generally expected to perform better given that the interaction terms would be incorporated in the residuals of the CFA model, i.e., are expected to have non-normal distributions, which is where the advantage of the MLR estimator is.

The results of the simulation study show that there is little difference between ML and MLR chi-square statistics and both reject the model 95% of the time. On the other hand, all approximate fit indices accept the model: the average value for the RMSEA is 0.02, the average value for the SRMR is 0.02, the average value for the CFI is 0.99, and the average value for the TLI is 0.98. One can conclude from this example that approximately fitting models, rejected by the exact chi-square test of fit, may indeed be models that have omitted interaction terms (among other types of minor misspecifications). Table 3 contains the results for the second- and third-factor loadings (the first-factor loading is fixed to 1) for the ML and MLR estimators with omitted interaction terms and the Bayesian estimator with the interaction terms included. First, we note that the Bayesian estimator yields low coverage for the first loading even though the bias is negligible. Usually, such situations can be resolved by running a longer MCMC sequence, instead of relying on the default convergence settings. The ML run shows bias for both loadings but particularly large bias for the third loading and substantial drop in coverage. Using the MLR estimator improves the coverage but not sufficiently. We conclude here that omitted interaction terms can change the factor structure and bias the factor loadings. This occurs even when the factors are uncorrelated. The model estimation with the omitted interaction terms will attempt to incorporate the interaction terms implied covariance within one of the existing factors which in turn will distort the measurement model for that factor.

Mooijaart and Satorra (2009) point out that for some SEM models the likelihood-ratio test cannot detect omitted interaction terms. As the above example shows, however, this does not apply to all models. If interaction terms do not affect directly the observed variables but only other latent variables, we can expect that the chi-square test will not reject the model even when the interaction terms are ignored.

Now we turn our attention to the effect of omitted interaction terms in EFA. We analyze the same data as above with a five-factor EFA model and a six-factor EFA model. Using the chi-square test of fit, we reject the five-factor model 93% of the time and reject the six-factor model 9% of the time, i.e., 84% of the time we conclude that the number of factors is 6. Thus, omitted interactions can lead to an incorrect number of factors in EFA. In addition, Table 4 shows the results for several factor loading estimates for the five-factor EFA model. Here the factor loadings are biased as well. This fact

Table 3. Factor Analysis with Omitted Interactions: Absolute Bias (Coverage)

Parameter	True Value	Bayes	ML	MLR
λ_{21}	1	.02(.81)	.04(.88)	.04(.93)
λ_{31}	1	.01(.92)	.15(.60)	.15(.67)

Table 4. EFA with Omitted Interactions: Absolute Bias (Coverage)

Parameter	True Value	MLR
λ_{11}	1	.11(.64)
λ_{21}	1	.12(.59)
λ_{31}	1	.11(.64)
λ_{22}	0	.12(.63)

has some implications regarding the question of how to include the interactions within the EFA estimation. One possible approach is to use the ESEM-within-CFA approach described in Marsh et al. (2013). Because of the biases shown in Table 4, however, such an approach may still result in biased loading structure even after including the interaction terms. Further adjustments might be necessary for such situations. The results in Table 4, see λ_{22} , also show that small cross-loadings can appear in the model due to the omitted interaction terms. It is also worth noting here that the six-factor EFA model, picked by the chi-square test of fit, has an additional (sixth) factor of somewhat uninterpretable quality. This factor has multiple medium-range loadings with large standard errors that appear to be statistically insignificant. This kind of phenomenon also appears quite often in real data EFA, i.e., it could potentially be due to omitted interaction terms.

This simulation study suggests the following estimation sequence for practical applications. First, estimate the standard EFA model with a different number of factors. Select the model with the largest number of factors that are interpretable and have a clear and statistically significant measurement structure. Suppose that the chi-square test of fit points out that additional factors are needed, but no such factors have a clear and interpretable measurement structure. At that point, the structural model can be augmented with interaction terms. The second step is to estimate the factor model as a CFA model according to the clear measurement structure suggested by the EFA model. Next, the CFA model can be augmented with latent variable interactions using the BSEM strategy discussed in the previous section. Note that the EFA model can still inform the choice of where interaction terms are needed. In the above example, the sixth uninterpretable factor has large loadings for variables Y_1 , Y_2 and Y_4 . This suggests that those are the variables where interaction terms are needed most and where the linear CFA is not sufficient.

One issue that may appear as a stumbling block for the Bayesian interaction modeling is the lack of fit statistics. Neither DIC nor PPP are available in Mplus at this time. It is possible however to make informed model modifications in the interaction framework by evaluating the significance of the interaction coefficients, i.e., if an interaction term has a significant effect as established by the credibility interval it should be included in the model and if the effect is insignificant the interaction terms are not needed and can be removed from the model.

Two-level moderation analysis

Preacher et al. (2016) describe several two-level moderation models with interactions among predictors at the within level, the between level, and across the two levels. The authors

used Mplus to estimate the models via maximum-likelihood with numerical integration. With the release of Mplus 8.3, these models can now be estimated with the Bayesian method. In this section, we compare the accuracy, speed, and robustness between the different estimation methods using simulation studies. The scripts we use for the simulation studies are taken directly from the supplemental materials of Preacher et al. (2016), although in certain cases we have simplified the inputs. Such simplifications, however, do not alter the models. We also preserve the notation used in that article for quick reference. For example, model A1 in Preacher et al. (2016) refers to the interaction model [Within part of L1 moderator] x [Within part of L1 predictor]. In the next eight sections, we present simulation studies on the first 8 examples in the supplemental materials in Preacher et al. (2016) and we preserve the order of these examples.

The simulation results illustrate that the Bayesian method allows us to more fully pursue these moderation models. The Bayesian estimation is faster, simpler, and more robust (more likely to converge) than the maximum-likelihood estimation.

Model A1: [Within part of L1 moderator] x [Within part of L1 predictor]

Suppose that Y_{ij} , X_{ij} and Z_{ij} are the observed variables for individual i in cluster j . The model can be described by the following equations. First, we decompose the variables X_{ij} and Z_{ij} as within-between

$$X_{ij} = X_i + X_j \quad (40)$$

$$Z_{ij} = Z_i + Z_j \quad (41)$$

where X_j and Z_j are the between-level parts of the variables (i.e., their cluster-specific means), which are assumed to be normally distributed latent variables. The moderation model is then given as follows:

$$Y_{ij} = \beta_{0j} + \beta_1 X_i + \beta_2 Z_i + \beta_3 X_i Z_i + \varepsilon_{ij} \quad (42)$$

where

$$\beta_{0j} = \gamma_{00} + \gamma_{01} X_j + \gamma_{02} Z_j + u_{0j} \quad (43)$$

and ε_{ij} and u_{0j} are normally distributed zero-mean residuals. To generate the data we use the model parameters in Preacher et al. (2016) supplemental materials. We generate 100 data sets with 100 clusters of size 10. The Bayesian estimator converged in all 100 replications and the computation takes only a few seconds for each replication. The maximum-likelihood estimation, based on quadrature integration as in Preacher et al. (2016), did not converge in all of the replications. This simulation is different from the one used in Preacher et al. (2016) because it is based on a smaller number of clusters and smaller cluster sizes. In Preacher et al. (2016), the number of clusters is 500 and the size of the clusters is 20. For larger samples, convergence can be achieved easier because the likelihood is smoother and more prominent and therefore easier to optimize with less precise computations. Using Monte Carlo integration (MLMC) for this estimation

did not yield any convergence as well. The results presented in Table 5 show that the Bayesian estimation performs very well.

It is important to point out here why the ML and MLMC estimations have convergence problems. The interaction term X_iZ_i in Equation (42) is not an observed quantity. It is essentially $(X_{ij} - X_j)(Z_{ij} - Z_j)$ where X_{ij} and Z_{ij} are observed but X_j and Z_j are not observed. X_j and Z_j represent the true means of these variables in cluster j (or equivalently the random intercept effect) which are different from the sample means, i.e., the averages of the observations in the cluster. Because the likelihood of this model involves the product of two latent variables, it has no closed-form expression and is computed through numerical integration. For the above model, the Mplus implementation requires five-dimensional integration which is very computationally demanding. To make the computation feasible, the number of quadrature points per dimension is reduced to 4 with the ML estimation. That, in turn, leads to poor precision in the computation of the log-likelihood which eventually leads to non-convergence. Similarly, the precision of the MLMC estimation is compromised as well.

The observed cluster averages \bar{X}_j and \bar{Z}_j are measurements for the true cluster means X_j and Z_j , which have measurement error. The smaller the cluster size the bigger the measurement error. If that measurement error is not accounted for, the regression coefficients can be biased. That bias is generally referred to as Lüdtke’s bias, see Lüdtke et al. (2008) and Asparouhov and Muthén (2019). The bias occurs when there is a contextual effect in the model and the cluster sizes are relatively small, i.e., less than 50. If there is no contextual effect or the contextual effect is small or if the cluster sizes are large, the bias does not occur and in such situations it is safe to use the sample cluster average in place of the true mean in the moderation model. If we replace X_j with the cluster average \bar{X}_j and Z_j with the cluster average \bar{Z}_j , all the covariates in the model X_i , Z_i , X_iZ_i , X_j , and Z_j become observed and the above model is essentially a simple univariate two-level regression which is very easy to estimate. Let us call this estimation method the MLO (maximum likelihood with observed centering).

In the above example, the contextual effect for X_{ij} and Z_{ij} is small because β_1 is close to γ_{01} and β_2 is close to γ_{02} . Therefore, we can expect that the MLO method performs well for this example. The results for the MLO method are also included in Table 5 and we can see that indeed the method works well. It yields fast convergence in all cases and the parameter estimates and standard errors are satisfactory.

We illustrate Lüdtke’s bias in the above model with one additional simulation study. We use parameters that are different

Table 5. Model A1: Absolute Bias (Coverage)

Parameter	True Value	Bayes	MLO
β_1	.1	.00(.95)	.00(.97)
β_2	.3	.00(.94)	.01(.96)
β_3	.2	.01(.93)	.01(.94)
γ_{00}	.1	.00(.94)	.00(.94)
γ_{01}	.2	.01(.98)	.02(.98)
γ_{02}	.2	.00(.93)	.01(.91)

from those specified in Preacher et al. (2016) Monte Carlo setups so that the variables have a contextual effect. For this simulation study, we generate 100 data sets with 500 clusters of size 10 using the following parameters $\beta_1 = .1$, $\beta_2 = -.6$, $\beta_3 = .6$, $\gamma_{00} = .1$, $\gamma_{01} = .7$, $\gamma_{02} = .9$, $Var(u_{0j}) = Var(\epsilon_{ij}) = .7$. The means of X_j and Z_j are set to 0, the variances to .7 and the covariance to .1. The means of X_i and Z_i are set to 0, the variances to 2.7 and the covariance to 1.5. The results of the simulation study are presented in Table 6. For this simulation, we also include the MLRO estimation, which is the same as MLO point estimation plus robust Huber-White sandwich standard errors.

The results show that the Bayesian estimator performs well while both MLO and MLRO perform poorly due to Lüdtke’s bias for all between-level parameters, which also results in poor coverage. On the within level, the results are unbiased for MLO but the standard errors are underestimated which results in poor coverage. In that respect, MLRO is better as it resolves this issue but only for the within-level parameters. Underestimation of the standard errors appears to be a problem unique to the moderation models. This problem does not occur with standard path analysis models, see Table 3 in Asparouhov and Muthén (2019). It is also important to note here that if random regression slopes are included in the model, the within-level parameters β_i may also be biased, see Table 4 in Asparouhov and Muthén (2019). This within-level bias will carry over to the moderation models as well.

Despite the fact that the MLO/MLRO estimators could be biased, we recommend that these estimators be used as a part of any moderation analysis. MLO/MLRO can be used as a first preliminary step, which can be followed by the Bayesian estimation. The simplicity of the MLO/MLRO estimation is a very desirable attribute that no other estimation can match. This is why the approach should not be dismissed when it is available, i.e., when there are no missing data for the predictor and the mediator. In addition, if the cluster sizes are 100 or more, see Asparouhov and Muthén (2019), these estimators can be used as the main method of estimation because they offer more options for model testing such as AIC/BIC and LRT.

Model A2: [Between part of L1 moderator] x [Within part of L1 predictor] (cross-level interaction)

The model is given by the following equations:

$$X_{ij} = X_i + X_j \tag{44}$$

$$Z_{ij} = Z_i + Z_j \tag{45}$$

$$Y_{ij} = \beta_{0j} + \beta_1X_i + \beta_2Z_i + \beta_3X_iZ_j + \epsilon_{ij} \tag{46}$$

Table 6. Lüdtke’s Bias in Model A1: Absolute Bias (Coverage)

Parameter	True Value	Bayes	MLO	MLRO
β_1	.1	.00(.84)	.00(.82)	.00(.96)
β_2	-.6	.00(.90)	.00(.72)	.00(.99)
β_3	.6	.01(.93)	.00(.72)	.00(.88)
γ_{00}	.1	.00(.88)	.09(.59)	.09(.60)
γ_{01}	.7	.01(.95)	.29(.00)	.29(.00)
γ_{02}	.9	.01(.93)	.43(.00)	.43(.00)

Table 7. Model A2: Absolute Bias (Coverage)

Parameter	True Value	Bayes
β_1	.1	.00(.97)
β_2	.3	.00(.97)
β_3	.2	.01(.91)
γ_{00}	.1	.01(.94)
γ_{01}	.2	.00(.99)
γ_{02}	.2	.01(.96)

$$\beta_{0j} = \gamma_{00} + \gamma_{01}X_j + \gamma_{02}Z_j + u_{0j}. \quad (47)$$

We generate 100 data sets with 100 clusters of size 10. We analyze the data with the Bayesian estimator, the ML estimator with numerical integration and 4 integration points per dimension and the ML estimator with Monte Carlo (MLMC) integration with 500 integration points. The ML and MLMC did not converge. The results for the Bayesian estimator are presented in Table 7. The Bayesian estimator performs very well. It is important to note here that the Bayesian estimator needs an additional option for this model: VARIANCE = 0.01. The role of this option is to prevent slow/poor mixing due to residual variances fixed to 0. The option refers to the minimal variance allowed in the model, which by default is 0.0001, and in some cases that default is too small. The option is generally needed when the input file utilizes fixing the residual variance of a variable to 0 with the Mplus language $Y@0;$. In such a situation, if the VARIANCE option is set to 0.01, Mplus estimates the model as if it is specified as $Y@0.01;$, i.e., the variance will be fixed to the option value instead of 0. If the VARIANCE option is too small, the mixing will be of poor quality and it will be very slow in terms of the number of MCMC iteration needed for convergence. The option can be increased to a larger value to facilitate better mixing but it should not be increased beyond what would be considered a reasonable approximation of zero.

Model A3: [Between part of L1 moderator] x [Between part of L1 predictor]

The model is given by the following equations:

$$X_{ij} = X_i + X_j \quad (48)$$

$$Z_{ij} = Z_i + Z_j \quad (49)$$

$$Y_{ij} = \beta_{0j} + \beta_1X_i + \beta_2Z_i + \varepsilon_{ij} \quad (50)$$

$$\beta_{0j} = \gamma_{00} + \gamma_{01}X_j + \gamma_{02}Z_j + \gamma_{03}X_jZ_j + u_{0j}. \quad (51)$$

We generate 100 data sets each containing 100 clusters of size 10. We analyze the data with the Bayesian estimator, the ML estimator with numerical integration and 4 integration points per dimension and the ML estimator with Monte Carlo (MLMC) integration with 1000 integration points. The results are presented in Table 8. All three estimators performed well in this situation. The Bayesian estimator is 10 times faster than the ML estimator and 30 times faster than the MLMC estimator and takes less than a second for each replication.

Model A1 and A2 combination

The model is given by the following equations:

$$X_{ij} = X_i + X_j \quad (52)$$

Table 8. Model A3: Absolute Bias (Coverage)

Parameter	True Value	Bayes	ML	MLMC
β_1	.1	.00(.95)	.00(.97)	.00(.96)
β_2	.3	.00(.94)	.01(.93)	.00(.95)
γ_{00}	.1	.00(.94)	.01(.94)	.01(.89)
γ_{01}	.2	.01(.98)	.02(.93)	.02(.95)
γ_{02}	.2	.00(.93)	.00(.98)	.00(.98)
γ_{03}	.2	.00(.93)	.02(.91)	.00(.90)

$$Z_{ij} = Z_i + Z_j \quad (53)$$

$$Y_{ij} = \beta_{0j} + \beta_1X_i + \beta_2Z_i + \beta_3X_iZ_i + \beta_4X_iZ_j + \varepsilon_{ij} \quad (54)$$

$$\beta_{0j} = \gamma_{00} + \gamma_{01}X_j + \gamma_{02}Z_j + u_{0j}. \quad (55)$$

We generate 100 data sets with 100 clusters of size 10. We analyze the data with the Bayesian, ML, and MLMC estimators. The ML and MLMC estimators did not converge. The results for the Bayesian estimator are presented in Table 9. The Bayesian estimator performs well for this model as well.

Model B1: [L2 moderator] x [Within part of L1 predictor] (cross-level interaction)

In this model, the moderator Z_{ij} is assumed to be a between-level variable, i.e., $Z_{ij} = Z_j$. The model is given by the following equations:

$$X_{ij} = X_i + X_j \quad (56)$$

$$Y_{ij} = \beta_{0j} + \beta_{1j}X_i + \beta_3X_iZ_j + \varepsilon_{ij} \quad (57)$$

$$\beta_{0j} = \gamma_{00} + \gamma_{01}X_j + \gamma_{02}Z_j + u_{0j}. \quad (58)$$

Note that unlike in the previous models, here we have a random slope β_{1j} . The model can be estimated with a nonrandom slope β_1 but we are following the fifth example from Preacher et al. (2016) where the model is with a random slope.

The presence of the random slope, however, complicates the identification of the model. In the earlier draft of Preacher et al. (2016), the model was specified as an unidentified model but in the current version of the supplemental materials the issue is resolved by a model modification. We illustrate these complications by considering first the simple situation where the random slope β_{1j} is regressed on Z_j . That is, we augment the above model with the equation

$$\beta_{1j} = \gamma_{10} + \gamma_{12}Z_j + u_{1j}. \quad (59)$$

If Equation (59) is substituted in Equation (57) we can clearly see that the coefficients γ_{12} and β_3 play the same role, i.e., these are the regression coefficient for the interaction term X_iZ_j . Thus,

Table 9. Model A1 Plus A2 Combination: Absolute Bias (Coverage)

Parameter	True Value	Bayes
β_1	.1	.00(.97)
β_2	.3	.00(.94)
β_3	.2	.00(.94)
β_4	.2	.01(.94)
γ_{00}	.1	.01(.91)
γ_{01}	.2	.00(.95)
γ_{02}	.2	.02(.95)

both of these coefficients cannot be identified at the same time. Only one of the two coefficients can be present in the model.

An alternative way that this unidentification can appear in the model is as follows. Instead of estimating the regression Equation (59) it is possible to estimate the variance-covariance structure for the random effect β_{1j} and Z_j , which includes the covariance parameter. Such a model, however, is a reparameterization of (59). Thus, we conclude that model B1 of Preacher et al. (2016) must have the covariance parameter between β_{1j} and Z_j fixed to 0. If the covariance parameter is not fixed to 0 the model would be unidentified because it would include the two essentially equivalent parameters: the covariance between β_{1j} and Z_j as well as β_3 . One of these two parameters must be fixed to zero.

In the following simulation, we estimate the above model, assuming that the covariance between β_{1j} and Z_j as well as the covariance between β_{1j} and X_j are not estimated, i.e., these covariance parameters are fixed to zero. Equivalently, we can assume that γ_{12} in Equation (59) is fixed to 0. The covariance between Z_j and X_j is estimated. We generate 100 data sets with 100 clusters of size 10. The ML and the MLMC estimation methods did not converge for this model and thus we report the results in Table 10 only for the Bayesian estimator. The Bayesian estimator performs well also for this example.

Model B2: [L2 moderator] x [Between part of L1 predictor]

In this model, the moderator is again assumed to be a between-level variable Z_j . The model is given by the following equations:

$$X_{ij} = X_i + X_j \tag{60}$$

$$Y_{ij} = \beta_{0j} + \beta_1 X_i + \epsilon_{ij} \tag{61}$$

$$\beta_{0j} = \gamma_{00} + \gamma_{01} X_j + \gamma_{02} Z_j + \gamma_{03} X_j Z_j + u_{0j}. \tag{62}$$

We generate 100 data sets with 100 clusters of size 10. The data are analyzed by the three estimators Bayesian, ML, MLMC and the results are reported in Table 11. All three estimators performed well for this model.

Model A1 with random slope for the interaction term

The model can be described by the following equations:

Table 10. Model B1: Absolute Bias (Coverage)

Parameter	True Value	Bayes
β_3	.2	.00(.92)
γ_{00}	.1	.01(.92)
γ_{01}	.2	.01(.94)
γ_{02}	.2	.00(.98)
γ_{10}	.1	.01(.96)

Table 11. Model B2: Absolute Bias (Coverage)

Parameter	True Value	Bayes	ML	MLMC
β_1	.2	.01(.93)	.00(.94)	.00(.95)
γ_{00}	.1	.01(.99)	.01(.95)	.01(.93)
γ_{01}	.2	.01(.95)	.01(.93)	.01(.91)
γ_{02}	.2	.02(.92)	.00(.93)	.00(.89)
γ_{03}	.2	.01(.99)	.01(.97)	.02(.87)

Table 12. Model A1 with Random Slope: Absolute Bias (Coverage)

Parameter	True Value	Bayes
β_1	.1	.00(.94)
β_2	.3	.00(.97)
γ_{00}	.1	.01(.96)
γ_{01}	.2	.02(.96)
γ_{02}	.2	.00(.97)
γ_{30}	.2	.02(.96)

$$X_{ij} = X_i + X_j \tag{63}$$

$$Z_{ij} = Z_i + Z_j \tag{64}$$

$$Y_{ij} = \beta_{0j} + \beta_1 X_i + \beta_2 Z_i + \beta_3 X_i Z_i + \epsilon_{ij} \tag{65}$$

$$\beta_{0j} = \gamma_{00} + \gamma_{01} X_j + \gamma_{02} Z_j + u_{0j} \tag{66}$$

$$\beta_{3j} = \gamma_{30} + u_{3j}. \tag{67}$$

We conduct a simulation study again using 100 samples with 100 clusters of size 10. Only the Bayesian estimator converged in this case. The results are presented in Table 12. The Bayesian estimator performs well for this model as well.

Model C: [L2 moderator] x [L2 predictor]

In this model, the moderator and the predictor are the between-level variables Z_j and X_j respectively. The model is given by the following equations:

$$Y_{ij} = \beta_{0j} + \epsilon_{ij} \tag{68}$$

$$\beta_{0j} = \gamma_{00} + \gamma_{01} X_j + \gamma_{02} Z_j + \gamma_{03} X_j Z_j + u_{0j}. \tag{69}$$

If the variables X_j and Z_j have no missing values, the model can be estimated as a regular two-level model (without the Mplus moderation command XWITH). The interaction term $X_j Z_j$ can be computed with the Mplus DEFINE command and be treated just like any other covariate. If there are missing data for these variables, however, the Mplus DEFINE command can not be used to simply multiply the two variables, and instead, the moderation model estimation has to be utilized.

In this simulation, we generate 100 data sets with 100 clusters of size 10. Missing data for the variable X_j are generated as follows:

$$Prob(X_j \text{ is missing}) = \frac{1}{1 + Exp(Z_j)}. \tag{70}$$

This method of generating missing data is MAR (and not MCAR). Likelihood-based estimators such as Bayes, ML, and MLMC are guaranteed to produced unbiased estimates for such missing data mechanisms.

The results of this simulation are reported in Table 13. All three estimators performed well for this model.

Multilevel moderated mediation

The multilevel moderated mediation model, discussed in Zyphur et al. (2019), is described as follows. Suppose that Y_{ij} , M_{ij} , X_{ij} and Z_{ij} are the observed variables for an individual

Table 13. Model C: Absolute Bias (Coverage)

Parameter	True Value	Bayes	ML	MLMC
Y_{00}	.1	.01(.90)	.01(.92)	.00(.94)
Y_{01}	.1	.00(.87)	.00(.93)	.00(.93)
Y_{02}	.2	.00(.98)	.00(.96)	.01(.95)
Y_{03}	.1	.01(.94)	.00(.94)	.01(.96)

i in cluster j . The variables are decomposed as within and between portions as follows:

$$Y_{ij} = Y_i + Y_j \quad (70)$$

$$M_{ij} = M_i + M_j \quad (72)$$

$$X_{ij} = X_i + X_j \quad (73)$$

$$Z_{ij} = Z_i + Z_j. \quad (74)$$

On the within level, the moderated mediation model is given by the following equations:

$$M_i = \beta_1 X_i + \beta_2 Z_i + \beta_3 X_i Z_i + \varepsilon_{1,ij} \quad (75)$$

$$Y_i = \beta_4 X_i + \beta_5 Z_i + \beta_6 M_i + \beta_7 X_i Z_i + \beta_8 M_i Z_i + \varepsilon_{2,ij}. \quad (76)$$

Similarly, on the between level the moderated mediation model is

$$M_j = \alpha_1 + \gamma_1 X_j + \gamma_2 Z_j + \gamma_3 X_j Z_j + \varepsilon_{3,j} \quad (77)$$

$$Y_j = \alpha_2 + \gamma_4 X_j + \gamma_5 Z_j + \gamma_6 M_j + \gamma_7 X_j Z_j + \gamma_8 M_j Z_j + \varepsilon_{4,j}. \quad (78)$$

This model can be estimated directly in Mplus 8.3 with the Bayesian estimator. Here we compare that estimation method with the MLO estimation method where all variables involved in interaction terms, i.e., M , X , and Z , are decomposed as within and between portion using observed centering. The interaction terms are formed by multiplying the observed quantities and the model is then estimated with the ML estimator. Numerical integration is not needed with this estimation method. We also consider the two-stage estimation method proposed in Zyphur et al. (2019). This method attempts to take into account the uncertainty in the centering by estimating plausible values for the between portions of the variables. The plausible values are generated using an unrestricted variance-covariance two-level model, i.e., by ignoring the interaction terms. The authors used 20 plausible value data sets, see Asparouhov and Muthén (2010b), which are subsequently analyzed using the standard imputation methodology. Just as in the MLO estimation, the interaction terms are formed by multiplying the plausible values, which allows us to convert the above two-level moderated mediation model into a standard two-level regression model that can be estimated with the ML estimator without numerical integration.

We evaluate the performance of the three estimation methods using the following simulation study. We generate 100 data sets with 200 clusters of size 10. The data are generated using the above model and the following parameter values. The values of α_i , β_i and γ_i are given in Table 14. The residual variances are set to 2 on the within level and to 0.7 on the between level. The

Table 14. Multilevel Moderated Mediation Model: Absolute Bias (Coverage)

Parameter	True Value	Bayes	Two-stage	MLO
α_1	.2	.00(.87)	.00(.94)	.02(.94)
α_2	.6	.00(.96)	.02(.96)	.04(.95)
β_1	-.6	.00(.90)	.02(.92)	.00(.83)
β_2	.3	.00(.96)	.00(.92)	.00(.90)
β_3	-.5	.00(.94)	.10(.00)	.06(.06)
β_4	-.4	.00(.98)	.05(.82)	.03(.90)
β_5	.2	.00(.90)	.07(.58)	.06(.45)
β_6	.4	.00(.92)	.10(.14)	.10(.06)
β_7	.3	.00(.94)	.09(.03)	.06(.38)
β_8	-.5	.00(.96)	.05(.10)	.02(.76)
γ_1	.7	.01(.96)	.02(.95)	.29(.06)
γ_2	.6	.02(.95)	.06(.95)	.07(.87)
γ_3	.6	.01(.91)	.29(.26)	.28(.12)
γ_4	.4	.03(.88)	.21(.83)	.09(.84)
γ_5	.5	.01(.95)	.17(.86)	.10(.79)
γ_6	.8	.02(.90)	.28(.48)	.05(.83)
γ_7	.7	.03(.94)	.32(.61)	.21(.37)
γ_8	.4	.00(.94)	.11(.89)	.10(.59)

covariance between X_i and Z_i is set to .1. The covariance between X_j and Z_j is set to .1. The means of X_j and Z_j are set to 0. Table 14 contains the results of the three estimation methods. The direct Bayesian estimation outperforms both the two-stage (plausible values) estimation and the MLO estimation. The bias for the Bayesian estimation is minimal and the coverage is near the nominal level. Both, the two-stage and the MLO estimators show fairly large bias and poor coverage for most of the model parameters. The two-stage estimation does not appear to be better than the MLO estimation. The plausible values generated with this approach ignore the interaction terms in the model and thus are of poor quality and are unable to improve the estimation as compared to the simpler MLO estimator. Further simulation studies, that are not reported here but can be reproduced using the online materials accompanying this article, reveal that the biases in the two-stage and the MLO estimators are affected primarily by the following factors: the cluster sample sizes, the ICC of the variables, and the size of the contextual effects. If the cluster sample sizes are 100 or more we can expect the biases to disappear. If the ICC of the variables is larger we can expect the biases to be smaller. If the contextual effects are smaller, i.e., the coefficients β_i are closer to the corresponding coefficients γ_i , we can expect the biases to be smaller. These findings are in line with the findings in Lüdtke et al. (2008) and Asparouhov and Muthén (2019) regarding latent variable centering for predictors in multilevel modeling.

Three-way interactions

The Bayesian model estimation described so far is specific for two-way interactions, i.e., the product of two variables. It is possible, however, using the same methodology to form three-way and higher-order interactions. Suppose that we want to include a term $\eta_1 \eta_2 \eta_3$ as a predictor of a variable Z . We can accomplish that by using a new latent variable η_{12} and 2 two-way interactions as follows:

$$\eta_{12} = \eta_1 \eta_2 + \varepsilon_{12} \quad (79)$$

$$Z = \beta_2 \eta_{12} \eta_3 + \varepsilon. \quad (80)$$

Table 15. Three-way Interactions: Absolute Bias (Coverage)

Parameter	True Value	Bayes
β_1	.5	.00(.94)
β_2	.7	.00(.92)
β_3	.4	.02(.89)

If we fix the variance of ε_{12} to zero then $\eta_{12}\eta_3 = \eta_1\eta_2\eta_3$ and we have the desired three-way interaction. With the Bayesian estimation in Mplus, however, fixing the variance to 0 is not an option (see earlier discussion on the VARIANCE option), and thus we have to fix it to a small positive value, which makes the above model an approximation of the three-way interaction model. The smaller the value is, the more precise the approximation but also the slower the mixing. In our experience, choosing a value that represents around 1% of the variance of Z works well. Alternatively, if the variances of η_1 , η_2 and η_3 are set to 1 fixing the variance of ε_{12} to 0.01 would work well too.

We illustrate the three-way interaction with the following single-level simulation study. Consider the following model with nine observed variables and three latent variables:

$$Y_i = v_i + \lambda_i\eta_1 + \varepsilon_i, i = 1, 2, 3 \quad (81)$$

$$Y_i = v_i + \lambda_i\eta_2 + \varepsilon_i, i = 4, 5, 6 \quad (82)$$

$$Y_i = v_i + \lambda_i\eta_3 + \varepsilon_i, i = 7, 8, 9. \quad (83)$$

The structural part of the model is given by the following equation which includes the three-way interaction (cubic term) $\eta_1^2\eta_2$

$$\eta_3 = \beta_1\eta_1 + \beta_2\eta_2 + \beta_3\eta_1^2\eta_2 + \xi. \quad (84)$$

We generate 100 data sets of size 1000 using the following model parameters: $\alpha_i = 0$, $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \lambda_7 = 1$, $\lambda_5 = \lambda_6 = .8$, $\lambda_8 = \lambda_9 = .9$, $\beta_1 = .5$, $\beta_2 = .7$, $\beta_3 = .4$, $Var(\eta_1) = Var(\eta_2) = Var(\varepsilon_i) = 1$, and $Var(\eta_3) = .5$. We analyze the data with the above model and the Bayesian estimator and present the results for a subset of the parameters in Table 15. The results indicate that the Bayesian estimation performs well.

Discussion

In this article, we show that the Bayesian estimation of latent variable interaction models outperforms the maximum-likelihood estimation. This is particularly the case for two-level models, where the larger dimensions of ML numerical integration lead to imprecision. Multilevel moderation models can now be reliably estimated with the Bayesian estimator in various situations within a general and flexible framework. The algorithms discussed here are implemented in Mplus 8.3 and all scripts for the simulation studies presented in this article are available online.¹

The models that we discussed here can easily accommodate categorical variables with one exception. In the multilevel moderation models, only the dependent variable can be categorical, while the predictors and the moderator variables are assumed to be normally distributed. The algorithms discussed here will not extend to categorical predictors and mediators in the context of moderation analysis. Such multilevel moderation situations might be addressed through alternative methodologies such as the MLO estimator based on observed centering or through multiple group multilevel analysis, see Asparouhov and Muthén (2012) and Kim and Cao (2015). If the moderators and the predictors have many categories they can be treated as continuous and the Bayesian estimation can be applied. If the variables are binary, however, such an approach is not recommended. In addition to the limitations of the estimation methods, there is an uncertainty regarding the scale on which the interaction term will be formed. The two options are: the latent scale using the underlying latent variables or the observed scale where the interaction term is formed by multiplying the observed categorical values. This issue arises in single-level models as well but is further complicated in multilevel models where we attempt to model separately individual-level effects and cluster-level effects. Further methodological development is needed to address these limitations.

The estimation method discussed in this article relies on distributional assumptions and is generally not expected to be robust to gross model or distributional misspecifications. The method is asymptotically equivalent to the LMS method discussed in Klein and Moosbrugger (2000). The mixture-based method of Kelava et al. (2014) models the non-normality of the factors and can be estimated in Mplus with the ML and the Bayes estimators. The Bayesian approach would allow the estimation of larger models with multiple interaction terms; however, the complexity of embedding the latent variable interaction methodology within the mixture framework makes it less practical than its ML counterpart.

Model fit evaluation remains a challenge for latent variable interaction models. The challenge lies in constructing an unstructured/unrestricted model that is general enough that a structural model can be compared to it, but is also well identifiable and easy to estimate. The more general an interaction model is, the more difficult it is to estimate it and the more poorly identifiable it is. The proposed Bayesian approach makes progress on this front due to the fact that many interaction terms can be included in the unrestricted model. On its own however such a model will be difficult to estimate. The model must be combined with the BSEM methodology discussed in Muthén and Asparouhov (2012) where tiny priors are included for most interaction terms to secure model identifiability. This approach can be further combined with the Bayesian version of the Wald test discussed in Asparouhov and Muthén (2020) to be able to test multiple interaction effects for significance. Undoubtedly, this topic requires further methodological development.

¹<http://statmodel.com/download/WebNote23.zip>.

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Appendix: Model estimated means and variances and standardization in latent variable interaction models

This section describes the computation of the model estimated means and variances as well as the standardization of the general model in Mplus when latent variable interactions are present. Suppose that Y is the vector of all dependent variables, X is the vector of all covariates, and η is the vector of all latent variables. All residual variables are assumed to be normally distributed.

Suppose that the variables (Y, η, X) are split into two disjoint sets of variables V_1 and V_2 , where V_1 represent all dependent variables that are not a part of an interaction term and V_2 represent all variables that are a part of an interaction term. Suppose that V_1 is a vector of size p_1 and V_2 is a vector of size p_2 . The SEM model is described by the following equations:

$$V_1 = \alpha_1 + B_1 V_1 + C_1 V_2 + \sum_{i=1}^k D_i (V_{2,f(i)} V_{2,g(i)}) + \varepsilon_1$$

$$V_2 = \alpha_2 + B_2 V_2 + \varepsilon_2,$$

where $\alpha_1, B_1, C_1, D_i, \alpha_2, B_2$ are model parameters. The vectors α_1, D_i are of length p_1 while the vector α_2 is of length p_2 . The matrices B_1, C_1 and B_2 are of size $p_1 \times p_1, p_1 \times p_2$ and $p_2 \times p_2$ respectively.

The residual variable ε_1 has zero mean and variance–covariance Θ and ε_2 has zero mean and variance–covariance Ψ . The covariance between ε_1 and ε_2 is denoted by F . The functions $f(i)$ and $g(i)$

simply define the interaction terms, i.e., $f(i)$ and $g(i)$ are integers between 1 and p_2 and k is the number of interaction terms in the model.

We can assume that all covariates X are in the V_2 vector and the V_1 vector consists only of η and Y variables that are regressed on interaction terms, while the remaining η and Y variables are in vector V_2 . We can compute the model implied mean and variance for these variables as follows. For the variables V_2 we get

$$E(V_2) = \mu_2 = (1 - B_2)^{-1} \alpha_2$$

$$\text{Var}(V_2) = \Sigma_2 = (1 - B_2)^{-1} \Psi ((1 - B_2)^{-1})^T.$$

For V_1 we get

$$\begin{aligned} E(V_1) &= (1 - B_1)^{-1} \alpha_1 + (1 - B_1)^{-1} C_1 \mu_2 \\ &+ (1 - B_1)^{-1} \sum_{i=1}^k D_i (\mu_{2,f(i)} \mu_{2,g(i)} + \Sigma_{2,f(i),g(i)}). \end{aligned}$$

Denote by

$$\begin{aligned} V_{20} &= V_2 - \mu_2 \\ \mu_{10} &= (1 - B_1)^{-1} \alpha_1 + (1 - B_1)^{-1} C_1 \mu_2 \\ &+ (1 - B_1)^{-1} \sum_{i=1}^k D_i (\mu_{2,f(i)} \mu_{2,g(i)}) \\ V_{10} &= (1 - B_1)^{-1} C_1 V_{20} + (1 - B_1)^{-1} \varepsilon_1 \\ &+ (1 - B_1)^{-1} \sum_{i=1}^k D_i (\mu_{2,f(i)} V_{20,g(i)}) \\ &+ (1 - B_1)^{-1} \sum_{i=1}^k D_i (V_{20,f(i)} \mu_{2,g(i)}). \end{aligned}$$

Then

$$V_1 = \mu_{10} + V_{10} + (1 - B_1)^{-1} \sum_{i=1}^k D_i (V_{20,f(i)} V_{20,g(i)}).$$

Another representation for V_{10} is

$$V_{10} = QV_{20} + (1 - B_1)^{-1} \varepsilon_1,$$

where the matrix Q combines all the coefficients from the terms involving V_{20} . The above equation is essentially the definition of Q . Note now that

$$\text{Cov}(\varepsilon_1, V_{20}) = F((1 - B_2)^{-1})^T$$

and thus

$$\begin{aligned} \text{Var}(V_{10}) &= Q \Sigma_2 Q^T + (1 - B_1)^{-1} \Theta ((1 - B_1)^{-1})^T \\ &+ Q(1 - B_2)^{-1} F^T ((1 - B_1)^{-1})^T \\ &+ (1 - B_1)^{-1} F ((1 - B_2)^{-1})^T Q^T. \end{aligned}$$

Using the fact that the covariance between $V_{20,f(i)} V_{20,g(i)}$ and V_{20} and the covariance between $V_{20,f(i)} V_{20,g(i)}$ and ε_1 are zero we get that

$$\begin{aligned} \text{Var}(V_1) &= \text{Var}(V_{10}) + \sum_{i,j} D_i \text{Cov}(V_{20,f(i)} V_{20,g(i)}, V_{20,f(j)} V_{20,g(j)}) D_j^T \\ &= \text{Var}(V_{10}) + \sum_{i,j} D_i D_j^T (\Sigma_{2,f(i),f(j)} \Sigma_{2,g(i),g(j)} \\ &+ \Sigma_{2,f(i),g(j)} \Sigma_{2,g(i),f(j)}). \end{aligned}$$

Note also that

$$\text{Cov}(V_1, V_2) = \text{Cov}(V_{10}, V_{20}) = Q \Sigma_2 + (1 - B_1)^{-1} F ((1 - B_2)^{-1})^T.$$

Once the estimated means and variances are computed, the standardization of the parameters is as in the standard SEM models with the exception of the parameters D_i which are standardized as follows. If j denotes the index $j = 1, \dots, p_1$ the standardized coefficient for D_{ij} is

$$D_{ij} \frac{\sqrt{\text{Var}(V_{2,f(i)})} \sqrt{\text{Var}(V_{2,g(i)})}}{\sqrt{\text{Var}(V_{1,j})}}.$$