THE INFLUENCE OF MISSPECIFICATION OF BETWEEN-SUBJECT AND WITHIN-SUBJECT COVARIANCE STRUCTURES IN HIERARCHICAL GROWTH MODELS

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IN HIERARCHICAL GROWTH MODELS

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Hierarchical growth models are widely used in longitudinal studies to investigate individual changes over time since the model can handle unbalanced design and missing data. Between-subject and within-subject covariance structures can also be flexibly modeled. However, the current methods for selecting the optimal covariance structure are inefficient. It is common that covariance structures are misspecified. This dissertation is to examine the influences on fixed and random effects due to the misspecification of between-subject and within-subject covariance structures in a two-level hierarchical quadratic growth model with one continuous level-two predictor via two simulations. In addition, whether the Standardized Root Mean square Residual (SRMR) can be used in selecting the optimal covariance is examined.

The results indicate that the estimates of fixed effects are unbiased. The estimates of random effects and standard errors of fixed effects are biased due to the misspecification of the covariance structures. The over-specification of the covariance structure at one-level cannot compensate due to the under-specification of the covariance structure at the other level. When the within-subject covariance is under-specified and the between-subject covariance is over-

specified, the relative biases of standard errors of fixed effects are smaller than those when the within-subject covariance structure is over-specified and the between-subject covariance structure is under-specified. When random slopes of a quadratic change cannot be modeled, we recommend to use an unspecified ***R*** matrix so that the fixed effects and their standard errors can be estimated bias-free. However, the over-specified between-subject covariance has little impact on fixed effects and their standard errors. There are biased estimations of random effects due to the misspecification of within-subject and between-subject covariance structures. If the random effects are of interest, different ***R*** matrices and ***G*** matrices should be examined. If there are large differences among the results when using different ***R*** matrices, the results should be interpreted carefully. The results suggest that BIC is the best method in detecting the optimal covariance structure under the designed factors no matter whether the within-subject and between-subject covariances are over- or under-specified. SRMR performs poorly in the covariance selection under the misspecification of covariance structures.

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PREFACE

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1.0 INTRODUCTION

Hierarchical Linear Growth Models (HLGM) are widely used in the fields of education, psychology, and medicine to analyze individual changes using collected data on the same subject over time (Bryk & Raudenbush, 1987). For example, in the educational field, if researchers are interested in students' progress in math achievements, repeated measures of math achievements (such as statewide standardized test scores) are collected. The scores on the tests at different occasions or times are nested within a student, who is then nested in a classroom or a school. Hierarchical growth models (Raudenbush & Bryk, 2002) can be used to model individual changes and predictors of such changes at student, classroom and/or school levels.

1.1 STATE OF THE PROBLEM

1.1.1 Background of the longitudinal study and its problems

The longitudinal study (Hedeker & Gibbons, 2006; Singer & Willett, 2003) is more powerful than cross-sectional studies as each subject can serve as his/her own control and provides more information than a single measure obtained from a single subject. However, longitudinal data are usually collected at unequal time intervals, and have more missing data, especially for the measures at later time points.

Three commonly used statistical approaches for repeated measures are univariate ANOVA, multivariate ANOVA, and multilevel modeling (or hierarchical growth model, or mixed model). Univariate ANOVA is a powerful statistical approach if the underlying assumption of sphericity is met. However, this assumption is too restrictive to be met in longitudinal datasets (Keselman, Algina, Kowalchuk, & Wolfinger, 1998). Multivariate ANOVA requires fewer assumptions than univariate ANOVA, but the disadvantage of the approach is the requirement for a balanced design without missing data. Multilevel modeling allows flexible treatments of time and missing data, and is thus a better approach for analyzing individual changes over time in a longitudinal study.

Latent growth curve modeling (Kaplan, 2009) is another way to investigate individual changes within a structure equation modeling framework, which is more flexible in modeling the change trajectory and provides more information about the model evaluation. However, hierarchical growth models and latent growth curve models generate the same results for the estimates of intercepts and slopes with slight differences in the estimates of the standard errors of the regression coefficients (Bauer, 2003; Curran, 2003; Wu, West, & Taylor, 2009). Compared to latent growth curve models, hierarchical growth models (Chou, Bentler, & Pentz, 1998) are more straightforward in modeling and more efficient in the model computation.

1.1.2 Advantages of hierarchical growth models

Two-level hierarchical growth models are commonly used in statistical analyses for studying changes over time in a longitudinal study. The level-1 model specifies how individuals change over time, and the level-2 model assesses how individual characteristics impact the individuals' change trajectory. Hierarchical growth models have several advantages that are described below (Diggle, Heagerty, Liang, & Zeger, 2002; Laird & Ware, 1982; R. Wolfinger, 1993).

Handling unbalanced data or design. Hierarchical growth models do not assume that subjects are measured at the same number of time points, or fixed time, or equal time intervals since the time is treated as a continuous variable. For example, observations may be collected every half years at the very beginning of a study and then collected every other year at later time points. The time variable can then be measured as a continuous variable like days, months or years.

Handling Missing data. Missing data on the outcome variable is either not a problem for the analyses using hierarchical growth models. Missing data are due to a participant either does not show up at the scheduled time or refuses for all following-up measures. As HGLMs do not assume equal numbers of observations, subjects with missing observations on the outcome variable can remain in the analysis. The results in larger samples compared to the MANOVA approaches, thus provide more precise estimates and more powerful statistical tests.

Flexibility of modeling covariance structures. Within-subject and between-subject covariance structures can be flexibly modeled separately and simultaneously in hierarchical growth models. The within-subject covariance structure defines the first-level variances and covariances. The between-subject covariance structure defines the second-level variances and covariances. Since the two different covariance structures are modeled separately, the effects of variables at different levels can be modeled.

In summary, hierarchical growth models can include subjects with missing values, and thus the statistical power is higher than traditional approaches (Hedeker & Gibbons, 2006). Estimates are more accurate than traditional approaches due to including all the collected data which better represents the population. The flexibility of modeling covariance structures makes hierarchical growth models more attractive. Hierarchical growth models can be used to describe the structure of the mean growth trajectory, to estimate the variation of growth among subjects, and to estimate the correlation between the initial status and the growth rate. Model selection becomes more important since the model will influence the estimation of individual growth. The misspecification of the covariance structure may lead to biased estimates of the fixed effects and random effects.

1.1.3 Selection and misspecification of covariance structures

To estimate individual changes accurately in hierarchical growth models, an optimal covariance structure should be carefully selected to better fit the data under the same fixed effects model. The Likelihood ratio test, information criteria (AIC, BIC, AICC, HQIC, and CAIC), and graphical methods can be used to serve this purpose. Different methods were examined in previous studies for the selection of a covariance structure (Bozdogan, 1987; Ferron, Dailey, & Yi, 2002; Gomez, Schaalje, & Fellingham, 2005; Liu, Rovine, & Molenaar, 2012; R. Wolfinger, 1993; Ye, 2005). However, AIC, BIC, AICC, HQIC, CAIC, and LRT perform poorly in identifying the correct covariance structure. The graphical method is usually used to complement the information criteria and LRT to make the final decision on choosing the correct covariance structure. More effective methods are needed for identifying the correct covariance.

Since the current methods are problematic, it is common that covariance structures are misspecified. How the estimates of fixed effects and random effects are influenced by the misspecification of both between-subject and within-subject covariance structures in hierarchical growth models should be comprehensively investigated.

Several studies (Ferron et al., 2002; Kwok, West, & Green, 2007; Y.-H. Lee, 2010; Maas & Hox, 2004) investigated the influence of the within-subject covariance misspecification on fixed and random effects in different situations using hierarchical linear growth modeling. The studies showed that the estimates of fixed effects were unbiased if the within-subject covariance structure was misspecified. However, the standard errors of fixed effects were biased due to the misspecification of the within-subject covariance structure. The under-specification and general misspecification of the within-subject covariance led to larger standard errors of fixed effects. The over-specification of the within-subject covariance did not impact the estimation of standard errors of fixed effects. However, standard errors of fixed effects were underestimated when the within-subject covariance was specified as unstructured and between-subject as null, in which the Type I error rates were inflated compared to the correct models.

Only one study examined (Lee, 2010) the influence of the misspecification of the within-subject and between-subject covariance simultaneously in a hierarchical linear model. Three different combinations were considered, including over-specified between-subject and under-specified within-subject covariance structures, under-specified between-subject and over-specified within-subject covariance structures, and generally misspecified between-subject and within-subject covariance structures. The study focused on a two-level hierarchical linear growth model without any other predictors except time points and it included a balanced design only. The within-subject covariance structure considered in the study was AR(1) only and the between-subject covariance structure had random effects of the intercept and growth rate with no correlation between the two random effects. It was found that the estimates of fixed effects were unbiased in all three different combinations. The estimates of standard errors of the initial status and growth rate were biased depending on the combination of under-specification or over-specification for within-subject and between-subject covariance structures. The only exception is that these estimates were also unbiased when the between-subject covariance was over-specified and the within-subject covariance was under-specified.

1.2 PURPOSE OF THE STUDY

The purpose of this dissertation was to investigate the influence on fixed and random effects in two-level hierarchical quadratic growth models due to the misspecification of the within-subject and between-subject covariance structures, and to test whether the standardized root mean square residual can be used as an indicator to select the optimal covariance structures in hierarchical quadratic growth models. Two simulation studies were conducted to examine the effects on the fixed and random effects due to misspecifying both within-subject and between-subject covariance structures. In simulation study 1, data were generated with a simple within-subject and a complex between-subject covariance structure, and analyzed with a complex within-subject covariance structures and a simple between-subject covariance structure. In simulation study 2, data were generated with a complex within-subject covariance structure and a simple between-subject covariance structure, and analyzed with a simple within-subject covariance structure and a complex between-subject covariance structure.

1.3 RESEARCH QUESTIONS

The study was based on two-level hierarchical quadratic growth models. Three main research questions were addressed in this dissertation.

Question 1: If the within-subject covariance structure is simple and the between-subject covariance structure is complex, once the between-subject covariance structure is under-specified, will the complex within-subject covariance structure recover the overall covariance structure? What is the impact on the fixed and random effects?

Question 2: If the within-subject covariance structure is complex and the between-subject covariance structure is simple, once the within-subject covariance structure is under-specified, will the complex between-subject covariance structure recover the overall covariance structure? What is the impact on the fixed and random effects?

Question 3: Does the standardized root mean square residual provide improvement over information criteria methods in searching for the optimal covariance structure using hierarchical quadratic growth models?

1.4 SIGNIFICANCE OF THE STUDY

The previous research on misspecification of the covariance structure in HGLMs has focused on the within-subject covariance structure. Only Lee (2010) assessed the misspecification for both the within-subject and between-subject covariance structures. However, Lee (2010) considered only the intercept and linear growth slope in the fixed effects, and AR(1) as the within-subject covariance. The current study aims to provide a more comprehensive examination of the simultaneous misspecification at both levels (within-subject and between-subject) by including a second-level predictor on both intercepts and slopes, and more complex and common between- and within-subject covariance structures. More specifically, the study examines the compensation of covariance due to the under-specification at one level with over-specification at another level. Simulation study 1 investigated that whether the under-specification of the second-level covariance structure can be compensated by the over-specification of the first-level covariance structure. The conclusion from this study can be applied not only in the field of education, but also in the fields of psychology, behavioral health, and medicine, particularly for those application with small sample sizes which limit the complex specification of the second level covariance structure. Simulation study 2 investigated whether the under-specification of the first-level covariance structure can be compensated by the over-specification of the second-level covariance structure. Under-specification of the first-level covariance structure is common when the attrition rate is high or when the study is unbalanced. These two simulation studies will provide guidance for applied researchers on the specification of the optimal within-subject and between-subject covariance structures.

The influence of misspecification of the within-subject covariance on fixed and random effects was intensively investigated in hierarchical linear growth models. However, the growth pattern can be more complex such as quadratic or piecewise (Anumendem, Verbeke, De Fraine, Onghena, & Van Damme, 2013; Brehaut et al., 2011; Chen & Jacobson, 2013). There were only a few simulations that studied the influence of misspecifying the within-subject covariance structure on fixed effects and associated standard errors in two level hierarchical quadratic growth models (Ferron et al., 2002; Kwok et al., 2007). The influence of misspecifying the covariance structure at the between-subject level and at both levels (within- and between-subject) in hierarchical quadratic growth models has not been investigated. The proposed two simulation studies provide some information on how fixed and random effects are impacted due to the misspecification of the within-subject and between-subject covariance structures in a more complex growth model, a hierarchical quadratic growth model. In addition, a level-2 continuous variable was added into the model to investigate how the fixed effects of the second-level variable were impacted due to the misspecification of the with-subject and between-subject covariance structures.

Lee (2010) first proposed and investigated whether the standardized root mean square residual can be used as an indicator for selecting an optimal within-subject covariance structure in hierarchical linear models. The results showed that the overall standardized root mean square residual selected the correct covariance structures at about 81% across all investigated conditions, which was much higher than AIC, BIC selections. Whether the standardized root mean square residual can be used as a measure for selecting the optimal covariance structure in more complex models and covariance structures was examined in the current study. This provides a guidance for applied researchers on which evaluation criteria to use when selecting the optimal covariance structure.

1.5 ORGANIZATION OF DISSERTATION

The dissertation is divided into five distinct sections. This section is the introduction section that provides a brief background of the topics, and states the study's purpose and research questions. Section 2 provides a comprehensive literature review of related previous studies, including the commonly used covariance structures, the selection of covariance structures, and the impact of misspecification of the within-subject and between-subject covariance structures. Section 3 discusses the methodology, including the research design, data generation, data analyses, data validation, and evaluation criteria. Section 4 discusses the results from the two simulations studies separately based on the fixed and random effects and their corresponding standard errors. Section 5 summarizes the overall results from both studies, compares the results with previous studies, and explains the limitations of the study.

2.0 LITERATURE REVIEW

In this chapter, literatures on hierarchical growth models are reviewed for the study. The literature review is organized into eight sections: 1) hierarchical linear growth models, 2) covariance structures and their implications, 3) selection of covariance structures, 4) misspecification of covariance structures, 5) influence of misspecification of the within-subject covariance, 6) influence of misspecification of the between-subject covariance structure, 7) influence of misspecification of between-subject and within-subject covariance structures, and 8) summary of literature review.

2.1 HIERARCHICAL LINEAR GROWTH MODELS

Hierarchical growth models can be used to model individual changes adjusted for the hierarchical structure. The individual changes can be represented through two-level hierarchical linear growth models. The level 1 model is defined in equation 1 that is within-subject level (Raudenbush & Bryk, 2002). The level 2 models are defined by equations 2 and 3, which are between-subject levels. The combined hierarchical linear growth model is represented by equation 4. Equation 5 shows the assumptions about the first-level residual e_{ti} and two second-level random effects of r_{0i} and r_{1i},

Equation 1

$$y_{ti} = \pi_{0i} + \pi_{1i}a_{ti} + e_{ti} \ ,$$

Equation 2

$$\pi_{0i} = \beta_{00} + \sum_{q=1}^{Q_0} \beta_{0q}X_{qi} + r_{0i} \ ,$$

Equation 3

$$\pi_{1i} = \beta_{10} + \sum_{q=1}^{Q_1} \beta_{1q}X_{qi} + r_{1i},$$

Equation 4

$$y_{ti} = \beta_{00} + \sum_{q=1}^{Q_0} \beta_{0q}X_{qi}\,\pi_{1i} + \beta_{10}a_{ti} + (\sum_{q=1}^{Q_1} \beta_{1q}X_{qi})a_{ti} + r_{0i} + r_{1i}a_{ti} + e_{ti},$$

Equation 5

$$e_{ti} \sim N(0, \sigma^2 I), \text{ and } \begin{bmatrix} r_{0i} \\ r_{1i} \end{bmatrix} \sim N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \tau_{00} & \tau_{01} \\ \tau_{10} & \tau_{11} \end{bmatrix}\right),$$

where y_{ti} is the observed status at time t for individual i, i = 1, …, N subjects, t = 1, …, T occasions or time points, α_{ti} is the time related variable (such as age or year) observed at time t for individual i, π_{0i} is the initial status, π_{1i} is the rate of the linear change (slope), β_{00} is the overall mean of the initial status, β_{0q} is the effect of X_q on the initial status, β_{10} is the overall mean of the growth rate, β_{1q} is the effect of X_q on the growth rate of the linear change, and X_{qi} is either a measured characteristic of the individual's background or an experimental treatment.

The first-level model describes the individual growth, and the second-level indicates whether there is variability in the growth rate among those individuals. The model in equation 4 can be generalized as the following equation (Raudenbush & Bryk, 2002; R. Wolfinger, 1993).

Equation 6

$$\boldsymbol{y} = \boldsymbol{X\beta} + \boldsymbol{Z\nu} + \boldsymbol{\varepsilon},$$

where $\boldsymbol{y}$ is the vector of observed data in a vector of length $N \times T$, $\boldsymbol{\beta}$ is an unknown vector of fixed effects with a known design matrix $\boldsymbol{X}$, $\mathbf{v}$ is an unknown vector of random effects with known design matrix $\boldsymbol{Z}$, and $\boldsymbol{\varepsilon}$ is an unobserved error vector. The variance in $\boldsymbol{y}$ is

Equation 7

$$\boldsymbol{V} = \boldsymbol{Z}\boldsymbol{G}\boldsymbol{Z}' + \boldsymbol{R}.$$

The covariance matrices of the first-level model errors ($\boldsymbol{R}_i$) and second-level random effects ($\boldsymbol{G}_i$) in equation 5 are block diagonal matrices in labeled $\boldsymbol{R}$ and $\boldsymbol{G}$, respectively. The $\boldsymbol{R}$ and $\boldsymbol{G}$ are also called as within-subject and between-subject covariances.

The assumptions for the first-level residual are usually violated in longitudinal studies due to the hierarchical structure in the longitudinal data. Within the hierarchical linear growth model framework, the $\boldsymbol{R}$ and $\boldsymbol{G}$ can be defined as different structures to fit the model. The flexibility of modeling the covariance structure in the hierarchical linear growth model is one of the advantages of estimating individual changes over other traditional methods.

Hierarchical linear growth models are also good at handling unbalanced data that include unbalanced time points or missing data as the nature of the longitudinal design and the data collection method. There is no requirement for collecting data at equal spaced time points or fixed time points. Based on the equations, Hierarchical linear growth models can be used to describe the structure of the mean growth trajectory, estimate the variation of the growth among subjects, and estimate the correlation between the initial status and the growth rate (Bryk & Raudenbush, 1987). The model selection becomes more important since the model will influence the estimation of the individual growth. The misspecification of covariance structures may lead to biased estimates of the fixed effects and random effects.

2.2 COVARIANCE STRUCTURES AND THEIR IMPLICATIONS

Table 1 shows commonly used covariance structures for ***R*** and ***G*** (Littell, Milliken, Stroup, wolfinger, & Schabenberger, 2006; Singer, 1998; Singer & Willett, 2003; R. Wolfinger, 1993) including IDentity structure (ID), Compound Symmetry (CS), First-order AutoRegressive (AR(1)), First-order AutoRegressive Moving Average structure (ARMA(1,1)), Spatial Power Law (SP(POW)), TOEPlitz (TOEP), and UNstructured (UN).

ID covariance structure specifies that the repeated measures are independent with the homogeneous variance. There are no correlation between all pairs of lags, which actually may not be the case in longitudinal studies.

CS covariance structure is required to estimate two parameters. The diagonal elements of $\boldsymbol{R}_i$ are homoscedastic with the variance $\sigma^2+\sigma_1^2$ and the off diagonal elements are homogeneous, too, assuming the correlation is constant regardless of the lag between pairs of repeated measures.

AR(1) covariance structure has the homogenous variance and the decreased covariances with the increase of lags. But the decrease rate of the covariances is the same with the correlation ρ between any two adjacent observations. ρ is called as an autocorrelation coefficient.

ARMA(1,1) is similar with AR(1) with an additional moving average constant γ as the increase of lags. γ is called as a multiplicative moving average.

TOEP covariance structure is also similar to AR(1) with bands of identical covariances that parallel to the main diagonal. However, TOEP does not constrain an identical correlation instead of that determined by data.

Table 1. Examples of commonly used covariance structure

Covariance Structures	Notation	Example	Number of parameters
Identity structure	ID	$\begin{bmatrix} \sigma^2 & 0 & 0 & 0 \\ 0 & \sigma^2 & 0 & 0 \\ 0 & 0 & \sigma^2 & 0 \\ 0 & 0 & 0 & \sigma^2 \end{bmatrix}$	1
Compound Symmetry	CS	$\begin{bmatrix} \sigma^2+\sigma_1^2 & \sigma_1^2 & \sigma_1^2 & \sigma_1^2 \\ \sigma_1^2 & \sigma^2+\sigma_1^2 & \sigma_1^2 & \sigma_1^2 \\ \sigma_1^2 & \sigma_1^2 & \sigma^2+\sigma_1^2 & \sigma_1^2 \\ \sigma_1^2 & \sigma_1^2 & \sigma_1^2 & \sigma^2+\sigma_1^2 \end{bmatrix}$	2
First-order Autoregressive	AR(1)	$\begin{bmatrix} \sigma^2 & \sigma^2\rho & \sigma^2\rho^2 & \sigma^2\rho^3 \\ \sigma^2\rho & \sigma^2 & \sigma^2\rho & \sigma^2\rho^2 \\ \sigma^2\rho^2 & \sigma^2\rho & \sigma^2 & \sigma^2\rho \\ \sigma^2\rho^3 & \sigma^2\rho^2 & \sigma^2\rho & \sigma^2 \end{bmatrix}$	2
First-order Autoregressive Moving Average	ARMA(1,1)	$\begin{bmatrix} \sigma^2 & \sigma^2\gamma & \sigma^2\gamma\rho & \sigma^2\gamma\rho^2 \\ \sigma^2\gamma & \sigma^2 & \sigma^2\gamma & \sigma^2\gamma\rho \\ \sigma^2\gamma\rho & \sigma^2\gamma & \sigma^2 & \sigma^2\gamma \\ \sigma^2\gamma\rho^2 & \sigma^2\gamma\rho & \sigma^2\gamma & \sigma^2 \end{bmatrix}$	3
Toeplitz	TOEP	$\begin{bmatrix} \sigma^2 & \sigma_1 & \sigma_2 & \sigma_3 \\ \sigma_1 & \sigma^2 & \sigma_1 & \sigma_2 \\ \sigma_2 & \sigma_1 & \sigma^2 & \sigma_1 \\ \sigma_3 & \sigma_2 & \sigma_1 & \sigma^2 \end{bmatrix}$	T
Banded Toeplitz	TOEP(2)	$\begin{bmatrix} \sigma^2 & \sigma_1 & 0 & 0 \\ \sigma_1 & \sigma^2 & \sigma_1 & 0 \\ 0 & \sigma_1 & \sigma^2 & \sigma_1 \\ 0 & 0 & \sigma_1 & \sigma^2 \end{bmatrix}$	2
Spatial Power Law	SP(POW)	$\begin{bmatrix} \sigma^2 & \sigma^2\rho^{d_{12}} & \sigma^2\rho^{d_{13}} & \sigma^2\rho^{d_{14}} \\ \sigma^2\rho^{d_{12}} & \sigma^2 & \sigma^2\rho^{d_{23}} & \sigma^2\rho^{d_{24}} \\ \sigma^2\rho^{d_{13}} & \sigma^2\rho^{d_{23}} & \sigma^2 & \sigma^2\rho^{d_{34}} \\ \sigma^2\rho^{d_{14}} & \sigma^2\rho^{d_{24}} & \sigma^2\rho^{d_{34}} & \sigma^2 \end{bmatrix}$	2
Unstructured	UN	$\begin{bmatrix} \sigma_1^2 & \sigma_{21} & \sigma_{31} & \sigma_{41} \\ \sigma_{21} & \sigma_2^2 & \sigma_{32} & \sigma_{42} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 & \sigma_{43} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_4^2 \end{bmatrix}$	$T(T+1)/2$

SP(POW) reflects the correlation change as the lag increases, and the change is based on the Euclidean distance between two adjacent time points. The covariance structures described above are homogeneous between groups, but may be heterogeneous between groups as well.

UN is the most complex covariance structure with different variances and covariances assuming the correlations among any pairs of lags are unique.

The covariance structures described above also have corresponding heterogeneous covariance structures (R. D. Wolfinger, 1996). ID covariance structure is the simplest one, and nested within CS covariance structure, which is nested within AR(1) that is nested within ARMA(1,1). ID is also nested within TOEP and SP(POW). Homogeneous covariance structures are nested within their corresponding heterogeneous covariance structures. Homogeneous covariance structures among groups are nested within their corresponding heterogeneous covariance structures. All covariance structures are nested within UN covariance structure.

2.3 SELECTION OF COVARIANCE STRUCTURES

Different covariance structures can be selected in an analysis using hierarchical growth models. This section introduces the methods selecting an appropriate covariance structure, the comparisons of selection methods, the factors influencing the performance of the selection methods, and the summary of the selection methods.

2.3.1 Methods for selecting covariance structures

To estimate the individual changes accurately in hierarchical linear growth models, the optimal covariance structure should be carefully selected to better fit the data under the same fixed effect model. The Likelihood ratio test, information criteria, standardized root mean square residual, and graphic methods can be used to serve this purpose. This section describes the methods to select the appropriate covariance structure among the alternatives.

2.3.1.1 Likelihood Ratio Test (LRT)

The LRT can be used for model comparisons among nested models based on either the Maximum log-likelihood (ML) or Restricted Maximum log-Likelihood (REML). ML and REML are estimated by the equations 8 and 9, respectively (Littell et al., 2006; R. Wolfinger, 1993),

Equation 8

$$-2ll(\boldsymbol{\theta}|\boldsymbol{y}) = \log|\mathbf{V}(\boldsymbol{\theta})| + (\boldsymbol{y} - \boldsymbol{X\beta}(\boldsymbol{\theta}))'\boldsymbol{V}(\boldsymbol{\theta})^{-1}(\boldsymbol{y} - \boldsymbol{X\beta}(\boldsymbol{\theta})) + n\log(2\pi),$$

Equation 9

$$-2ll_R(\boldsymbol{\theta}|\boldsymbol{y}) = \log|\mathbf{V}(\boldsymbol{\theta})| + \left(\boldsymbol{y} - \boldsymbol{X\beta}(\boldsymbol{\theta})\right)'\boldsymbol{V}(\boldsymbol{\theta})^{-1}\left(\boldsymbol{y} - \boldsymbol{X\beta}(\boldsymbol{\theta})\right)$$

$$+\log|\boldsymbol{X}'\boldsymbol{V}(\boldsymbol{\theta})^{-1}\boldsymbol{X}| + (n-p)\log(2\pi),$$

Equation 10

in which $$\beta(\theta) = |\boldsymbol{X}'\boldsymbol{V}(\boldsymbol{\theta})^{-1}\boldsymbol{X}|^{-1}\boldsymbol{X}'\boldsymbol{V}(\boldsymbol{\theta})^{-1}\boldsymbol{y},$$

where $\boldsymbol{V(\theta)}$ is used to denote explicit dependence of $\boldsymbol{V}$ on a vector of unknown variance-covariance parameters $\boldsymbol{\theta}$, $\boldsymbol{y}$ is the observed status, $\boldsymbol{X}$ is the design matrix. Maximizing $ll(\boldsymbol{\theta}|y)$ or $ll_R(\boldsymbol{\theta}|\boldsymbol{y})$ to estimate $\boldsymbol{\theta}$ can provide the elements of $\boldsymbol{\theta}$ to evaluate the parameter matrix $\boldsymbol{\beta}(\boldsymbol{\theta})$. REML is preferred over ML. There are some advantages using REML to estimate parameters (Kutner, Nachtsheim, Neter, & Li, 2005), such as REML estimators do not seem to be as sensitive to outliers in the data as they are in ML estimators. Also, REML takes into account the degree of freedom of the fixed effects in a model.

After the models are fitted by ML or REML, LRT can be performed to compare log-likelihood between the full model and reduced models. In order to do the comparisons, the reduced models should be nested within the full model. For example, the model with a TOEP covariance structure can only be compared to the models with ID or UN covariance structures. The LRT statistic is defined by equation 11 (Diggle et al., 2002),

Equation 11

$$D = 2ll(\widehat{\boldsymbol{\theta}}|\boldsymbol{y}) - 2ll(\widehat{\boldsymbol{\theta}}_{\mathbf{0}}|\boldsymbol{y}),$$

where $\widehat{\boldsymbol{\theta}}_{\mathbf{0}}$ and $\widehat{\boldsymbol{\theta}}$ are the ML or REML estimates of $\boldsymbol{\theta}$ in the full model and a reduced model under the null hypothesis, respectively. Assuming the null hypothesis is correct, the sampling distribution of *D* is approximately a Chi-squared distribution with the degree of freedom that is equal to the difference between the numbers of parameters estimated in the compared two models.

Under a specified α value, if the test statistics are smaller than the critical value in the Chi-squared distribution, then a simpler model is preferred, which means that the simpler covariance structure should be used in the analysis.

2.3.1.2 Akaike Information Criteria (AIC)

AIC is used to compare non-nested models, such as comparing the model with TOEP covariance structure to a model with AR(1) or ARMA(1,1) covariance structures. AIC is defined by equation 12 (Akaike, 1974).

Equation 12

$$AIC = -2ll(\widehat{\boldsymbol{\theta}}|\boldsymbol{y}) + 2q,$$

where q is the number of parameters in a covariance structure. It is a penalty for over-parameterization (R. D. Wolfinger, 1996). REML $\left(-2ll_R(\widehat{\boldsymbol{\theta}}|\boldsymbol{y})\right)$ can also be used in equation 12 to get AIC_R. The smaller the AIC or AIC_R, the better the model fits, which means the model is fitted with a better covariance structure choice.

2.3.1.3 Bayesian Information Criteria (BIC)

BIC is defined by equation 13 (Schwarz, 1978) for the comparisons between non-nested models. The smaller the BIC is, the better the model fits.

Equation 13

$$BIC = -2ll(\widehat{\boldsymbol{\theta}}|\boldsymbol{y}) + q\log(n-p),$$

where n is the sample size, p is the rank of X, q is the number of covariance parameters. BIC prefers parsimony models since the correction of the sample size and the number of covariance parameters is added in the equation.

2.3.1.4 Other criteria: AICC, HQIC, CAIC

AICC is an extension of AIC (Hurvich, Simonoff, & Tsai, 1998) defined by equation 14. The smaller the AICC, the better the model fits.

Equation 14

$$AICC = -2ll(\widehat{\boldsymbol{\theta}}|\boldsymbol{y}) + \frac{2(q+1)n}{n-q-2}.$$

where n is the sample size, q is the number of parameters in the model.

CAIC is Consistent Akaike Information Criterion defined by equation 15 (Bozdogan, 1987). It is another extension of AIC adjusting for the sample size. The smaller the CAIC, the better the model is, which is the same as AIC.

Equation 15

$$CAIC = -2ll(\widehat{\boldsymbol{\theta}}|\boldsymbol{y}) + q\ (\log(n) + 1),$$

where n is the sample size, q is the number of parameters in the model.

HQIC is Hannan and Quinn Information Criterion (Hannan & Quinn, 1979) defined by equation 16. The smaller the HQIC, the better the model is.

Equation 16

$$HQIC = -2ll(\widehat{\boldsymbol{\theta}}|\boldsymbol{y}) + 2q\ (\log(\log(n))),$$

where n is the sample size, q is the number of parameters in the model.

2.3.1.5 Standardized Root Mean square Residual (SRMR)

SRMR (Bentler, 1995) is calculated by equation 17, which is a measure of the averaged difference of the standardized residuals between the observed and model based covariance matrices.

Equation 17

$$\mathrm{SRMR} = \sqrt{\frac{\left\{2\sum_{i=1}^{T}\sum_{j=1}^{i}\left[{(s_{ij}-\hat{\sigma}_{ij})}/{(s_{ii}s_{jj})}\right]^2\right\}}{T(T+1)}},$$

where T is the total number of repeated measures (waves), s_{ij} is the element of the i^{th} row and the j^{th} column in the total covariance matrix of the generated data, and $\hat{\sigma}_{ij}$ is the corresponding element for the model based covariance matrix. It is considered as a good fit model when SRMR is smaller than .08, indicating the selected covariance structure is optimal.

2.3.1.6 Graphical method

Plotting the variances and covariances in the data can help visualize the pattern of covariances (Kincaid, 2005; Littell et al., 2006). At first, the residual correlation, variances and covariances are estimated in fitting a hierarchical linear growth model with a UN covariance structure. All variances and covariances are sorted by the time points and plotted over time started at time 0, then the lag 1 covariance, the lag 2 covariance, and so on. If the pattern of covariances decreases with increasing lags in linear trend, AR(1) covariance structure may be a better choice for the model. If covariances in different lags overlay, the constant variance may fit the model better since there is no evidence showing the change of the variance and covariance over time. In this case, choosing AR(1), TOEP, and UN covariance structure may not be necessary to over fit the data.

After checking the plot of the variances and covariances over time separated by lags, one possible covariance structure is chosen. Then another model should be fitted with the selected covariance structure. The estimated variances and covariances, as well as the correlation between lags can be compared with the plot. If the pattern of variances and covariances is similar as in the graph, the selected covariance structure will be the final decision.

2.3.2 Comparisons of methods for selecting covariance structures

Hierarchical linear growth models have flexibility to specify the covariance structure comparing to other methods in modeling individual changes. Information criteria and the graphical method can be used to select an optimal covariance structure to fit models. Previous studies have compared different methods in terms of success rates for selecting an appropriate covariance structure, and the Type I error rates on the estimations of fixed and random effects by using the selected covariance.

Wolfinger (1993) compared AIC, BIC and LRT methods in terms of selecting an appropriate covariance structure including 18 conditions in two real datasets. For the first dataset, three factors investigated are the ***G*** matrix with two levels (none and heterogeneous between groups), the ***R*** matrix with four levels (ID, AR(1), TOEP(5), SP(POW)), and five different ***X*** matrices designs (no predictor, one main effect, two-way interaction, three-way interaction, and four-way interaction). The results of the first example showed that AIC selected a two-way interaction model with a heterogeneous structure as the between-subject (***G***) covariance, and a TOEP(5) as the within-subject covariance (***R***). BIC selected a simpler model, having one main effect and an SP(POW) as the ***R*** matrix without random effects. LRT carried out 4 favor models, including the models chosen by AIC and BIC. Since the models are not nested, LRT was not able to do the comparisons among the models and could not give more detail information. The second example in the study had more choices for the ***G*** matrix. LRT favored AR(1) for the ***G*** matrix and an AR(1) was the common covariance as the ***R*** matrix, while AIC_R and BIC_R chose the same model as that by LRT.

Bozdogan (1987) conducted a Monte Carlo study to compare AIC, and CAIC for selecting the correct model. Three factors were considered, including the sample size with three levels (n = 50, 100, and 200), the within-subject covariance structure with three levels (σ^2 = 0.25, 0.50, and 1.00), and the degree of freedom for a polynomial model with six levels (*df* = 1, 2, 3, 4, 5, and 6). CAIC performed better than AIC in almost all the conditions in the study. The study recommended that CAIC is more consistent for large samples, and sometimes it may choose a simpler model.

In another study (Keselman et al., 1998), AIC and BIC were compared for selecting a covariance structure in balanced and unbalanced designs. Six factors were investigated, which were the type of covariance structures with six levels (UN, AR(1), RC and their corresponding heterogeneous group structures) to generate the data, the type of covariance structures to fit the model with eleven levels, the sample size with three levels (n = 30, 45, and 60), the balanced or unbalanced design with two levels, the group sample size with three levels (the degree of unbalanced), and normal and nonnormal data. The results showed that AIC selected a covariance structure only by 47% correctly across the 26 conditions, and BIC selected the correct models only by 35 on average. However, in 14 out of the 26 conditions, the correct covariances were never selected by BIC. AR(1) with heterogeneous among groups was more frequently selected than the correct covariance structures by AIC. The larger sample size had more power to identify the correct covariance structure. Non-normal data seemed to have no obvious effects on the selection by AIC. The study suggested that AIC, and in particular BIC more frequently chose a wrong covariance structure than the correct one.

Ferron, Dailey & Yi (2002) conducted a simulation study to compare LRT, AIC, and BIC in identifying the optimal covariance structure, in which AR(1) was used to generate data. The factors in the study included the autocorrelation with two levels (ρ = .3 and ρ = .6), the number of time points with five levels (t = 3, 4, 6, 8, and 12), the sample size with three levels (n = 30, 100, and 500), and the value of first-level covariance with three levels (σ^2 = 0.01, 1, and 100). All conditions in the study were obtained to fit two-level hierarchical linear growth models including the random intercept and slope with only one predictor in the second-level. The parameters β_{00}, β_{01}, β_{10}, and β_{11} were set to zero. For each condition, 10,000 data sets were simulated. The results showed that AIC, BIC and LRT correctly identified the model by 79%, 66%, and 71% of the time on average, respectively. In most of the conditions, AIC is the most sensitive one out of the three, and LRT was more sensitive than BIC. For the small sample size and 3 repeated measures with smaller intraclass correlation, the success rates were 6.3%, 0.1%, and 0.2% by AIC, BIC, and LRT, respectively. For the medium sample size and 4 repeated measures with a large intraclass correlation, the success rates were 87%, 55%, and 72% by AIC, BIC, and LRT, respectively. The study concluded that the success rates were higher when the condition was in the combination of a larger sample size, more repeated measures, a higher intraclass correlation, and larger value of the first-level covariance.

Another simulation study that compared AIC and BIC performances was a four factor design (Gomez et al., 2005). The factors included the treatment effect with three levels, the number of time points with two levels (t = 3, 5), the covariance structure with fifteen levels, and the fitting covariance structure from the fifteen covariance structures. The study did the comparisons by balanced and unbalanced sample sizes among treatment groups separately. For the equal sample size study, Type I error rates for models fitted with the selected covariance structures by AIC and BIC, were higher than the target value of 0.05 for all covariance structures and sample sizes. The Type I error rates from the best BIC models were closer to the target value than those from the best AIC models. The selected structures by AIC and BIC were not affected by the unbalanced data. The Type I error rates for treatment were even smaller in unbalanced conditions than those in balanced designs. The success rates of AIC and BIC were generally low regardless of the sample sizes and covariance structures. AIC had a higher success rate than BIC for complicated covariance structures. However, BIC was better than AIC for simpler covariance structures. The results showed there were no effects on success rates due to the unbalanced sample size as well.

Using two real samples of job satisfaction and simulated datasets, the comparisons were investigated between AIC and BIC performances for selecting the optimal covariance structure among CS, AR(1), TOEP, ARMA(1,1), their corresponding heterogeneous variance, and UN structures (Liu et al., 2012). AIC preferred more complex covariance structures than BIC did. AIC and BIC selected UN and TOEP with heterogeneous variance most of the time in the example using real datasets. For the simulation study, three factors were included in the study. They were the sample size with three levels (n = 20, 100, 200), the effect size with two levels (η^2 = 0.5, and 0.8)), and the intraclass correlation with three levels (ρ = 0.2, 0.5, and 0.8). AIC and BIC performed well for selecting correct models, and they were always at the lowest values when an AR(1) covariance structure was used to fit the models. The success rates were higher when the sample size was larger, the effect size was greater, and the intraclass correlation was higher. In the optimal combination, the success rates of AIC and BIC were very high. In addition, the study suggested that AIC and BIC selected almost the same models, and the result patterns were identical indicating they were doing equally well. The results were similar with a study using real data (Eyduran & Akbas, 2010), in which AIC, AICC, and BIC were used to select covariances.

Ye (2005) compared AIC, BIC, AICC, HQIC, and CAIC performances and the Type I error rates in a simulation study. Three factors were the number of time points with three levels (t = 3, 5, and 7), the sample size with three levels (n = 5, 10, and 15 per treatment), and the covariance structure with twelve levels. The results showed that the success rates increased as the number of subjects per treatment and total sample size increased. As the number of repeated measures per subject increased, the success rates increased as well. When TOEP was the correct covariance, it was selected by AIC only 3.3% of the time out of the simulated datasets, while

AIC selected EXP instead of TOEP about 15.6% of the time. AR(1) was mistakenly selected by AIC as a Spherical spatial covariance structure at 26.9%. AIC's performance was better than other methods when the correct covariance structures were complex. BIC had a higher success rate than AIC when covariance structures were simpler. AICC performed between AIC and BIC. AICC was better than AIC when covariance was homogenous among the treatment groups, while AICC was better than BIC when covariance was heterogeneous among the groups. The HQIC performance was close to AIC. The CAIC performance was close to BIC when covariances were homogenous among the groups. However, the CAIC performance was poor in general when covariances were heterogeneous among the groups. The Type I error rates using selected covariance structures by AIC, BIC, AICC, HQIC and CAIC in HLGMs were significantly greater than the target value of 0.05. Type I error rates were influenced by the sample sizes and the number of repeated measures. Typically, AIC, BIC, AICC, HQIC, and CAIC performed similarly on the Type I error rates.

Lee (2010) investigated whether SRMR can be used as an indicator for selecting the optimal within-subject covariance structure for two level hierarchical linear growth models in a simulation study. Six factors included were the sample size with two levels (30 and 210), the number of repeated measures with two levels (4 and 8), the magnitude of growth rates with three levels (0, 0.05, and 0.16), the amount of between-subject covariance (***G*** matrix: small and medium), and the within-subject covariance structures (***R*** matrix: ID, TOEP(2), AR(1), and ARMA(1,1)). A total of 500 replications were generated for each condition. The SRMR selected the correct within-subject covariance at 81% across all the conditions. The hit rates of SRMR were better than AIC and BIC which were at 62% and 66% across all the conditions, respectively. Also SRMR gave more information than AIC and BIC indicating the discrepancy between the real data and the estimations of total variances and covariances. The study reported SRMR outperformed other fit statistics in the selection of the within-subject covariance structure.

2.3.3 Factors influencing the performance of selection methods

The factors that had an impact on the performance of selection methods based on the previous studies, were the sample size, the number of waves, the intraclass correlation, covariance structures, and the missing and unbalanced design.

2.3.3.1 Sample size

Based on the previous studies in selecting the covariance structure for hierarchical linear growth models by AIC, BIC, AICC, HQIC, and CAIC, the sample size influenced on selections, especially for small number of repeated measures. Usually, larger sample size provided more power to identify the optimal covariance structure in hierarchical linear growth models for all the selection methods. Ferron et al. (2004) reported that the percentages of identifying the correct covariance was between 8% and 59% when the sample sizes changed from 30 to 500 based on 3 repeated measures in the data. When the number of repeated measures was large, such as for 12 repeated measures, the percentage of correctly identifying the correct models was between 99.9% and 100%, which meant that the sample size effect was not apparent when the number of repeated measures was large. Ye’s (2005) study had similar results indicating that the success rates increased as the number of subjects per treatment increased, which agreed with the studies by Gomez et al. (2005) and Liu et al. (2012).

2.3.3.2 Number of waves

The number of repeated measures in longitudinal studies was also an important factor for selecting a covariance structure by IC methods and LRT. For example, AIC identified the correct models from 31% to 99% with the number of repeated measures from 3 to 12 when the sample size was 100 in the study by Ferron et al. (2004). And the success rates were high for all methods when the number of repeated measures was large regardless of the other factors in the study. Ye (2005) agreed with the results and reported that the success rates increased from 59% to 66% when the number of repeated measures changed from 5 to 10 with the sample size of 3 per treatment.

2.3.3.3 Intraclass correlation

The larger the effect size and intraclass correlation were, the more sensitive to the correct covariance by all methods. For example, in Ferron et al. (2004) study, when the sample size was 100 with 4 repeated measures, the success rates increased from 54% to 87%, from 17% to 55%, and from 32% to 72% when intraclass correlation changed from 0.3 to 0.6 by AIC, BIC, and LRT, respectively. Liu et al. (2012) also reported that the success rates were increased as the intraclass correlation increased.

2.3.3.4 Covariance structures

Covariance structures and their values in studied data sets had effects on the selection based on the previous studies (Ferron et al., 2004; Ye, 2005). For the sample size of 100 and repeated measures of 4 with an intraclass correlation of 0.3, if the covariance changed from 0.01 to 1 and 100, the success rates changed from 44% to 55% and 72%, from 12% to 18% and 29%, from 24% to 33% and 50% by AIC, BIC and LRT (Ferron et al., 2004), respectively. Ye (2005) summarized that some covariance structures, such as CS and Gaussian covariance structures, were more consistently selected by all methods, and others were rarely selected. Whether others were selected or not depended on the sample size and the method used. Gomez et al. (2005) also pointed out that AIC did better than BIC when the correct covariance was more complex, and BIC did better when the correct covariance was simpler. In Liu et al. (2012) study, the influences of a true covariance structure on selecting the model covariance by AIC and BIC were reported as well indicating that the performances of AIC and BIC were influenced by the similarity between the true error structure and the competing error structure.

2.3.3.5 Missing data and unbalanced design

Missing data are common in longitudinal studies, which would be well handled by hierarchical linear growth models in estimating individual changes. The unbalanced design was not a problem neither, such as unfixed time points, unequal intervals between repeated measures, or unequal numbers of subjects per treatment. The previous studies showed that there were very limited effects on selecting the correct covariance structure. In Gomez et al. (2005) study, the results showed that there was no effect by an unbalanced design, which was agreed with the study by Keselman et al. (1998).

2.3.4 Conclusion on the methods for selecting covariance structures

Hierarchical linear growth models can be applied either in experimental and quasi-experimental designs for analyzing individual changes. However, the estimations of fixed and random effects or their hypothesis tests are affected by the choice of the covariance structure. AIC, BIC, AICC, HQIC, CAIC, LRT, and graphical methods are usually used to identify an appropriate covariance structure in order to fit hierarchical linear growth models in estimating individual changes. The success rates of selection and the Type I error rates are influenced by the sample size that includes number of subjects in each treatment group and the total sample size in a study, the number of repeated measures, the effect size, the intraclass correlation, and the covariance structure in studied dataset.

The sample size had important influences on the success rates in selecting the correct covariance for all IC methods. The greater the sample sizes are, the better the IC performance is. The larger number of repeated measures can help hierarchical linear growth models account for measurement errors, and estimate fixed and random effects more accurately.

AIC generally had better success rates for the data that have heterogeneous covariance structures among treatment groups, while BIC did better than AIC when a covariance structure was simpler and homogenous among groups. LRT is used to compare nested models.

Generally speaking, the larger number of time points, the larger sample size, and the greater autocorrelation led to higher proportion in identifying the correct covariance structure. SRMR did better than AIC and BIC. AIC did better than BIC and LRT in selecting the correct models in most of the conditions. AIC, BIC, AICC, HQIC, CAIC, and LRT perform poorly in identifying the correct covariance structures. The graphical method is usually used to help the IC methods and LRT make the final decision for choosing the correct covariance structure. More effective methods are needed for identifying the correct covariance structure in future studies.

2.4 MISSPECIFICATION OF COVARIANCE

Hierarchical growth models can investigate the structure of the individual growth and properties of the growth trajectory, discover the relationship between the initial status and the growth rate, examine the reliability of repeated measures to account for measurement errors, and also conduct hypothesis tests for fixed and random effects (Bryk & Raudenbush, 1987). To estimate the growth trajectory more accurately and perform the hypothesis tests correctly, identifying the optimal $\boldsymbol{R}$ and $\boldsymbol{G}$ is important since the misspecification of the $\boldsymbol{R}$ and $\boldsymbol{G}$ may lead to biased results. However, the methods used in identifying the correct covariance structure, such as Akaike information criteria, Bayesian information criteria and likelihood ratio test, are not promising and effective. Hierarchical growth models are usually miss-specified with alternative covariance structures instead of the correct ones. How the estimates of fixed effects and random effects are influenced by the misspecification of both between-subject and within-subject covariance structures in hierarchical growth models should be comprehensively investigated.

2.4.1 Types of misspecification of covariance

The misspecification of the $\boldsymbol{G}$ and $\boldsymbol{R}$ in hierarchical linear growth models for longitudinal studies is classified into three categories (Kwok et al., 2007), which are under-specification, over-specification, and general misspecification of covariance structures. The under-specification occurs when the true covariance structure is more complex than the selected one for the analysis and the selected covariance is nested within the true one. The over-specification occurs when the true covariance structure is more constrained than the selected one and the true covariance is nested within the selected one. The general misspecification occurs when true covariance structure and selected one are not nested. Table 2 shows some examples for the three types of covariance structure misspecifications.

Table 2. Three types of the misspecification of covariance structures

Specified covariance structure in Analysis	True covariance structure					
	ID	CS	AR(1)	ARMA(1,1)	TOEP(2)	UN
ID	X	Under	Under	Under	Under	Under
CS	Over	X	Under	Under	General	Under
AR(1)	Over	Over	X	Under	General	Under
ARMA(1,1)	Over	Over	Over	X	General	Under
TOEP(2)	Over	General	General	General	X	Under
UN	Over	Over	Over	Over	Over	X

2.4.2 Misspecification of the within-subject covariance (*R* matrix)

The ***R*** matrix is defined in equation 18 (Kwok et al., 2007).

Equation 18

$$\boldsymbol{R} = \begin{bmatrix} \boldsymbol{R_i} & 0 & \cdots & 0 \\ 0 & \boldsymbol{R_i} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \boldsymbol{R_i} \end{bmatrix}_{NT\times NT},$$

Equation 19

in which

$$\boldsymbol{R_i} = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1T} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2T} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{T1} & \sigma_{T2} & \cdots & \sigma_T^2 \end{bmatrix}_{T\times T},$$

where N is the total number of subjects, and T is the number of repeated measures.

The Misspecification of the within-subject covariance structure means that $\boldsymbol{R}_i$ is miss-specified. The three types of misspecifications are applied here.

2.4.3 Misspecification of the between-subject covariance (*G* matrix)

The ***G*** Matrix is defined in equation 20 (Kwok et al., 2007).

Equation 20

$$\boldsymbol{G} = \begin{bmatrix} \boldsymbol{G_i} & 0 & \cdots & 0 \\ 0 & \boldsymbol{G_i} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \boldsymbol{G_i} \end{bmatrix}_{QN \times QN},$$

Equation 21

in which

$$\boldsymbol{G_i} = \begin{bmatrix} \tau_{00} & \tau_{01} & \cdots & \tau_{0Q} \\ \tau_{10} & \tau_{11} & \cdots & \tau_{1Q} \\ \vdots & \vdots & \ddots & \vdots \\ \tau_{Q0} & \tau_{Q1} & \cdots & \tau_{QQ} \end{bmatrix}_{Q \times Q},$$

where N is the total number of subjects, *Q* is the number of random effects.

The misspecification of the between-subject covariance structure means that $\boldsymbol{G}_i$ is miss-specified. The three types of misspecifications are applied here as well.

2.4.4 Misspecification of Between-subject and within-subject covariances

When using hierarchical growth models to estimate fixed and random effects for individual changes, ***G*** and ***R*** matrices need to be specified simultaneously. There are fifteen possibilities of misspecifications between the within-subject and between-subject covariance structures, which are listed in Table 3.

Table 3. Misspecifications of between-subject and with-subject covariance structures

Specification of between-subject G	Specification of within-subject covariance structure R			
	Correct specification	Under-specification	Over-specification	General misspecification
Correct specification	Correct	Correct-G & Under-R	Correct-G & Over-R	Correct-G & General-R
Under-specification	Under-G & Correct-R	Under-G & Under-R	Under-G & Over-R	Under-G & General-R
Over-specification	Over-G & Correct-R	Over-G & Under-R	Over-G & Over-R	Over-G & General-R
General misspecification	General-G & Correct-R	General-G & Under-R	General-G & Over-R	General-G & General-R

2.4.5 Evaluation criteria

Three evaluation criteria were mostly used in previous simulation studies for investigating the effects of misspecifications of the within-subject and between-subject covariance structures. They were the convergence rate, the relative bias and simple bias of parameters, the Type I error rate and the power rate of the fixed effects.

2.4.5.1 Convergence rate of replications

The percentage of converged models is calculated over the total number of models running HLMs by selected covariance structures. This is used to evaluate whether the selected covariance structure is appropriate. If selected covariance is too complex to fit the data, the maximum likelihood or restricted maximum likelihood may not be able to be identified.

2.4.5.2 Relative bias of the estimates of the fixed and random effects

The relative bias (*RB*) of parameters usually is examined for all fixed effects, their associated standard errors, and random effects in the models when the examined true parameters are not equal to zero, while simple bias (SB) is used when true parameters are zero. The relative bias of parameters is defined by equation 22 and the simple bias of parameters is defined by equation 23

Equation 22

$$RB = \frac{\hat{\beta} - \beta}{\beta},$$

Equation 23

$$SB = \hat{\beta} - \beta,$$

where $\hat{\beta}$ is the estimated parameters by fitting HLMs using the selected covariance structure, and β is the true parameter value.

2.4.5.3 Type I error rate and power rate

The Type I error rate is defined as the percentage of the number of performed models with significant effects over the total number of the models in the condition that the true parameter values of fixed or random effects are equal to zero.

The power rate is defined as the percentage of the number of performed models with significant effects over the total number of the models in the condition when the true parameter values are greater than zero.

2.5 INFLUENCE OF MISSPECIFICATIONS OF THE WITHIN-SUBJECT COVARIANCE STRUCTURE

The influence of the misspecification of the within-subject covariance structure has been investigated in several studies. This section discusses the previous studies about the design, the related factors, and the impact of the misspecification of the within-subject covariance structure.

In Kasim & Raudenbush (1998) study, heterogeneous within-subject covariances were investigated to examine the influence of the misspecification of the $\boldsymbol{R}$ on fixed effects by the Gibbs sampling approach. Four data sets were generated based on the degree of heterogeneity of covariance with two levels (θ = 0.02 and 0.2) and the number of groups with two levels (n = 15 and 100). The study was also applied in real datasets. When the models were fitted by the homogenous $\boldsymbol{R}$, the convergence rates increased as the sample size increased. The results showed that the estimations of fixed effects were not biased due to the misspecification of the $\boldsymbol{R}$. However, the standard errors of fixed effects and random effects were biased.

Ferron et al. (2002) conducted a simulation study to investigate how the misspecification of the within-subject covariance influenced the estimates of fixed and random effects. The simulation study had three factors that were the autocorrelation with two levels (ρ = .3 and ρ = .6), the number of time points with five levels (t = 3, 4, 6, 8, and 12), and the sample size with three levels (n = 30, 100, and 500). The datasets were generated using an AR(1) as the within-subject covariance structure in which σ^2 = 0.01, 1 and 100, and $\boldsymbol{G_i} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$. The models were fitted with an ID covariance structure, meaning that the within-subject covariance structure in all models were under-specified.

The results showed that the estimations of fixed effects (initial status β_{00} and growth rate β_{10}) were very close to the true values in all conditions indicating that the fixed effects were not biased due to the under-specification of the ***R*** matrix, which was agreed with the studies by Chi & Reinsel (1989) and Lange & Laird (1989).

The random effects were overestimated for all conditions due to the under-specification of the ***R*** matrix. The covariance in the ***G*** matrix was estimated to be negative in all conditions as well. The biased random effects were slightly greater when the number of repeated measures and the sample size were smaller and the autocorrelation was higher. The overestimates of the ***G*** matrix in the between-subject level in turn led to the underestimate in the variability (σ^2) of the within-subject level. The biased estimates of the within-subject variance were greater as the sample size and the number of repeated measures decreased and the autocorrelation increased. For example, under 4 time points and the medium sample size with small autocorrelation, the estimations of random effects ($\boldsymbol{G_i}$) were increased from $\begin{bmatrix} 1.00 & 0.00 \\ 0.00 & 1.00 \end{bmatrix}$ to $\begin{bmatrix} 1.43 & -0.13 \\ -0.13 & 1.08 \end{bmatrix}$ and $\begin{bmatrix} 43.82 & -12.69 \\ -12.69 & 9.46 \end{bmatrix}$ and the underestimated σ^2 was from 0.0076 to 0.75 and 75.56 if the first-level true variability (σ^2) was used to generate the data increased from 0.01 to 1 and 100.

The Type I error was slightly inflated in most of the conditions and increased as the sample size increased, the number of repeated measures increased and the autocorrelation increased.

Missing data and unequally spaced observations were also investigated in the study. For the missing data, 50% of the participants were randomly missing one of four observations. For the unequal space condition, four observations were randomly selected from eight time points. An ARMA(1,1) was used to generate the data that made the study more complex. The results showed that the estimates of fixed effects were not biased as the complete data. The Type I error rates were not influenced by the missing data or unequal time points.

The study also examined whether the estimations of fixed and random effects were biased by adding more predictors into the models, in which some predictors were related to the outcome and some were not. Again, the estimations of the fixed effects were not biased due to the misspecification of the $\boldsymbol{R}$ matrix. The Type I error rates were close to the target value. In addition, quadratic growth models were conducted with a single predictor and eight time points. The biased estimates of fixed effects occurred in some conditions that had unequally spaced observations due to the misspecification of the $\boldsymbol{R}$ matrix, which may need to pay more attention. The Type I error rates were inflated for many of the conditions, especially for smaller sample size, lower autocorrelation and fewer time points.

Kwok et al. (2007) intensively investigated the influences of the three types of misspecifications of the within-subject covariance structures on linear and quadratic two-level growth models, respectively. For the linear growth models, five factors were simulated, which were two levels of the number of participants (30 and 210), two levels of the time points (4 and 8), three levels of the growth parameter β_{10} (0, 0.05 and 0.16), two levels of the second level random effects $\boldsymbol{G_i}$ ($\begin{bmatrix} .100 & .025 \\ .025 & .050 \end{bmatrix}$ and $\begin{bmatrix} .200 & .050 \\ .050 & .100 \end{bmatrix}$), and four types of the $\boldsymbol{R}$ matrix for generating the data (ID, TOEP(2), AR(1), and ARMA(1,1)). Each dataset was performed in a two-level HLM with five different with-subject covariance structures (ID, TOEP(2), AR(1), ARMA(1,1), and UN) separately. The between-subject covariance structure was defined as UN for all analyses except when the $\boldsymbol{R}$ matrix was specified as UN, in which the $\boldsymbol{G}$ matrix was specified as null. In the case of $\boldsymbol{G}$ specified as null, it was assumed that there was no random effects in which the $\boldsymbol{R}$ matrix captured all variability.

When specified $\boldsymbol{R}$ was ID, AR(1) and UN, all fitted models were converged, only 99.7% of the models specified by TOEP(2) were converged, while the models specified with ARMA(1,1) had the lowest convergence rate at 95.6%.

For fixed effects, the mean relative bias and simple bias were close to zero for the initial status (β_{00}) and the growth rate (β_{10}) regardless of the misspecifications of covariance structures. The relative bias of standard errors of fixed effects was influenced by the type of misspecifications. A large overestimation of standard errors of the initial status (β_{00}) was observed when the $\boldsymbol{R}$ matrix was either under-specified or general misspecified. There were no significant differences on the relative bias of standard errors of fixed effects when the $\boldsymbol{R}$ was over-specified and correctly specified. Comparing specified by a UN when $\boldsymbol{G}$ was null to correct-specification, the standard errors of fixed effects were usually underestimated. For random effects, under-specified and general misspecified $\boldsymbol{R}$ led to larger overestimation of random effects, especially under small $\boldsymbol{G}$ matrix. Over-specified $\boldsymbol{R}$ usually resulted in the smallest random effects.

The Type I rates detecting fixed effects were not significantly influenced by the five factors. Controlling the other factors, the Type I error rate for the models specified by UN with the null $\boldsymbol{G}$ was significantly larger than those from the models of correct-specified $\boldsymbol{R}$. The statistical power rates detecting the initial status (β_{00}) was higher when the $\boldsymbol{R}$ was over-specified. There was no influence on the power of detecting growth rate (β_{10}) by type of misspecification of the $\boldsymbol{R}$ matrix.

For the quadratic growth models, a similar pattern of the results were detected. There were no influences on the fixed effects due to the misspecification of the $\boldsymbol{R}$, while the standard errors of fixed effects were impacted by the misspecification of the $\boldsymbol{R}$. Again, overestimated standard errors of fixed effects occurred when the within-subject ***R*** was under-specified or general misspecified. The similar patterns of results of random effects were also detected as in linear models. A substantially overestimated variance for random effects occurred when the ***R*** was under-specified and general misspecified, especially when the ***G*** matrix was small.

The Type I error rates of the intercept and linear growth were not influenced by the misspecification of the ***R*** matrix, while the type I error rate for the growth acceleration (quadratic coefficient) was inflated when the within-subject ***R*** was specified as a UN. The pattern of power rates for fixed effects was also similar to the pattern from linear models.

Addition of one level-2 predictor was examined for the influence on fixed and random effects due to the misspecification of the ***R*** (Murphy & Pituch, 2009). AR(1) and ARMA(1,1) were used to generate the first level ***R***. The autocorrelation had two levels ($\rho = 0.5$ and 0.8), and the moving average parameter had two levels ($\gamma = 0.3$ and -0.3). The specified ***R*** were AR(1), ARMA(1,1), VC (Variance Components: no autocorrelation among different time points within each subject), and UN. The results were agreed with Ferron et al. (2002) and Kwok et al. (2007) regarding the fixed effects with unbiased estimations. The Type I error rates were inflated when the ***R*** was specified as a UN. Under other conditions the Type I error rates were close to the target value. The random effects were bias estimated for all conditions if the true ***R*** was an ARMA(1,1), even when the true models were performed. The overestimations of random effects (τ_{00} and τ_{11}) were larger as the sample size and the number of repeated measures decreased, and the autocorrelation and the average moving parameter increased. τ_{10} was always negative values comparing to the true value which was zero, even when the ***R*** was correctly specified. The variability of the first level ***R*** was in turn underestimated in almost all the conditions. When the true ***R*** was AR(1), the results agreed with Ferron et al. (2002) study.

The influence on the fixed effects due to a more complex ***R*** without ***G***, and a non-normal distribution of the first-level residual were investigated (LeBeau, 2013). The examined models included one first-level time-vary predictor, and one second-level continuous predictor. The residual distribution included three levels (Normal, Chi-squared, and Laplace). The within-subject covariance was generated with five levels (ID, AR(1), MA(1) (Moving Average), MA(2) and ARMA(1,1)). The results showed that the convergence rates were low when the ***R*** was over-specified, especially when the specified covariance structures were an AR(1) and ARMA(1,1). The estimated fixed effects were close to their corresponding true values. The estimates of standard errors of fixed and random effects were biased and agreed with the previous studies (Ferron et al., 2002; Kwok et al., 2007; Murphy & Pituch, 2009), indicating that the biased estimation of τ_{00} was greater than the estimations of other random effects and there were no significant effects due to the non-normal distribution of the first-level residual. In addition, there were no influences on the fixed effects since the ***G*** was null.

2.6 INFLUENCE OF MISSPECIFICATION OF THE BETWEEN-SUBJECT COVARIANCE STRUCTURE

Most of the studies focused on the influence of misspecification of the within-subject covariance structure. Maas & Hox (2004) investigate if there were influences on the estimation of fixed effects when the second-level residuals were not independent and the distribution was not normal based on simulated data. The results showed that there were little or no effect on the estimations of fixed effects. However, the non-normal distribution of the second level residual did have an effect on the estimations of random effects.

2.7 INFLUENCE OF MISSPECIFICATIONS OF BETWEEN-SUBJECT AND WITHIN-SUBJECT COVARIANCE STRUCTURES

Only a few studies examined the influence of misspecifications of the between-subject and within-subject covariance structures simultaneously. Lee (2010) simulated longitudinal data with true AR(1) within-subject $\boldsymbol{R}$ and between-subject covariance $\boldsymbol{G_i} = \begin{bmatrix} \tau_{00} & 0 \\ 0 & \tau_{11} \end{bmatrix}$ without correlation between the intercept and slope to investigate the consequence of misspecifications of covariance structures at within-subject and between-subject levels, and the relationship of misspecifications between within-subject and between-subject covariance structures. Four factors were considered that were the sample size with two levels (30 and 210), the number of repeated measures with two levels (4 and 8), the magnitude of growth rates with three levels (0, 0.05, and 0.16), and the autocorrelation with three levels (0.2, 0.5, and 0.8). The model was defined as two level hierarchical linear growth models. In the study, three different combinations of misspecifications of the within-subject and between-subject covariances were investigated including influences of over-specified on the between-subject covariances and under-specified on the within-subject covariances (Over-G & Under-R), influences of under-specified on the between-subject covariance and over-specified on the within-subject covariance (Under-G & Over-R), and influences of general specified on the between-subject and the within-subject covariance (General-G & General-R).

For Over-G & Under-R, HLMs were fitted by the between-subject covariance $\boldsymbol{G_i} = \begin{bmatrix} \tau_{00} & \tau_{01} \\ \tau_{10} & \tau_{11} \end{bmatrix}$ and ID as the within-subject covariance. For Under-G & Over-R, HLMs were fitted by the between-subject covariance $\boldsymbol{G_i} = \begin{bmatrix} \tau_{00} & 0 \\ 0 & 0 \end{bmatrix}$ and an ARMA(1,1) as the within-subject covariance. For General-G & General-R, HLMs were fitted by the between-subject covariance $\boldsymbol{G_i} = \begin{bmatrix} \sigma_1^2 & \sigma_2^2 \\ \sigma_2^2 & \sigma_1^2 \end{bmatrix}$ and a TOEP(2) as the within-subject covariance.

The convergence rate was 100% for correct models, for Over-G & Under-R, and for generally misspecified $\boldsymbol{G}$ & $\boldsymbol{R}$, while the convergence rate for Under-G & Over-R was 99.97%. The models were not converged under the combinations of the small sample size, the small number of repeated measures, and the low autocorrelation.

The simple bias and relative bias of the initial status (β_{00}) were close to zero for all conditions. The mean relative biases of the growth rate (β_{10}) were close to zero for all conditions as well. The smallest relative bias was observed for Under-G & Over-R, and then for general misspecified $\boldsymbol{G}$ & $\boldsymbol{R}$, and largest bias was for Over-G & Under-R. The standard errors of fixed effects were influenced by the misspecification of covariance structures. The relative bias of standard errors of the initial status and growth rate were close to zero for the correct models. The relative bias of standard errors of the growth rate was underestimated for Under-G & Over-R, overestimated for Over-G & Under-R and general misspecified $\boldsymbol{G}$ & $\boldsymbol{R}$, especially with a larger number of repeated measures and high autocorrelation. The relative bias of standard errors of the initial status was overestimated for Under-G & Over-R or Over-G & Under-R as the number of repeated measures and autocorrelation increased, while it was underestimated for general-misspecified $\boldsymbol{G}$ & $\boldsymbol{R}$. The results were similar to Ferron et al. (2002) and Kwok et al. (2007) studies that the overestimates of the $\boldsymbol{G}$ matrix in the between-subject level occurred because of the under-specified of $\boldsymbol{R}$, in turn led to the underestimation in the variability of the within-subject level.

The Type I error rates for the growth rate were close to the target value ($\alpha = 0.05$) for the true models and Over-G & Under-R, while the rates were inflated for Under-G & Over-R.

General misspecification of ***G*** & ***R*** had lower Type I error rates than true models. The statistical power of parameters was influenced by the misspecification of covariances. For the initial status, Under-G & Over-R had the lowest power, while general misspecification ***G*** & ***R*** had the highest power. The power rates for Under-G & Over-R were decreased as the sample size decreased and the number of repeated measures increased. However, for general misspecification ***G*** & ***R***, the power rates increased as the sample size and the number of repeated measures increased. For the growth rate, the statistical power was estimated in a completely different direction. The power rates were higher for Under-G & Over-R, while they were lower for general misspecification ***G*** & ***R***.

2.8 SUMMARY OF THE LITERATURE REVIEW

This section provides the summary about the influence of misspecifications of the within-subject and between-subject covariances on fixed and random effects in previous studies, about the limitations in previous simulation studies, and about applied longitudinal studies.

2.8.1 Summary of the influence of misspecifications of covariances

The influences on estimates of fixed and random effects due to the misspecification of within-subject covariance structure were investigated in previous studies (Ferron et al., 2002; Kwok et al., 2007). The estimates of fixed effects were not influenced and unbiased for under-specification, over-specification, and general misspecification of the within-subject covariance structures comparing to the correct linear models, which are indicated in Table 4. The standard errors of fixed effects were influenced and biased due to the misspecification of the ***R*** matrix. Under-specification and general misspecification of the within-subject covariance led to larger standard errors of fixed effects. Over-specification of the ***R*** did not impact the estimates of standard errors of fixed effects comparing to the correct models. However, standard errors of fixed effects were underestimated when the ***R*** was specified as a UN and ***G*** was null. The Type I errors were not influenced by the specification of the ***R*** except when the ***R*** was specified as a UN and the ***G*** was null. In this condition, the Type I error rates were inflated comparing to the correct models. The power rate for the initial status (β_{00}) was lower when the ***R*** was under-specified or generally misspecified. The power rate for the growth rate (β_{10}) was not influenced by the misspecification of the ***R*** matrix.

Table 4. Influences of misspecification in Previous Simulation Studies

Misspecification of covariance structures		Fixed effects	Standard error of fixed effects		Random effects	
Within-subject	Between-subject		Intercept	Linear growth rate	First-level	Second-level
Unstructured	Null	Unbiased	Underestimates	Underestimates	–	–
Over-specification	Unstructured	Unbiased	Underestimates Similar to correct model	Underestimates Similar to correct model	Overestimates	Overestimates
Under-specification	Unstructured	Unbiased	Overestimates	Overestimates	Overestimates	Overestimates
General specification	Unstructured	Unbiased	Overestimates	Overestimates	Overestimates	Overestimates
Over-specification	Under-specification	Unbiased	Overestimates	Underestimates	–	–
Under-specification	Over-specification	Unbiased	Overestimates Similar to correct model	Overestimates Similar to correct model	–	–
General specification	General specification	Unbiased	Underestimates	Overestimates	–	–

In examining the influence of the fixed effects due to the misspecification of the within-subject and between-subject covariance simultaneously (Lee, 2010), the estimations of fixed effects were unbiased at all conditions. The standard errors of the initial status (β_{00}) were overestimated and the standard errors of the growth rate (β_{10}) were underestimated at Under-G & Over-R. In addition, the power rates for testing the initial status was lower and the Type I error for detecting the growth rate was inflated. However, general misspecification of the within-subject and between-subject covariances influenced the estimations of standard errors of fixed effects in an opposite direction. There were almost no influences on the estimates of standard errors of fixed effects due to Over-G & Under-R compared to the correct models.

2.8.2 Limitation and future research of studies on misspecification of within-subject and between-subject covariance structures

In Ferron (2002) study, the within-subject covariance that generated the data was AR(1) and the selected covariance to fit the models was ID. The analysis was all about the under-misspecification of the $\boldsymbol{R}$. In addition, all coefficients were set to zero that may be questionable for the results about the unbiased estimations of fixed effects. In Kwok et al. (2007) study, more types of misspecifications of the $\boldsymbol{R}$ matrix were considered. However, only two levels hierarchical growth models were considered in the previous studies. The number of predictors in the models and the distribution (normal or non-normal) of the first-level residual also need to be examined. Adding more second-level predictors may explain some variability for the between-subject covariance that may change the pattern of the underestimations or overestimations of random effects.

In Lee (2010) study about the influence of misspecification of covariance structures at both the within-subject and between-subject levels, only three possibilities of the relationships between the within-subject and between-subject covariance structures were investigated. The number considered in the study was much smaller than the number of possibilities listed in Table 3. Therefore, more studies should be conducted to examine the relationship between the misspecifications of ***G*** & ***R*** matrices.

Most of the studies focused on two-level hierarchical linear growth models. This dissertation was to investigate the influence of misspecification of ***G*** & ***R*** matrices on fixed and random effects in hierarchical quadratic growth models.

2.8.3 Literature review of applied studies in hierarchical growth model

A literature review on applied studies using hierarchical growth models was conducted. Using the keyword ‘Longitudinal study’ to search full-text articles between 2011 and 2014 in the database of PsycINFO resulted with a total of thirty-eight applied longitudinal studies in *Developmental Psychology*, *Journal of Behavioral medicine*, *American Journal of Public Health*, etc. (Allor, Mathes, Roberts, Cheatham, & Al Otaiba, 2014; Anumendem et al., 2013; Attout, Noël, & Majerus, 2014; Bielak, Cherbuin, Bunce, & Anstey, 2014; Bookwala, 2014; Brehaut et al., 2011; Browning, Gardner, Maimon, & Brooks-Gunn, 2014; Chen & Jacobson, 2013; Chow, Krahn, & Galambos, 2014; Csizmadia & Ispa, 2014; Diehl et al., 2014; Eisenberg, Hofer, Sulik, & Liew, 2014; Fauth, Gerstorf, Ram, & Malmberg, 2014; Fuhs, Nesbitt, Farran, & Dong, 2014; Geary, 2011; Hayward & Krause, 2013; Kelly & El-Sheikh, 2014; Kuzucu, Bontempo, Hofer, Stallings, & Piccinin, 2014; R. Lee, Zhai, Brooks-Gunn, Han, & Waldfogel, 2014; Liu et al., 2012; Michel, Babik, Sheu, & Campbell, 2014; Nærde, Ogden, Janson, & Zachrisson, 2014;

O'Donnell, Glover, Barker, & O'Connor, 2014; Orth, Robins, Widaman, & Conger, 2014; Pössel, Rudasill, Sawyer, Spence, & Bjerg, 2013; Rawana & Morgan, 2014; Reitz, Motti-Stefanidi, & Asendorpf, 2014; Riggins, 2014; Sargent-Cox, Anstey, & Luszcz, 2014; Solmeyer, McHale, & Crouter, 2014; Tavernier & Willoughby, 2014; Taylor & Mailick, 2014; Titzmann, Silbereisen, & Mesch, 2014; Tucker-Drob, Reynolds, Finkel, & Pedersen, 2014; van Lissa et al., 2014; Vansteenkiste, Soenens, Van Petegem, & Duriez, 2014; Verboom, Sijtsema, Verhulst, Penninx, & Ormel, 2014; Young et al., 2011). Table 5 shows the sample size, the number of waves, the models used, and the ***G*** & ***R*** matrices for reviewed applied studies. It is noted that 26 out of the 38 studies chose hierarchical linear or quadratic growth models to perform the analyses. The number of waves ranges from 2 to 14. Some of the studies provided the ***G*** & ***R*** matrices.

Based on the literature review for the applied studies, hierarchical quadratic growth models are also widely used in addition to hierarchical linear growth models. This dissertation focused on the influence of misspecifications of covariance structures in hierarchical quadratic growth models which have been understudied.

Table 5. Examples of applied Studies Using Hierarchical Growth Model

Author	Sample Size	Waves	Models	***R*** matrix	***G*** matrix
Allor, Mathes, Roberts, Cheatham, & Al Otaiba (2014)	141	4	Linear	ID (6.1 – 210.6)	
Anumendem et al. (2013)	6000	6	Quadratic	AR(1)	
Attout, Noël, & Majerus (2014)	68	3	Piecewise		
Bielak, Cherbuin, Bunce, & Anstey (2014)	7485	3	Linear	ID (5.38)	$\begin{bmatrix} 2.97 & 0 \\ 0 & 0 \end{bmatrix}$
Bookwala (2014)	1704	2	Linear		
Brehaut et al. (2011)	9401	6	Quadratic	ID (15.56)	$\begin{bmatrix} 11.58 & 0 & 0 \\ 0 & 1.86 & 0 \\ 0 & 0 & 0.06 \end{bmatrix}$

Table 5 (continued)

Author	Sample Size	Waves	Models	***R*** matrix	***G*** matrix
Browning, Gardner, Maimon, & Brooks-Gunn (2014)	1227	3	3 level linear		
Chen & Jacobson (2013)	9988	4	Quadratic		
Chow, Krahn, & Galambos (2014)	404	5	Latent growth curve		
Csizmadia & Ispa (2014)	293	5	Linear Quadratic	ID (0.16)	$\begin{bmatrix} 0.33 & 0 \\ 0 & 0.01 \end{bmatrix}$
Diehl et al. (2014)	392	4	Linear	ID (3.67)	$\begin{bmatrix} 5.00 & -0.02 \\ -0.02 & 0.0004 \end{bmatrix}$
Eisenberg, Hofer, Sulik, & Liew (2014)	32	14	Piecewise		
Fauth, Gerstorf, Ram, & Malmberg (2014)	453	6	Quadratic		
Fuhs, Nesbitt, Farran, & Dong (2014)	562	3	SEM		
Geary (2011)	177	6	Quadratic		
Hayward & Krause (2013)	1500	4	Linear	ID (3.97)	$\begin{bmatrix} 4.51 & 0 \\ 0 & 0.03 \end{bmatrix}$
Kelly & El-Sheikh (2014)	176	3	SEM		
Kuzucu, Bontempo, Hofer, Stallings, & Piccinin (2014)	464	8	Quadratic	ID (0.15 – 0.20	$\begin{bmatrix} 0.1602 & -0.08 \\ -0.08 & 0.0058 \end{bmatrix}$
Lee, Zhai, Brooks-Gunn, Han, & Waldfogel (2014)	6950	4	Linear		
Liu et al. (2012)	110	4	Quadratic	CS, AR(1)	
Michel, Babik, Sheu, & Campbell (2014)	328	9	Latent growth Quadratic		
Nærde, Ogden, Janson, & Zachrisson (2014)	1159	8	Quadratic Cubic	ID (1.586)	$\begin{bmatrix} 0.790 & 0.006 \\ 0.006 & 0.019 \end{bmatrix}$
O'Donnell, Glover, Barker, & O'Connor (2014)	7499	6	Quadratic		
Orth, Robins, Widaman, & Conger (2014)	674	2	Latent growth curve		

Table 5 (continued)

Author	Sample Size	Waves	Models	***R*** matrix	***G*** matrix
Pössel, Rudasill, Sawyer, Spence, & Bjerg (2013)	4341	5	Linear		
Rawana & Morgan (2014)	4359	6	Linear Quadratic	ID (40.35)	
Reitz, Motti-Stefanidi, & Asendorpf (2014)	609	3	SEM		
Riggins (2014)	135	3	Linear		
Sargent-Cox, Anstey, & Luszcz (2014)	1507	5	Linear		
Tavernier & Willoughby (2014)	942	3	SEM		
Taylor & Mailick (2014)	161	6	Linear		
Titzmann, Silbereisen, & Mesch (2014)	607	3	Latent growth curve		
Tucker-Drob, Reynolds, Finkel, & Pedersen (2014)	857	5	Latent growth curve		
Solmeyer, McHale, & Crouter (2014)	393	5	Linear Quadratic	ID (0.016)	$\begin{bmatrix} 0.042 & 0 \\ 0 & 0.002 \end{bmatrix}$
van Lissa et al. (2014)	474	4	SEM		
Vansteenkiste, Soenens, Van Petegem, & Duriez (2014)	532	2	Linear and SEM		
Verboom, Sijtsema, Verhulst, Penninx, & Ormel (2014)	2230	3	SEM		
Young et al. (2011)	248	3	Linear Quadratic		

3.0 METHODS

The purpose of this study was to use Monte Carlo study to investigate how the misspecification of the within-subject covariance structure (***R*** matrix) and the between-subject covariance structure (***G*** matrix) impacts the fixed and random effects in two-level hierarchical quadratic growth models. Three main research questions were addressed in this dissertation.

Question 1: If the within-subject covariance structure is simple and the between-subject covariance structure is complex, once the between-subject covariance structure is under-specified, will the complex within-subject covariance structure recover the overall covariance structure? What is the impact on the fixed and random effects?

Question 2: If the within-subject covariance structure is complex and the between-subject covariance structure is simple, once the within-subject covariance structure matrix is under-specified, will the complex between-subject covariance structure recover the overall covariance structure? What is the impact on the fixed and random effects?

Question 3: Does the standardized root mean square residual provide improvement over information criteria methods in searching for the optimal covariance structure using hierarchical quadratic growth models?

Two simulation studies were conducted to examine the impact of misspecifications of covariance structures which answered the first two research questions. The third research question was also addressed by the two simulation studies. The two studies, including data generations, data validations, and analyses, were performed in SAS 9.4. The SAS programs for the two simulations are attached in Appendix A and B.

This chapter presents in five parts: 1) Hierarchical quadratic growth models; 2) Simulation study 1; 3) Simulation study 2; 4) Evaluation criteria; and 5) Data validation. Each simulation study is organized in the following four sections 1) Design of the study; 2) Data generation; 3) Analysis of the simulated data; and 4) Summary of simulation study

3.1 HIERARCHICAL QUADRATIC GROWTH MODELS

The two simulation studies were based on two-level hierarchical quadratic growth models including one level-2 predictor. The level-1 model was defined in equation 24, which was within-subject level to model individual changes over time (Raudenbush & Bryk, 2002). The level-2 models were defined in equations 25, 26, and 27, which were between-subject level to model differences and predictors of individual changes. The combined equation was represented with equation 28. Equation 29 shows the assumptions about the first-level residual e_{ti} and three second-level random effects r_{0i}, r_{1i}, and r_{2i}.

Equation 24

$$y_{ti} = \pi_{0i} + \pi_{1i} a_{ti} + \pi_{2i} a_{ti}^2 + e_{ti} \ ,$$

Equation 25

$$\pi_{0i} = \beta_{00} + \beta_{01} W_i + r_{0i} \ ,$$

Equation 26

$$\pi_{1i} = \beta_{10} + \beta_{11} W_i + r_{1i},$$

Equation 27

$$\pi_{2i} = \beta_{20} + \beta_{21}W_i + r_{2i},$$

Equation 28

$$y_{ti} = \beta_{00} + \beta_{01}W_i + \beta_{10}a_{ti} + \beta_{11}W_i a_{ti} + \beta_{20}a_{ti}^2 + \beta_{21}W_i a_{ti}^2 + r_{0i} + r_{1i}a_{ti} + r_{2i}a_{ti}^2 + e_{ti},$$

Equation 29

$$e_{ti} \sim N(0, \sigma^2 I), \text{ and } \begin{bmatrix} r_{0i} \\ r_{1i} \\ r_{2i} \end{bmatrix} \sim N\left(\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \tau_{00} & \tau_{01} & \tau_{02} \\ \tau_{10} & \tau_{11} & \tau_{12} \\ \tau_{20} & \tau_{21} & \tau_{22} \end{bmatrix}\right),$$

where y_{ti} is the observed status or repeated measures at time t for individual i, i = 1, …, N subjects, t = 1, …, T occasions or time points, α_{ti} is the time related variable (such as age or year) observed at time t for individual i, W_i is a measured characteristic of an individual's background for individual i, π_{0i} is the initial status, π_{1i} is the instantaneous growth rate of the linear change (linear slope) when α_{ti} is 0, π_{2i} is the acceleration rate of the curvature change (quadratic slope), β_{00} is the overall mean of the initial status, β_{01} is the effect of W on the initial status, β_{10} is the overall mean of the growth rate, β_{11} is the effect of W on the growth rate of the linear change, β_{20} is the overall mean of the acceleration rate, β_{21} is the effect of W on the acceleration rate of the quadratic slope.

The models used in the study included only one level-2 continuous variable as a predictor in the equations for the intercept, the linear and quadratic slopes. Other level-2 covariates were not included as the impact of the misspecification of the between-subject and within-subject covariance structures is similar for all level-2 predictors.

3.2 SIMULATION STUDY 1

Simulation study 1 was designed to answer the first research question. This section provides the study design, the data generation, the analysis of simulated data, and the summary of simulation study 1.

3.2.1 Design of simulation study 1

To answer the first research question, the study was designed to generate the data by using complex between-subject covariance structures and simple within-subject covariance structures. In the analysis, the covariance structures were misspecified, in which the between-subject covariance structure was under-specified and the within-subject covariance structure was over-specified.

Figure 1 shows the research design for simulation study 1. The data generation was based on the complex ***G*** matrix and simple ***R*** matrix. This indicated that the three random effects were present in the data and $\boldsymbol{G}_i = \begin{bmatrix} \tau_{00} & \tau_{01} & \tau_{02} \\ \tau_{10} & \tau_{11} & \tau_{12} \\ \tau_{20} & \tau_{21} & \tau_{22} \end{bmatrix}$ is the i^{th} element on the diagonal of the ***G*** matrix. The simple ***R*** matrix, such as an ID covariance structure, indicated that the repeated measures within an individual over time were independent. When analyzing the data using such a complex ***G*** matrix, due to some reasons, such as the sample size is not big enough, or the random effects are very small to be distinguished by the analysis, or the analysis is too complicated to perform in the real situations, it is more likely that the model will not be converged. In this condition, using a complex ***R*** matrix to analyze individual changes with a simple ***G*** matrix is an alternative approach, and the simulation study 1 examined the influence of such misspecification of covariance structures on the fixed effects and random effects.

True model:

$$G_i = \begin{bmatrix} \tau_{00} & \tau_{01} & \tau_{02} \\ \tau_{10} & \tau_{11} & \tau_{12} \\ \tau_{20} & \tau_{21} & \tau_{22} \end{bmatrix}, R_i = \begin{bmatrix} \sigma^2 & 0 & 0 & 0 & 0 \\ 0 & \sigma^2 & 0 & 0 & 0 \\ 0 & 0 & \sigma^2 & 0 & 0 \\ 0 & 0 & 0 & \sigma^2 & 0 \\ 0 & 0 & 0 & 0 & \sigma^2 \end{bmatrix}$$

(G = complex, R = ID)

Misspecification conditions:

$$G_i = \begin{bmatrix} \tau_{00} & \tau_{01} & 0 \\ \tau_{10} & \tau_{11} & 0 \\ 0 & 0 & 0 \end{bmatrix}, R_i = \begin{bmatrix} \sigma^2+\sigma_1^2 & \sigma_1^2 & \sigma_1^2 & \sigma_1^2 & \sigma_1^2 \\ \sigma_1^2 & \sigma^2+\sigma_1^2 & \sigma_1^2 & \sigma_1^2 & \sigma_1^2 \\ \sigma_1^2 & \sigma_1^2 & \sigma^2+\sigma_1^2 & \sigma_1^2 & \sigma_1^2 \\ \sigma_1^2 & \sigma_1^2 & \sigma_1^2 & \sigma^2+\sigma_1^2 & \sigma_1^2 \\ \sigma_1^2 & \sigma_1^2 & \sigma_1^2 & \sigma_1^2 & \sigma^2+\sigma_1^2 \end{bmatrix}$$

(G = simple, R = CS)

$$R_i = \begin{bmatrix} \sigma_1^2 & \sigma_{21} & \sigma_{31} & \sigma_{41} & \sigma_{51} \\ \sigma_{21} & \sigma_2^2 & \sigma_{32} & \sigma_{42} & \sigma_{52} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 & \sigma_{43} & \sigma_{53} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_4^2 & \sigma_{54} \\ \sigma_{51} & \sigma_{52} & \sigma_{53} & \sigma_{54} & \sigma_5^2 \end{bmatrix}$$

(G = null, R = UN)

$$G_i = \begin{bmatrix} \tau_{00} & \tau_{01} & 0 \\ \tau_{10} & \tau_{11} & 0 \\ 0 & 0 & 0 \end{bmatrix}, R_i = \begin{bmatrix} \sigma^2 & \sigma^2\rho & \sigma^2\rho^2 & \sigma^2\rho^3 & \sigma^2\rho^4 \\ \sigma^2\rho & \sigma^2 & \sigma^2\rho & \sigma^2\rho^2 & \sigma^2\rho^3 \\ \sigma^2\rho^2 & \sigma^2\rho & \sigma^2 & \sigma^2\rho & \sigma^2\rho^2 \\ \sigma^2\rho^3 & \sigma^2\rho^2 & \sigma^2\rho & \sigma^2 & \sigma^2\rho \\ \sigma^2\rho^4 & \sigma^2\rho^3 & \sigma^2\rho^2 & \sigma^2\rho & \sigma^2 \end{bmatrix}$$

(G = simple, R = AR(1))

$$G_i = \begin{bmatrix} \tau_{00} & \tau_{01} & 0 \\ \tau_{10} & \tau_{11} & 0 \\ 0 & 0 & 0 \end{bmatrix}, R_i = \begin{bmatrix} \sigma^2 & \sigma_1 & 0 & 0 & 0 \\ \sigma_1 & \sigma^2 & \sigma_1 & 0 & 0 \\ 0 & \sigma_1 & \sigma^2 & \sigma_1 & 0 \\ 0 & 0 & \sigma_1 & \sigma^2 & \sigma_1 \\ 0 & 0 & 0 & \sigma_1 & \sigma^2 \end{bmatrix}$$

(G = simple, R = TOEP(2))

Figure 1. The design for simulation study 1

3.2.2 Data generation

Based on the design of simulation study 1, data sets were generated based on the complex between-subject (***G***) and simple within-subject (***R***) matrices. First, manipulated simulation design factors were discussed including the sample size, the number of time points, the complete or missing data, the effect size of growth parameters, and effect size of between-subject covariance structures. Secondly, ***X***, ***Z***, ***G***, and ***R*** matrices were defined. Then generation of the variable *W* at the individual level, and residuals in the first-level and second level was presented.

3.2.2.1 Manipulated simulation design factors

As discussed in the literature review, the main factors that impact the selection of covariance structures and estimations of parameters included the sample size, the number of waves, the unbalanced design or missing data. These three factors were considered in the simulation study 1. In addition, the effect sizes of coefficients in growth trajectories and the effect sizes of the ***G*** matrix were also manipulated as the significance tests of fixed and random effects depend on the effect size magnitude.

Sample size. Based on the review of thirty-eight applied longitudinal studies, the sample sizes ranged from 32 to 9988 with the mean of 1963 and median of 585. Table 6 shows the descriptive statistics of the sample size and number of waves in the reviewed thirty-eight applied longitudinal studies.

Table 6. Sample size and number of waves in Applied Studies

Variable	Mean	Minimum	Q1	Median	Q3	Maximum
Sample size	1963	32	293	585	1704	9988
Time point	5	2	3	4	6	14

The sample sizes of 500 and 2000 were chosen for the simulation study since the median and mean of sample sizes are about 500 and 2000 based on the literature review of applied longitudinal studies in the educational and psychological fields. In addition, the sample sizes of 2000 are sufficient for the analyses based on the power study using Optimal Design for Longitudinal and Multilevel research (Raudenbush & Liu, 2001).

Number of time points (*waves*). Table 6 shows that the median of time points was 4 and the range was from 2 to 14 in the reviewed studies. The number of time points 4 and 7 were chosen in the study. Since the model used is Hierarchical growth models with a time-square term, the time variable is centered. The element of the i^{th} individual in ***X*** and ***Z*** matrices for the 4 and 7 waves are displayed as:

Equation 30

$$X(T=4)=\begin{bmatrix}1 & W_i & -1.5 & -1.5W_i & 2.25 & 2.25W_i\\ 1 & W_i & -0.5 & -0.5W_i & 0.25 & 0.25W_i\\ 1 & W_i & 0.5 & 0.5W_i & 0.25 & 0.25W_i\\ 1 & W_i & 1.5 & 1.5W_i & 2.25 & 2.25W_i\end{bmatrix},$$

and $$Z(T=4)=\begin{bmatrix}1 & -1.5 & 2.25\\ 1 & -0.5 & 0.25\\ 1 & 0.5 & 0.25\\ 1 & 1.5 & 2.25\end{bmatrix},$$

Equation 31

$$X(T=7)=\begin{bmatrix}1 & W_i & -1.5 & -1.5W_i & 2.25 & 2.25W_i\\ 1 & W_i & -1 & -W_i & 1 & W_i\\ 1 & W_i & -0.5 & -0.5W_i & 0.25 & 0.25W_i\\ 1 & W_i & 0 & 0 & 0 & 0\\ 1 & W_i & 0.5 & 0.5W_i & 0.25 & 0.25W_i\\ 1 & W_i & 1 & W_i & 1 & W_i\\ 1 & W_i & 1.5 & 1.5W_i & 2.25 & 2.25W_i\end{bmatrix},$$

and $$Z(T=7)=\begin{bmatrix}1 & -1.5 & 2.25\\ 1 & -1 & 1\\ 1 & -0.5 & 0.25\\ 1 & 0 & 0\\ 1 & 0.5 & 0.25\\ 1 & 1 & 1\\ 1 & 1.5 & 2.25\end{bmatrix},$$

where *T* is the number of time points, W_i is a continuous variable at the individual level (second-level).

The first, third, and fifth columns in the ***X*** matrices were associated with the fixed effects in the design that are the intercept, the linear growth slope, and the quadratic growth slope, respectively. The second, fourth, and sixth columns in ***X*** matrices were associated with the effects of the individual level variable W_i on the intercept, linear slope and quadratic slope, respectively. The three columns in the ***Z*** matrices were associated with the random effects in the intercept, linear slope, and quadratic slope, respectively.

Missing data. Based on the literature review, hierarchical growth models can handle the missing data or unbalanced designs well. How the missing data influence the estimations of parameters due to the misspecification of covariance structures was investigated. In applied longitudinal studies, about 10% to 40% observations might be missing over time (Hayward & Krause, 2013; O'Donnell et al., 2014). The simulation study compared the results between complete data and missing data. The missing data in the study had the attrition rate of 10% in the repeated measures since this rate is common in longitudinal studies. Then the datasets had 72.9% and 53.1% observations left at the fourth and seventh visits, respectively.

Effect size of growth parameters. Two levels of standardized effect sizes of growth parameters were considered in the study except the intercept, which was hold as a constant that was equal to 10. The two effect sizes were 0 and 0.5 indicating no effect and large effect sizes (Kwok et al., 2007). Based on the equation 32 (Raudenbush & Liu, 2001), the coefficients to generate the data were determined.

Equation 32

$$\delta = \frac{\beta_{pi}}{\sqrt{\tau_{pp}}},$$

where δ is the standardized effect size, β_{pi} is the growth coefficient for the intercept, the linear slope, the quadratic slope, and effects of W, τ_{pp} is the variance of the random effects associated with the growth coefficients.

*Effect size of the **G** matrix*. Based on previous studies, small and medium sizes of the ***G*** matrices were selected (Ferron et al., 2002; Kwok et al., 2007; Lenzenweger, Johnson, & Willett, 2004; Zvoch & Stevens, 2003). The correlation between random effects was hold as a constant of 0.4. In the study, the small random effect was defined as $\boldsymbol{G}_i = \begin{bmatrix} 0.5 & 0.141 & 0.1 \\ 0.141 & 0.25 & 0.071 \\ 0.1 & 0.071 & 0.125 \end{bmatrix}$, and the medium one was $\boldsymbol{G}_i = \begin{bmatrix} 1 & 0.283 & 0.2 \\ 0.283 & 0.5 & 0.141 \\ 0.2 & 0.141 & 0.25 \end{bmatrix}$.

3.2.2.2 Fixed factors

R** matrix*. In simulation study 1, the ***R matrix was selected as an ID covariance structure indicating the repeated measures within individual were independent.

W_i distribution: The individual level variable was manipulated as a continuous variable with a standard normal distribution to reflect individuals' characteristics.

The first-level residual e_{ti} and three second-level random effects r_{0i}, r_{1i}, and r_{2i} were manipulated with the mean of 0 and variance of the ***R*** matrix and ***G*** matrix, respectively. e_{ti} had a normal distribution, and r_{0i}, r_{1i}, and r_{2i} had multivariate normal distributions.

3.2.3 Analysis of simulated data

The generated data were analyzed in SAS by Proc Mixed using the restricted maximum likelihood estimation (REML) (Littell et al., 2006; Singer, 1998). In the study, the generated data had complex ***G*** and simple ***R*** matrices. For the analysis, the ***G*** matrix was simple that only had random effects of the intercept and the linear slope assuming that the quadratic slope was fixed. A complex ***R*** matrix was selected in the analysis to recover the total covariances, which included CS, AR(1), TOEP(2), and UN covariance structures. When an UN was used, the models were saturated and the ***G*** matrix had to be null, indicating there were no variations on the intercept and the linear slope among individuals. AR(1) was the most commonly used ***R*** matrix in the previous applied studies. CS and TOEP(2) structures were selected as they were examined in previous simulation studies. The ID structure was also performed as the correct models to compare with other models.

3.2.4 Summary of simulation study 1

Simulation study 1 was designed to investigate whether the fixed and random effects were impacted by the misspecification of within-subject and between-subject covariance structures in two-level hierarchical quadratic growth models, in which a complex ***G*** matrix and a simple ***R*** matrix were adopted in the simulated data, and a simple ***G*** and a complex ***R*** were used for the analysis. This was a six factorial design that is summarized in Table 7. There were 160 combinations with 2 levels of the sample size (500 and 2000), by 2 levels of the number of time points (4 and 7), by two levels of missing or balanced data (complete and missing data), by 2 levels of effect sizes of the growth parameters (0, and 0.5), by 2 levels of effect sizes of the ***G*** matrix (small and medium), and by 5 levels of the ***R*** matrix (ID, CS, AR(1), TOEP(2), and UN) in the analyses that included the correct models. Each condition of the design was replicated 500 times. Therefore, a total of 80,000 analyses were performed for simulation study 1.

Table 7. Factorial design in simulation study 1

Factors	Levels	Values
Sample size	2	500, 2000
Number of time point	2	4, 7
Missing data	2	complete, missing (attrition rate = 10%)
Effect size of growth parameters	2	0, 0.5
Effect size of ***G*** matrix	2	small $\begin{bmatrix} 0.5 & 0.141 & 0.1 \\ 0.141 & 0.25 & 0.071 \\ 0.1 & 0.071 & 0.125 \end{bmatrix}$, medium $\begin{bmatrix} 1 & 0.283 & 0.2 \\ 0.283 & 0.5 & 0.141 \\ 0.2 & 0.141 & 0.25 \end{bmatrix}$
R matrix	5	ID, CS, AR(1), TOEP(2), UN

3.3 SIMULATION STUDY 2

Simulation study 2 was designed to answer the second research question. This section provides the study design, the data generation, the analysis of simulated data, and the summary of simulation study 2.

3.3.1 Design of simulation study 2

To answer the second research question, the study was designed to generate the data using a simple between-subject covariance structure and complex within-subject covariance structures. In the analysis, the covariance structures were misspecified, in which the between-subject covariance structure was over-specified and the within-subject was under-specified.

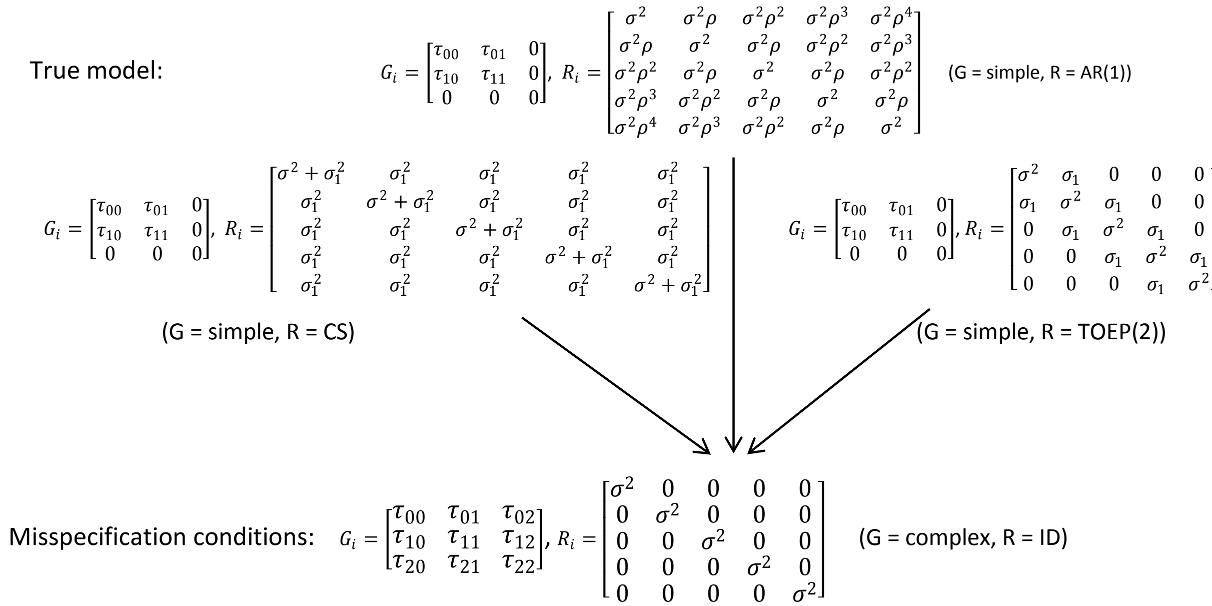

Figure 2. The design for simulation study 2

Figure 2 shows the research design for simulation study 2. The data generation was based on a simple $\boldsymbol{G}$ matrix and complex $\boldsymbol{R}$ matrices. The $\boldsymbol{G}_i$ matrix that is the i^{th} element on the diagonal of the $\boldsymbol{G}$ matrix, is equal to $\begin{bmatrix} \tau_{00} & \tau_{01} & 0 \\ \tau_{10} & \tau_{11} & 0 \\ 0 & 0 & 0 \end{bmatrix}$ indicating that the random effects of the intercept and the linear slope were present, and there was no random effect in the quadratic slope. The complex $\boldsymbol{R}$ matrices indicated that there were some relationships among the repeated measures over time within an individual. In the literature review, I found that for hierarchical growth models, little effort had been taken to assess alternative $\boldsymbol{R}$ matrices. In addition, the most popular software specifically designed for multilevel modeling, HLM7, considers only homogeneous, heterogeneous, and AR(1) structures for the $\boldsymbol{R}$ matrix. The alternative complex $\boldsymbol{R}$ matrices may be present. Simulation study 2 examined the influence of misspecifying such data with a complex $\boldsymbol{G}$ matrix and a simple $\boldsymbol{R}$ matrix. When using the mixed procedure in SAS to analyze the data, the ***G*** matrix is directly assumed as an UN(specified) structure, the most complex one allowed, and the most common one adopted in the applied research.

3.3.2 Data generation

According to the design of simulation study 2, data sets were generated with simple between-subject (***G***) and complex within-subject (***R***) matrices. Firstly, simulation design factors were discussed, including the sample size, the number of time points, the complete or missing data, the effect size of growth parameters, and within-subject covariance structures. Secondly, ***X***, ***Z***, ***G***, and ***R*** matrices were defined. Then the predictor *W* at the second-level, and residuals in the first-level and second-level were discussed.

3.3.2.1 Simulation design factors

The same factors were considered as in simulation study 1.

Sample size. The same sample size of 500 and 2000 were chosen for the simulation study as in simulation study 1.

Number of time points (*waves*). The same numbers of time points of 4 and 7 were chosen as in simulation study 1. The ***X*** matrix was the same as in simulation study 1. The element of the i^{th} individual in the ***X*** and ***Z*** matrices for the 4 and 7 waves are displayed as:

Equation 33

$$\boldsymbol{X}(T=4)=\begin{bmatrix}1 & W_i & -1.5 & -1.5W_i & 2.25 & 2.25W_i\\ 1 & W_i & -0.5 & -0.5W_i & 0.25 & 0.25W_i\\ 1 & W_i & 0.5 & 0.5W_i & 0.25 & 0.25W_i\\ 1 & W_i & 1.5 & 1.5W_i & 2.25 & 2.25W_i\end{bmatrix},$$

$$\text{and} \qquad \boldsymbol{Z}(T=4) = \begin{bmatrix} 1 & -1.5 \\ 1 & -0.5 \\ 1 & 0.5 \\ 1 & 1.5 \end{bmatrix},$$

Equation 34

$$\boldsymbol{X}(T=7) = \begin{bmatrix} 1 & W_i & -1.5 & -1.5W_i & 2.25 & 2.25W_i \\ 1 & W_i & -1 & -W_i & 1 & W_i \\ 1 & W_i & -0.5 & -0.5W_i & 0.25 & 0.25W_i \\ 1 & W_i & 0 & 0 & 0 & 0 \\ 1 & W_i & 0.5 & 0.5W_i & 0.25 & 0.25W_i \\ 1 & W_i & 1 & W_i & 1 & W_i \\ 1 & W_i & 1.5 & 1.5W_i & 2.25 & 2.25W_i \end{bmatrix},$$

$$\text{and} \qquad \boldsymbol{Z}(T=7) = \begin{bmatrix} 1 & -1.5 \\ 1 & -1 \\ 1 & -0.5 \\ 1 & 0 \\ 1 & 0.5 \\ 1 & 1 \\ 1 & 1.5 \end{bmatrix},$$

where *T* is the number of time points, W_i is a continuous variable at the individual level (second-level).

The first, third, and fifth columns in ***X*** matrices were associated with the fixed effects in the design that are the intercept, the linear growth slope, and the quadratic slope, respectively. The second, fourth, and sixth columns in ***X*** matrices were associated with the effects of the individual level variable W_i on the intercept, the linear slope, and the quadratic slope, respectively.

The two columns in ***Z*** matrices were associated with the random effects in the intercept and the linear slope, respectively.

Missing data. The missing data had the same attrition rate of 10% in the repeated measures as in simulation study 1.

Effect size of growth parameters. The two effect sizes were 0 and 0.5 indicating no effect and large effect sizes, which were the same as in the simulation study 1.

***R** matrix structure.* Based on the design of simulation study 2, three covariance structures were used in the data generation including CS, AR(1), TOEP(2) structures.

CS covariance structure for 4 and 7 time points were equal to

$$\begin{bmatrix} 1 & 0.5 & 0.5 & 0.5 \\ 0.5 & 1 & 0.5 & 0.5 \\ 0.5 & 0.5 & 1 & 0.5 \\ 0.5 & 0.5 & 0.5 & 1 \end{bmatrix} \text{ and } \begin{bmatrix} 1 & 0.5 & 0.5 & 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 1 & 0.5 & 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 1 & 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 & 1 & 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 & 0.5 & 1 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 & 0.5 & 0.5 & 1 & 0.5 \\ 0.5 & 0.5 & 0.5 & 0.5 & 0.5 & 0.5 & 1 \end{bmatrix}\text{, respectively.}$$

AR(1) covariance structure for 4 and 7 time points were equal to

$$\begin{bmatrix} 1 & 0.8 & 064 & 0.512 \\ 0.8 & 1 & 0.8 & 0.64 \\ 0.64 & 0.8 & 1 & 0.8 \\ 0.512 & 0.64 & 0.8 & 1 \end{bmatrix} \text{ and}$$

$$\begin{bmatrix} 1 & 0.8 & 064 & 0.512 & 0.4096 & 0.3277 & 0.2621 \\ 0.8 & 1 & 0.8 & 0.64 & 0.512 & 0.4096 & 0.3277 \\ 0.64 & 0.8 & 1 & 0.8 & 0.64 & 0.512 & 0.4096 \\ 0.512 & 0.64 & 0.8 & 1 & 0.8 & 0.64 & 0.512 \\ 0.4096 & 0.512 & 0.64 & 0.8 & 1 & 0.8 & 0.64 \\ 0.3277 & 0.4096 & 0.512 & 0.64 & 0.8 & 1 & 0.8 \\ 0.2621 & 0.3277 & 0.4096 & 0.512 & 0.64 & 0.8 & 1 \end{bmatrix}\text{, respectively, in}$$

which $\rho = 0.8$.

TOEP(2) covariance structure for 4 and 7 time points were equal to

$$\begin{bmatrix} 1 & 0.5 & 0 & 0 \\ 0.5 & 1 & 0.5 & 0 \\ 0 & 0.5 & 1 & 0.5 \\ 0 & 0 & 0.5 & 1 \end{bmatrix} \text{ and } \begin{bmatrix} 1 & 0.5 & 0 & 0 & 0 & 0 & 0 \\ 0.5 & 1 & 0.5 & 0 & 0 & 0 & 0 \\ 0 & 0.5 & 1 & 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 1 & 0.5 & 0 & 0 \\ 0 & 0 & 0 & 0.5 & 1 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0.5 & 1 & 0.5 \\ 0 & 0 & 0 & 0 & 0 & 0.5 & 1 \end{bmatrix}\text{, respectively.}$$

3.3.2.2 Fixed factors

W_i distribution: The individual level variable is manipulated as a normally distributed continuous variable to reflect individuals' characteristics, which is the same as in simulation study 1.

*Effect size of **G** matrix*. The medium size of the ***G*** matrix was selected in simulation study 2, which was $\boldsymbol{G}_i = \begin{bmatrix} 1 & 0.283 & 0 \\ 0.283 & 0.5 & 0 \\ 0 & 0 & 0 \end{bmatrix}$. The correlation between the intercept and the linear growth rate was 0.4.

The first-level residual e_{ti} and two second-level random effects r_{0i} and r_{1i} were manipulated with the mean of 0 and variance of the ***R*** matrix and the ***G*** matrix, respectively. e_{ti} had a multivariate normal distributions and were generated separately for different time points, and r_{0i} and r_{1i} had a bivariate normal distributions.

3.3.3 Analysis of simulated data

The generated data sets were analyzed in SAS by Proc Mixed using the restricted maximum likelihood estimation (REML) as for simulation study 1. In the study, the generated data had a simple ***G*** matrix and a complex ***R*** matrix. For the analysis, a simple ***R*** matrix was selected in the analysis since most of applied longitudinal studies treated the repeated measures as independent measures within an individual, especially for unbalanced designs. A complex ***G*** matrix was selected assuming there were random effects of the intercept, the linear slope, and the quadratic slope to investigate whether the complex ***G*** could recover the total covariances when the ***R*** matrix was under-specified.

3.3.4 Summary of simulation study 2

Simulation study 2 was designed to answer the research question 2 by investigating whether the fixed and random effects were impacted by the misspecification of within-subject and between-subject covariance structures in two level hierarchical quadratic growth models. This was a five way factorial design that is summarized in Table 8. There were 48 combinations with 2 levels of the sample size (500 and 2000), by 2 levels of the number of time points (4 and 7), by two levels of missing or balanced data (complete and missing data), by 2 levels of effect sizes of growth parameters (0, and 0.5), and by 3 levels of the ***R*** matrix (CS, AR(1), and TOEP(2)). Each condition of the design was replicated 500 times. Therefore, totally 24,000 data sets were generated and analyzed for simulation study 2.

Table 8. Factorial design in simulation study 2

Factors	Levels	Values
Sample size	2	500, 2000
Number of time point	2	4, 7
Missing data	2	complete, missing (attrition rate = 10%)
Effect size of growth parameters	2	0, 0.5
R matrix	3	CS, AR(1), TOEP(2)

3.4 EVALUAION CRITERIA

Several evaluation criteria were used in the two simulation studies to evaluate the effects of the misspecification of within-subject and between-subject covariance structures in hierarchical quadratic growth models.

3.4.1 Convergence rate

The convergence rate is calculated by the number of converged models over the total number of replications for each simulation condition.

3.4.2 Standardized Root Mean square Residual (SRMR)

The SRMR (Bentler, 1995) is calculated by equation 35, which is a measure of the averaged difference of the standardized residuals between the observed and model based covariance matrices.

Equation 35

$$\mathrm{SRMR} = \sqrt{\frac{\left\{2\sum_{i=1}^{T}\sum_{j=1}^{i}\left[{(s_{ij}-\hat{\sigma}_{ij})}\big/{(s_{ii}s_{jj})}\right]^2\right\}}{T(T+1)}},$$

where T is the total number of repeated measures (waves), s_{ij} is the element of i^{th} row and j^{th} column in the total covariance matrix of the generated data, and $\hat{\sigma}_{ij}$ is the corresponding element for the model based covariance matrix. Models with the SRMR smaller than .08 are considered as good fit models, indicating the selected covariance structure is optimal.

3.4.3 Relative bias of parameters and relative bias of standard errors

The Relative Bias (RB) of parameters for each generated data set is calculated by:

Equation 36

$$RB = \frac{\widehat{\theta_{ij}} - \theta_{ij}}{\theta_{ij}}, i = 1, 2, \ldots, K \; and \; j = 1, 2, \ldots, 500,$$

where θ_{ij} is the true parameters value of the *i*th parameter ($\theta_i \neq 0$) in *j*th replication, $\widehat{\theta_{ij}}$ is the corresponding estimated parameters, K is the total number of estimated parameters. If RB is positive for a parameter, the parameter is overestimated indicating that the estimated value is greater than the true value. Otherwise, the parameter is underestimated.

The relative bias of parameters and the relative standard error bias (Hoogland & Boomsma, 1998) for the simulation study in each condition over the 500 replications, $B(\hat{\theta}_i)$ and $B(\widehat{se}_{\hat{\theta}_i})$, are calculated by:

Equation 37

$$B(\hat{\theta}_i) = \frac{\overline{\hat{\theta}_i} - \theta_i}{\theta_i}, i = 1, 2, \ldots, K,$$

Equation 38

$$B(\widehat{se}_{\hat{\theta}_i}) = \frac{\overline{\widehat{se}_{\hat{\theta}_i}} - \widehat{se}_{\hat{\theta}_i}}{\widehat{se}_{\hat{\theta}_i}}, i = 1, 2, \ldots, K,$$

where $\overline{\hat{\theta}_i}$ is the mean of estimated the *i*th parameter, θ_i is the true value of the *i*th parameter, $\widehat{se}_{\hat{\theta}_i}$ is the empirical standard error for each coefficient estimated across 500 iterations and $\overline{\widehat{se}_{\hat{\theta}_i}}$ is the average standard error for $\hat{\theta}_i$. It is recommended the cut-off values of .05 and .10 for the relative parameter bias and the relative standard error bias, respectively. Analysis of variance (ANOVA) was conducted to investigate which designed factors contributed to the observed relative bias. Partial eta squared (η_p^2; Cohen, 1973) was reported as a measure of practival significance.

3.4.4 Type I error rate

The Type I error rate is the percentage of the number of performed models with significant effects over the total number of replications in each condition that the true parameter values of fixed or random effects are equal to zero.

3.5 DATA VALIDATION

The validation of data sets with the large sample size (n = 2000), no effect, and the medium effect size of coefficients (δ = 0 and 0.5) for the 7 waves were displayed as examples in the simulation study 1 for which the ***G*** matrix is unstructured and the ***R*** matrix is ID.

To validate the generated datasets, the following methods were used:

First, check the distributions of the first-level and second-level residuals to confirm if the distributions were what the study designed. Table 9 shows the distribution of residuals indicating the first-level and second-level residuals were multivariate normally distributed for seven time points.

Second, check the correlation between random effects and between different time points of first-level residuals to make sure if the correlations were what the study designed.

Table 10 and Table 11 show the correlations between residuals for the seven time points. The correlations show that there were no correlations among the first-level residuals, no correlation between the first-level and second-level residuals as stated in the data generation models.

By running the correct model to compare the parameters with generated parameters, the smaller the difference, the better the generated data were.

Table 12 shows the SRMR for the seven time points. The table shows the best models when the ***R*** matrix were IDs, the covariance structure used in the data generation.

Table 9. Distribution of residuals at the small G matrix with seven waves

Variables		No effect of Growth parameters					Large effect of Growth parameters				
		Mean	SD	Shapiro-Wilk (p values)	Mardia Test		Mean	SD	Shapiro-Wilk (p values)	Mardia Test	
					Skewness	Kurtosis				Skewness	Kurtosis
First level residuals	e0	-0.00	0.97	0.1138	0.2566	0.2527	-0.00	1.00	0.7338	0.3786	0.9307
	e1	0.00	0.99	0.9713			0.00	1.01	0.2039		
	e2	-0.07	0.99	0.0850			-0.01	0.98	0.3932		
	e3	0.00	1.01	0.7092			0.00	1.03	0.7650		
	e4	-0.01	0.99	0.8669			-0.03	0.99	0.8716		
	e5	-0.03	0.99	0.8764			-0.01	1.01	0.2714		
	e6	0.06	0.99	0.4870			0.02	0.99	0.1311		
Second-level residuals	r_{0i}	0.01	0.71	0.4698	0.3985	0.1645	-0.00	0.71	0.5000	0.6124	0.1923
	r_{1i}	0.01	0.51	0.4919			0.01	0.50	0.3403		
	r_{2i}	-0.00	0.36	0.7987			-0.01	0.36	0.0163		

Table 10. Correlation between residuals at small G matrix with no effect of growth parameters and seven waves

Correlation and p values	No effect of Growth parameters									
	First level residuals					Second-level residuals				
	e0	e1	e2	e3	e4	e5	e6	r_{0i}	r_{1i}	r_{2i}
e0	1.00	-0.00 0.85	0.01 0.66	-0.00 0.83	-0.01 0.75	0.01 0.78	-0.03 0.22	0.03 0.24	0.01 0.78	0.02 0.45
e1		1.00	0.04 0.11	-0.03 0.23	0.01 0.55	-0.02 0.43	-0.02 0.38	0.01 0.68	-0.00 0.91	0.01 0.51
e2			1.00	-0.02 0.27	0.03 0.24	-0.05 0.02	-0.02 0.42	-0.00 0.98	-0.02 0.27	0.03 0.13
e3				1.00	-0.01 0.76	-0.05 0.02	0.03 0.18	0.00 0.83	0.00 0.85	-0.01 0.77
e4					1.00	0.02 0.34	-0.01 0.69	-0.03 0.19	-0.01 0.55	-0.02 0.39
e5						1.00	-0.01 0.58	-0.01 0.76	-0.00 0.94	-0.03 0.23
e6							1.00	-0.03 0.12	-0.01 0.57	-0.01 0.72
r_{0i}								1.00	0.44 <.0001	0.36 <.0001
r_{1i}									1.00	0.43 <.0001
r_{2i}										1.00

Table 11. Correlation between residuals at small G matrix with large effect of growth parameters and seven waves

Correlation and p values	No effect of Growth parameters									
	First level residuals							Second-level residuals		
	e0	e1	e2	e3	e4	e5	e6	r_{0i}	r_{1i}	r_{2i}
e0	1.00	-0.02 0.31	-0.03 0.15	0.00 0.96	0.04 0.08	-0.01 0.71	0.03 0.17	-0.01 0.65	0.02 0.38	-0.01 0.66
e1		1.00	0.00 0.85	0.04 0.06	0.01 0.72	-0.01 0.53	-0.01 0.62	-0.02 0.27	0.00 0.98	-0.02 0.27
e2			1.00	0.01 0.56	0.02 0.46	0.01 0.77	0.01 0.67	0.01 0.76	0.03 0.14	0.06 0.008
e3				1.00	-0.07 0.002	0.01 0.59	0.02 0.42	0.00 0.88	0.01 0.62	0.01 0.69
e4					1.00	-0.04 0.11	-0.02 0.38	-0.01 0.77	-0.02 0.37	-0.01 0.53
e5						1.00	0.01 0.63	-0.01 0.72	-0.01 0.70	-0.01 0.58
e6							1.00	-0.01 0.57	0.02 0.30	-0.00 0.88
r_{0i}								1.00	0.38 <.0001	0.37 <.0001
r_{1i}									1.00	0.38 <.0001
r_{2i}										1.00

Table 12. SRMR of correct model at small G matrix with seven waves

Growth parameter	Model fit of ***R*** matrix	SRMR
No effect	Correct model by Correct R = ID	0.053
	Fixed time^2 by R = CS	0.061
	Fixed time^2 by R = AR(1)	0.066
	Fixed time^2 by R = TOEP(2)	0.066
	Fixed time^2 by R = UN	0.086
Large effect	Correct model by Correct R = ID	0.055
	Fixed time^2 by R = CS	0.061
	Fixed time^2 by R = AR(1)	0.067
	Fixed time^2 by R = TOEP(2)	0.066
	Fixed time^2 by R = UN	0.084

4.0 RESULTS

In this chapter, the results from the two simulation studies are presented separately that answer the three research questions. Simulation study 1 aimed to explore whether the under-specification of the between-subject (***G***) covariance structure can be compensated by the over-specification of the within-subject (***R***) covariance structure in hierarchical growth models. Simulation study 2 aimed to explore whether the under-specification of the within-subject (***R***) covariance structure can be compensated by the over-specification of the between-subject (***G***) covariance structure. The SRMR was also compared with information criterion methods in selecting the optimal within-subject covariance structures in both studies.

The results for each simulation study are organized in the following six sections: 1) Convergence rate; 2) Standardized root mean square residual; 3) Fixed effects; 4) Random effects; 5) Type I error rate; and 6) Singularity rate. For the sections 3) and 4), the influences on the fixed effects and their associated standard errors were discussed first, and then the results for random effects were addressed.

4.1 SIMULATION STUDY 1

In simulation study 1, the data generation was based on the complex ***G*** matrix and the simple ***R*** matrix. In the generated ***G*** matrix, the correlation between random effects was 0.4 and there were random effects of the intercept, linear slope, and quadratic slope. The ***R*** matrix was assigned as an ID structure, the simplest covariance structure. In the analysis, the random effects of the intercept and linear slope in the ***G*** matrix were considered and four types of covariance structures as the ***R*** matrix were performed, including CS, AR(1), TOEP(2), and UN covariance structures. To compare the results, the correct models were also performed. The results showed the influences of the over-specification of the ***R*** matrix and the under-specification of the ***G*** matrix on the fixed and random effects. The methods of specification of the optimal covariance structure were compared under the condition of the under-specification of the ***G*** matrix and the over-specification of the ***R*** matrix. In the tables of this section, the correct models referred to the models that were the same as the data generation models. The optimal covariance structure was the ID structure.

4.1.1 Convergence rate

Table 13 shows the convergence rates of the under-specification of the ***G*** matrix and the over-specification of the ***R*** matrix in simulation study 1. The overall convergence rate is 98.88%. A total of 899 cases did not converge out of 80,000 cases including correct models, in which 898 cases did not converge when TOEP(2)s were used as the ***R*** matrix across all the conditions. There were no differences between the converged and unconverged conditions in terms of the number of time points, complete or missing data, the effect sizes of growth parameters, the effect sizes of the ***G*** matrix, and the sample sizes. The convergence rates were 100% when ID, AR(1), and UN structures were used as the ***R*** matrix in the analysis. Only 1 case (0.01%) did not converge when the ***R*** matrix was a CS structure.

Table 13. Convergence rates in simulation study 1

Converged	***R*** matrix used in analysis					Total
	Correct model	CS	AR(1)	TOEP(2)	UN	
Yes	16000 (100.00%)	15999 (99.99%)	16000 (100.00%)	15102 (94.39%)	16000 (100.00%)	79101 (98.88%)
No	0 (0.00%)	1 (0.01%)	0 (0.00%)	898 (5.61%)	0 (0.00%)	899 (1.12%)

4.1.2 Standardized Root Mean square Residual (SRMR)

In stimulation study 1, the correct ***R*** matrix was an ID. The AIC, AICC, BIC, and SRMR were compared on the specification of the optimal ***R*** matrix when the ***R*** matrix was over-specified and the ***G*** matrix was under-specified. There were large discrepancies in magnitude of information criteria among the analysis models. For example, the average of BIC for the correct models was 21026, for the models with CS, AR(1), TOEP(2), and UN as the ***R*** matrix were 21399, 21373, 21654, and 21097, respectively. The average of AIC for the correct models was 20992, for models with CS, AR(1), TOEP(2), and UN as the ***R*** matrix were 21375, 21348, 21630, and 21004, respectively. The average of SRMR for the correct models was 0.07, for models with CS, AR(1), TOEP(2), and UN as the ***R*** matrix were 0.12, 0.13, 0.13, 0.01, respectively. Table 14 shows the results across all the conditions. BIC was the best method in selecting the optimal covariance matrix in the analysis with simulated data. The correct rates in selecting the optimal covariance structures were 94.09%, 94.25%, and 39.92% by AIC, AICC, and SRMR, respectively. SRMR tended to select the most complex covariance structure (UN) at 60.08%. The specification patterns were similar among the number of time points, complete or missing data, effect sizes of growth parameters, effect sizes of the ***G*** matrix, and sample sizes.

Table 14. Selection rates in simulation study 1

Selected models	AIC	AICC	BIC	SRMR
Correct model ***R*** matrix = ID	15055 (94.09%)	15080 (94.25%)	16000 (100%)	6387 (39.92%)
R matrix = UN	945 (5.91%)	920 (5.75%)	0 (0.00%)	9613 (60.08%)

4.1.3 Fixed effects

The fixed effects included the intercept (β_{00}), the effect of *W* on the initial status (β_{01}), the overall mean of the growth rate (β_{10}), the effect of *W* on the growth rate of the linear change (β_{11}), the overall mean of the acceleration rate (β_{20}), and the effect of *W* on the acceleration rate of the quadratic slope (β_{21}) in equation 28, in which *W* is a level-2 continuous variable with a standard normal distribution. The results of the relative bias of fixed effects for each condition and each sample, and their corresponding standard errors are presented in this section when the ***R*** matrix was over-specified and the ***G*** matrix was under-specified.

4.1.3.1 Relative bias of parameter estimates

The relative bias of parameters for each condition was calculated by the equation 37 and presented in Tables 15.

Intercept (β_{00}). The relative biases of the intercept for each condition were very small and close to 0 across all the conditions with the range from -0.0002 to 0.0004.

Overall mean of the growth rate (β_{10}). The relative biases of β_{10} for each condition were small with the range from -0.008 to 0.006.

Overall mean of the acceleration rate (β_{20}). The relative biases of β_{20} for each condition were small with the range from -0.006 to 0.004.

Effect of W on the initial status (β_{01}). The relative biases of β_{01} for each condition were small across all the conditions with the range from -0.009 to 0.001.

Effect of W on the growth rate of the linear change (β_{11}). The relative biases of β_{11} for each condition were very small with the range from -0.007 to 0.003.

Effect of W on the acceleration rate of the quadratic slope (β_{21}). The relative biases of β_{21} for each condition were small with the range from 0.002 to 0.013. The largest relative biases of β_{21} were presented when the **G** matrix was small. However, they were in the acceptable range.

In summary, the relative biases of the fixed effects were very small, which were not impacted by the over-specification of the ***R*** matrix and under-specification of the ***G*** matrix. Therefore, the estimation of the fixed effects was unbiased across all the designed factors under the over-specification of the ***R*** matrix and under-specification of the ***G*** matrix.

Table 15. Relative bias of parameters for each condition in study 1

Complete or missing	**Sample size**	**Time point**	***G* matrix**	***R* matrix**	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Complete	500	4	Small	ID	0.000	-0.006	0.000	-0.003	-0.006	0.010
Complete	500	4	Small	CS	0.000	-0.006	0.000	-0.003	-0.006	0.010
Complete	500	4	Small	AR(1)	0.000	-0.006	0.000	-0.003	-0.006	0.010
Complete	500	4	Small	TOEP(2)	0.000	-0.006	0.000	-0.003	-0.006	0.010
Complete	500	4	Small	UN	0.000	-0.005	0.000	-0.003	-0.006	0.009
Complete	500	4	Medium	ID	0.000	0.003	0.002	-0.003	-0.004	0.009
Complete	500	4	Medium	CS	0.000	0.003	0.002	-0.003	-0.004	0.009
Complete	500	4	Medium	AR(1)	0.000	0.003	0.002	-0.003	-0.004	0.009
Complete	500	4	Medium	TOEP(2)	-0.000	0.004	0.002	-0.004	-0.006	0.007
Complete	500	4	Medium	UN	0.000	0.003	0.001	-0.003	-0.004	0.009
Complete	500	7	Small	ID	0.000	-0.003	0.002	-0.005	-0.001	0.012
Complete	500	7	Small	CS	0.000	-0.003	0.002	-0.005	-0.001	0.012
Complete	500	7	Small	AR(1)	0.000	-0.003	0.002	-0.005	-0.002	0.013
Complete	500	7	Small	TOEP(2)	0.000	-0.003	0.002	-0.005	-0.002	0.013
Complete	500	7	Small	UN	0.000	-0.002	0.002	-0.004	-0.001	0.013
Complete	500	7	Medium	ID	0.000	0.002	0.001	0.001	-0.002	0.004
Complete	500	7	Medium	CS	0.000	0.002	0.001	0.001	-0.002	0.004
Complete	500	7	Medium	AR(1)	0.000	0.003	0.001	0.000	-0.003	0.004
Complete	500	7	Medium	TOEP(2)	0.000	0.003	0.001	0.000	-0.002	0.004
Complete	500	7	Medium	UN	0.000	0.002	0.001	0.000	-0.002	0.004

Table 15 (continued)

Complete or missing	**Sample size**	**Time point**	***G* matrix**	***R* matrix**	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Complete	2000	4	Small	ID	-0.000	0.003	-0.003	0.000	-0.004	0.009
Complete	2000	4	Small	CS	-0.000	0.003	-0.003	0.000	-0.004	0.009
Complete	2000	4	Small	AR(1)	-0.000	0.003	-0.003	0.000	-0.004	0.009
Complete	2000	4	Small	TOEP(2)	-0.000	0.003	-0.003	0.000	-0.004	0.009
Complete	2000	4	Small	UN	-0.000	0.003	-0.003	-0.000	-0.004	0.009
Complete	2000	4	Medium	ID	-0.000	0.000	-0.004	-0.004	-0.003	0.005
Complete	2000	4	Medium	CS	-0.000	0.000	-0.004	-0.004	-0.003	0.005
Complete	2000	4	Medium	AR(1)	-0.000	0.000	-0.004	-0.004	-0.003	0.005
Complete	2000	4	Medium	TOEP(2)	-0.000	0.000	-0.004	-0.004	-0.003	0.005
Complete	2000	4	Medium	UN	-0.000	0.000	-0.004	-0.004	-0.003	0.005
Complete	2000	7	Small	ID	0.000	0.003	-0.006	0.000	0.000	0.011
Complete	2000	7	Small	CS	0.000	0.003	-0.006	0.000	0.000	0.011
Complete	2000	7	Small	AR(1)	0.000	0.003	-0.006	0.000	0.000	0.011
Complete	2000	7	Small	TOEP(2)	0.000	0.003	-0.006	0.000	0.000	0.011
Complete	2000	7	Small	UN	0.000	0.003	-0.006	0.000	0.001	0.011
Complete	2000	7	Medium	ID	-0.000	0.001	-0.002	-0.002	-0.003	0.002
Complete	2000	7	Medium	CS	-0.000	0.001	-0.002	-0.002	-0.003	0.002
Complete	2000	7	Medium	AR(1)	-0.000	0.001	-0.002	-0.003	-0.003	0.002
Complete	2000	7	Medium	TOEP(2)	-0.000	0.001	-0.002	-0.002	-0.003	0.002
Complete	2000	7	Medium	UN	-0.000	0.001	-0.002	-0.002	-0.003	0.002

Table 15 (continued)

Complete or missing	**Sample size**	**Time point**	***G* matrix**	***R* matrix**	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Missing	500	4	Small	ID	0.000	-0.007	-0.004	-0.000	-0.004	0.009
Missing	500	4	Small	CS	0.000	-0.007	-0.005	-0.001	-0.005	0.008
Missing	500	4	Small	AR(1)	0.000	-0.007	-0.005	-0.001	-0.005	0.008
Missing	500	4	Small	TOEP(2)	0.000	-0.006	-0.005	-0.001	-0.004	0.008
Missing	500	4	Small	UN	0.000	-0.006	-0.004	-0.000	-0.004	0.009
Missing	500	4	Medium	ID	-0.000	0.004	0.004	-0.003	-0.007	0.006
Missing	500	4	Medium	CS	0.000	0.005	0.004	-0.004	-0.006	0.007
Missing	500	4	Medium	AR(1)	0.000	0.005	0.004	-0.004	-0.006	0.007
Missing	500	4	Medium	TOEP(2)	0.000	0.006	0.004	-0.009	-0.004	0.004
Missing	500	4	Medium	UN	-0.000	0.004	0.003	-0.003	-0.007	0.006
Missing	500	7	Small	ID	-0.000	-0.008	0.001	-0.004	-0.005	0.009
Missing	500	7	Small	CS	-0.000	-0.008	0.001	-0.003	-0.004	0.009
Missing	500	7	Small	AR(1)	-0.000	-0.008	0.001	-0.003	-0.005	0.009
Missing	500	7	Small	TOEP(2)	-0.000	-0.008	0.001	-0.004	-0.005	0.009
Missing	500	7	Small	UN	-0.000	-0.007	0.002	-0.003	-0.004	0.010
Missing	500	7	Medium	ID	0.000	0.002	-0.001	-0.002	0.002	0.011
Missing	500	7	Medium	CS	0.000	0.003	0.000	-0.002	0.001	0.010
Missing	500	7	Medium	AR(1)	0.000	0.002	-0.000	-0.002	0.001	0.010
Missing	500	7	Medium	TOEP(2)	0.000	0.002	-0.000	-0.002	0.001	0.010
Missing	500	7	Medium	UN	0.000	0.002	-0.001	-0.002	0.003	0.012

Table 15 (continued)

Complete or missing	**Sample size**	**Time point**	***G* matrix**	***R* matrix**	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Missing	2000	4	Small	ID	-0.000	0.002	-0.005	-0.000	-0.003	0.010
Missing	2000	4	Small	CS	-0.000	0.002	-0.005	-0.001	-0.003	0.010
Missing	2000	4	Small	AR(1)	-0.000	0.002	-0.005	-0.000	-0.003	0.010
Missing	2000	4	Small	TOEP(2)	-0.000	0.002	-0.005	-0.000	-0.003	0.010
Missing	2000	4	Small	UN	-0.000	0.002	-0.005	-0.000	-0.003	0.010
Missing	2000	4	Medium	ID	0.000	0.001	-0.004	-0.003	-0.002	0.005
Missing	2000	4	Medium	CS	0.000	0.002	-0.004	-0.003	-0.002	0.005
Missing	2000	4	Medium	AR(1)	0.000	0.001	-0.004	-0.003	-0.002	0.005
Missing	2000	4	Medium	TOEP(2)	0.000	-0.002	-0.005	-0.005	-0.004	0.004
Missing	2000	4	Medium	UN	0.000	0.001	-0.004	-0.003	-0.002	0.005
Missing	2000	7	Small	ID	-0.000	0.005	-0.002	0.001	0.003	0.013
Missing	2000	7	Small	CS	-0.000	0.005	-0.001	0.001	0.002	0.012
Missing	2000	7	Small	AR(1)	-0.000	0.005	-0.001	0.001	0.002	0.013
Missing	2000	7	Small	TOEP(2)	-0.000	0.005	-0.001	0.001	0.002	0.013
Missing	2000	7	Small	UN	-0.000	0.004	-0.002	0.001	0.003	0.013
Missing	2000	7	Medium	ID	-0.000	0.000	-0.001	-0.003	0.000	0.006
Missing	2000	7	Medium	CS	-0.000	0.001	-0.001	-0.003	-0.000	0.005
Missing	2000	7	Medium	AR(1)	-0.000	0.001	-0.001	-0.003	-0.000	0.006
Missing	2000	7	Medium	TOEP(2)	-0.000	0.001	-0.001	-0.003	-0.000	0.006
Missing	2000	7	Medium	UN	-0.000	0.000	-0.001	-0.003	0.000	0.005

4.1.3.2 Relative bias of standard errors of fixed effects

The relative bias of standard errors of the fixed effects was calculated by equation 38. Table 16 shows the relative bias of standard errors of the fixed effects for each condition. The estimations of standard errors of fixed effects were biased. A series of Mixed ANOVAs were performed to test the effects of simulation factors on the relative bias of standard errors of fixed effects due to the under-specification of the ***G*** matrix and the over-specification of the ***R*** matrix. The mixed ANOVAs tested all the five designed factors and their two-way and three-way interaction effects. The four between-subject factors included the sample size, the number of time points, complete or missing data, and the effect size of the ***G*** matrix. The within-subject factor was the ***R*** matrix used in the analysis. Given the large sample size, the significant tests would not be informative. Only the effects with partial η_p^2 greater than 0.1 were further interpreted. The mixed ANOVA results are presented in Table 17.

Intercept (β_{00}). The relative biases of standard errors of the intercept were greater than 0.1 for most of the conditions in Table 16, except when ID or UN structures were used in the analysis. Using CS, AR(1), and TOEP(2) as the ***R*** matrix in the analysis, the standard errors of the intercept were over-estimated for all the conditions.

Table 16. Relative bias of standard errors of fixed effects for each condition in study 1

Complete or missing data	**Sample size**	**Time point**	***G* matrix**	***R* matrix**	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Complete	500	4	Small	ID	0.001	-0.046	-0.042	0.059	0.056	0.042
Complete	500	4	Small	CS	0.214	-0.046	-0.125	0.284	0.056	-0.048
Complete	500	4	Small	AR(1)	0.214	-0.046	-0.126	0.283	0.055	-0.049
Complete	500	4	Small	TOEP(2)	0.212	-0.046	-0.126	0.282	0.055	-0.049
Complete	500	4	Small	UN	-0.004	-0.047	-0.047	0.055	0.052	0.043
Complete	500	4	Medium	ID	-0.019	-0.039	-0.040	0.055	0.052	0.027
Complete	500	4	Medium	CS	0.262	-0.039	-0.168	0.357	0.052	-0.111
Complete	500	4	Medium	AR(1)	0.286	-0.039	-0.157	0.383	0.051	-0.099
Complete	500	4	Medium	TOEP(2)	0.330	-0.031	-0.132	0.429	0.059	-0.080
Complete	500	4	Medium	UN	-0.020	-0.042	-0.038	0.055	0.048	0.025
Complete	500	7	Small	ID	-0.015	-0.040	-0.006	0.062	0.062	0.041
Complete	500	7	Small	CS	0.174	-0.040	-0.177	0.265	0.062	-0.138
Complete	500	7	Small	AR(1)	0.201	-0.041	-0.136	0.297	0.065	-0.097
Complete	500	7	Small	TOEP(2)	0.197	-0.040	-0.140	0.293	0.065	-0.101
Complete	500	7	Small	UN	-0.019	-0.049	-0.019	0.045	0.053	0.038
Complete	500	7	Medium	ID	-0.025	-0.073	-0.041	0.042	0.036	0.014
Complete	500	7	Medium	CS	0.204	-0.073	-0.290	0.286	0.036	-0.249
Complete	500	7	Medium	AR(1)	0.259	-0.071	-0.220	0.344	0.042	-0.170
Complete	500	7	Medium	TOEP(2)	0.241	-0.072	-0.235	0.325	0.041	-0.187
Complete	500	7	Medium	UN	-0.036	-0.080	-0.049	0.033	0.025	0.005

Table 16 (continued)

Complete or missing data	**Sample size**	**Time point**	***G* matrix**	***R* matrix**	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Complete	2000	4	Small	ID	-0.050	0.018	-0.002	0.006	0.054	0.052
Complete	2000	4	Small	CS	0.156	0.018	-0.088	0.224	0.054	-0.039
Complete	2000	4	Small	AR(1)	0.154	0.017	-0.089	0.222	0.054	-0.040
Complete	2000	4	Small	TOEP(2)	0.153	0.017	-0.090	0.220	0.053	-0.041
Complete	2000	4	Small	UN	-0.050	0.015	-0.001	0.006	0.053	0.051
Complete	2000	4	Medium	ID	-0.032	-0.033	-0.042	0.033	0.067	0.080
Complete	2000	4	Medium	CS	0.247	-0.033	-0.170	0.332	0.067	-0.065
Complete	2000	4	Medium	AR(1)	0.271	-0.034	-0.159	0.357	0.068	-0.052
Complete	2000	4	Medium	TOEP(2)	0.300	-0.039	-0.143	0.379	0.068	-0.026
Complete	2000	4	Medium	UN	-0.033	-0.033	-0.042	0.032	0.067	0.078
Complete	2000	7	Small	ID	-0.043	0.002	0.015	0.032	0.030	0.020
Complete	2000	7	Small	CS	0.141	0.002	-0.161	0.231	0.030	-0.157
Complete	2000	7	Small	AR(1)	0.169	0.002	-0.119	0.259	0.034	-0.114
Complete	2000	7	Small	TOEP(2)	0.165	0.002	-0.123	0.255	0.033	-0.118
Complete	2000	7	Small	UN	-0.047	0.001	0.012	0.035	0.030	0.018
Complete	2000	7	Medium	ID	-0.052	-0.028	-0.048	0.050	0.047	0.044
Complete	2000	7	Medium	CS	0.170	-0.028	-0.297	0.296	0.047	-0.228
Complete	2000	7	Medium	AR(1)	0.225	-0.027	-0.229	0.355	0.045	-0.146
Complete	2000	7	Medium	TOEP(2)	0.207	-0.028	-0.243	0.335	0.045	-0.164
Complete	2000	7	Medium	UN	-0.052	-0.032	-0.051	0.048	0.042	0.039

Table 16 (continued)

Complete or missing data	**Sample size**	**Time point**	***G* matrix**	***R* matrix**	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Missing	500	4	Small	ID	0.005	-0.040	-0.035	0.073	0.031	0.028
Missing	500	4	Small	CS	0.195	-0.070	-0.121	0.280	0.010	-0.068
Missing	500	4	Small	AR(1)	0.184	-0.071	-0.128	0.269	0.010	-0.076
Missing	500	4	Small	TOEP(2)	0.175	-0.070	-0.132	0.254	0.010	-0.084
Missing	500	4	Small	UN	-0.004	-0.040	-0.041	0.066	0.031	0.029
Missing	500	4	Medium	ID	-0.031	-0.021	-0.024	0.082	0.054	0.052
Missing	500	4	Medium	CS	0.216	-0.053	-0.154	0.358	0.012	-0.093
Missing	500	4	Medium	AR(1)	0.221	-0.054	-0.151	0.365	0.011	-0.091
Missing	500	4	Medium	TOEP(2)	0.269	-0.094	-0.136	0.380	0.022	-0.066
Missing	500	4	Medium	UN	-0.033	-0.026	-0.026	0.080	0.049	0.048
Missing	500	7	Small	ID	0.010	-0.053	-0.025	0.065	0.055	0.050
Missing	500	7	Small	CS	0.160	-0.090	-0.163	0.215	-0.003	-0.115
Missing	500	7	Small	AR(1)	0.174	-0.088	-0.146	0.230	-0.001	-0.097
Missing	500	7	Small	TOEP(2)	0.173	-0.088	-0.146	0.229	-0.001	-0.098
Missing	500	7	Small	UN	0.003	-0.066	-0.045	0.056	0.041	0.038
Missing	500	7	Medium	ID	-0.024	-0.068	-0.041	0.054	0.002	0.018
Missing	500	7	Medium	CS	0.155	-0.135	-0.260	0.249	-0.084	-0.214
Missing	500	7	Medium	AR(1)	0.184	-0.131	-0.218	0.285	-0.077	-0.170
Missing	500	7	Medium	TOEP(2)	0.177	-0.131	-0.223	0.278	-0.078	-0.175
Missing	500	7	Medium	UN	-0.031	-0.081	-0.050	0.046	-0.025	-0.010

Table 16 (continued)

Complete or missing data	**Sample size**	**Time point**	***G* matrix**	***R* matrix**	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Missing	2000	4	Small	ID	-0.039	-0.023	0.008	-0.015	0.036	0.055
Missing	2000	4	Small	CS	0.150	-0.043	-0.070	0.175	0.004	-0.042
Missing	2000	4	Small	AR(1)	0.139	-0.044	-0.077	0.163	0.003	-0.050
Missing	2000	4	Small	TOEP(2)	0.126	-0.045	-0.084	0.148	0.002	-0.057
Missing	2000	4	Small	UN	-0.040	-0.025	0.008	-0.017	0.034	0.052
Missing	2000	4	Medium	ID	-0.022	-0.016	-0.027	0.022	0.053	0.059
Missing	2000	4	Medium	CS	0.226	-0.058	-0.163	0.270	0.025	-0.090
Missing	2000	4	Medium	AR(1)	0.231	-0.058	-0.160	0.276	0.025	-0.087
Missing	2000	4	Medium	TOEP(2)	0.280	-0.023	-0.177	0.314	0.022	-0.036
Missing	2000	4	Medium	UN	-0.023	-0.017	-0.029	0.021	0.051	0.056
Missing	2000	7	Small	ID	-0.029	0.026	-0.020	0.015	0.020	0.067
Missing	2000	7	Small	CS	0.110	-0.015	-0.156	0.158	-0.022	-0.092
Missing	2000	7	Small	AR(1)	0.123	-0.015	-0.138	0.172	-0.021	-0.073
Missing	2000	7	Small	TOEP(2)	0.122	-0.015	-0.138	0.171	-0.021	-0.073
Missing	2000	7	Small	UN	-0.030	0.026	-0.023	0.014	0.013	0.067
Missing	2000	7	Medium	ID	-0.041	0.016	-0.035	0.023	0.042	0.062
Missing	2000	7	Medium	CS	0.139	-0.063	-0.257	0.199	-0.035	-0.182
Missing	2000	7	Medium	AR(1)	0.169	-0.060	-0.216	0.229	-0.032	-0.134
Missing	2000	7	Medium	TOEP(2)	0.164	-0.060	-0.221	0.222	-0.033	-0.139
Missing	2000	7	Medium	UN	-0.045	0.012	-0.040	0.019	0.037	0.058

Table 17. ANOVA results for the relative biases of standard errors of fixed effects in study 1

Factors	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
R matrix (R)	**0.989**	**0.887**	**0.985**	**0.988**	**0.876**	**0.984**
Complete or missing data (CM)	**0.152**	**0.131**	0.005	**0.174**	**0.247**	0.011
Sample size (SS)	**0.273**	**0.441**	0.096	**0.254**	0.001	0.096
Number of time point (T)	**0.256**	0.035	**0.516**	0.056	0.089	**0.394**
Effect size of ***G*** matrix (G)	**0.323**	**0.146**	**0.666**	**0.311**	0.005	**0.172**
R*CM	**0.481**	**0.902**	**0.159**	**0.545**	**0.901**	**0.105**
R*SS	0.019	**0.165**	0.053	0.069	**0.110**	0.023
R*T	**0.420**	**0.331**	**0.798**	**0.357**	**0.449**	**0.792**
R*G	**0.708**	**0.347**	**0.717**	**0.688**	**0.210**	**0.652**
CM*SS	0.011	0.011	–	0.061	0.004	0.005
CM*T	–	–	0.005	0.020	0.019	0.052
CM*G	0.034	0.014	0.029	0.001	0.005	–
SS*T	0.001	**0.112**	0.019	0.046	0.001	0.002
SS*G	0.100	0.025	**0.170**	0.025	0.047	0.030
T*G	**0.148**	0.050	**0.165**	0.075	0.035	0.089
R*CM*SS	0.002	**0.249**	0.005	0.014	0.036	0.008
R*CM*T	0.039	**0.410**	**0.183**	0.061	**0.518**	0.095
R*CM*G	0.025	**0.379**	0.035	0.023	**0.249**	0.035
R*SS*T	0.003	**0.279**	0.018	0.002	0.057	0.023
R*SS*G	0.003	**0.152**	0.019	0.002	0.035	0.023
R*T*G	**0.288**	**0.111**	**0.195**	**0.224**	**0.140**	**0.240**
CM*SS*T	0.010	0.055	–	–	0.007	0.024
CM*SS*G	0.013	0.018	–	0.003	0.002	0.025
CM*T*G	–	0.017	0.039	–	0.013	0.007
SS*T*G	0.026	0.027	0.053	–	0.019	0.005

Note: Partial Eta-Square ($\eta_p{}^2$) is reported in the table.

–: indicates that the $\eta_p{}^2$<0.001

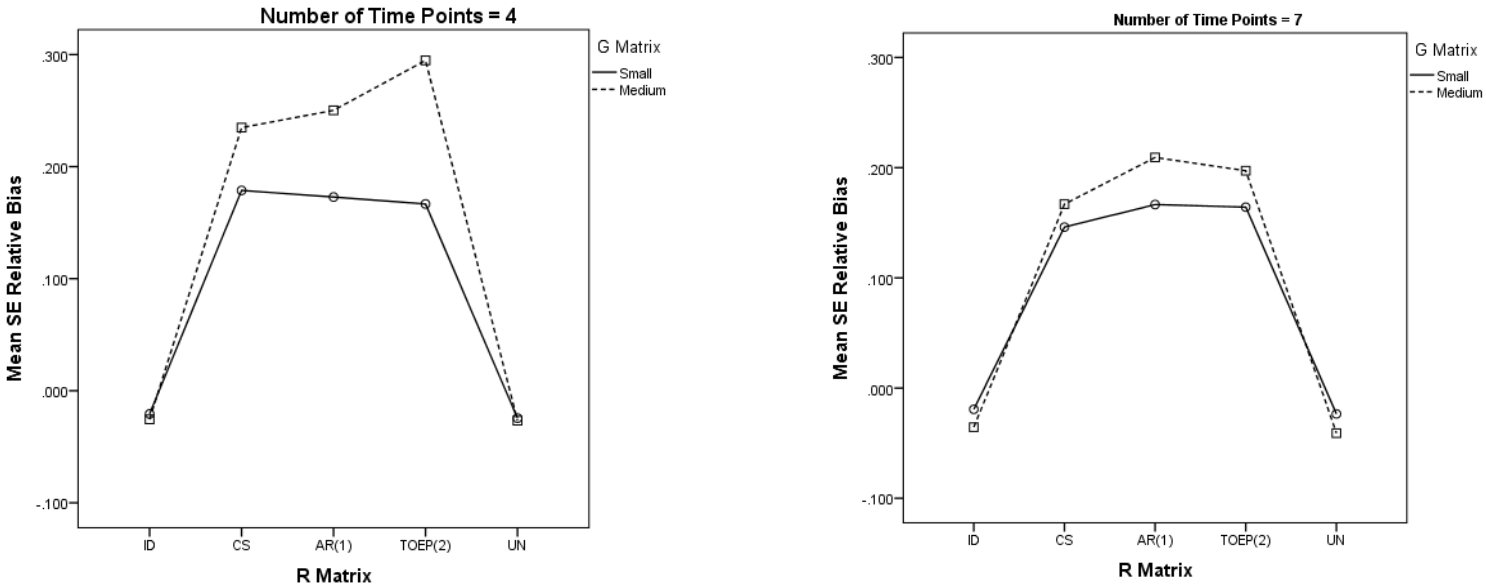

Figure 3. Mean standard error bias of the intercept as a function of the number of time points, ***G*** matrix, and ***R*** matrix in study 1

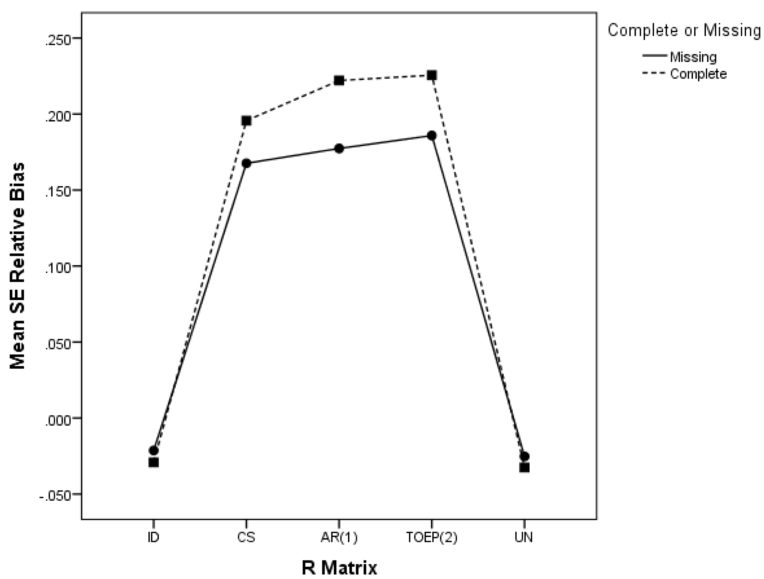

Figure 4. Mean standard error bias of the intercept as a function of the ***R*** matrix and complete or missing data in study 1

According to the ANOVA results in Table 17, the type of the ***R*** matrix used in the analysis had the largest impact on the relative bias of standard errors of the intercept (η_p^2 = 0.989). There were four two-way and one three-way interaction effects whose η_p^2 were greater than 0.1. The three-way interaction effect was among the ***R*** matrix used in the analysis, the ***G*** matrix, and the number of time points (η_p^2 = 0.288). The four two-way interaction effects included the interaction effect between the ***R*** matrix and the complete or missing data (η_p^2 = 0.481), the interaction between the ***R*** matrix and the number of time points (η_p^2 = 0.420), the interaction between the ***R*** matrix and the ***G*** matrix (η_p^2 = 0.708), and the interaction between the number of time points and the ***G*** matrix (η_p^2 = 0.148). Figure 3 illustrated the three-way interaction effect among the ***R*** matrix, the ***G*** matrix, and the number of time points. All conditions with ID or UN as the ***R*** matrix had close to zero bias values, while conditions with the other ***R*** matrices (CS, AR(1), TOEP(2)) had significantly larger biases. For these three ***R*** matrices, conditions with larger ***G*** matrix had larger biases than those with smaller ***G*** matrix, while such difference decreased for more time points. Figure 4 presented the two-way interaction effect between the ***R*** matrix and the complete or missing data and suggested that conditions with missing data had smaller biases than those with complete data for CS, AR(1), and TOEP(2) matrices.

Overall mean of the growth rate (β_{10}). The relative biases of standard errors of β_{10} were relatively smaller than the relative biases of standard errors of the other parameters for most of the conditions. The standard errors of β_{10} were slightly under-estimated for most of the conditions. Among the total 80 conditions, only 3 have biased standard error estimates (>.1) with CS, AR(1), and TOEP(2) structures as ***R*** matrices for missing data, 500 subjects, 7 time points, and the medium size ***G*** matrix.

According to the ANOVA results, six three-way interaction effects were significant in the analysis, including the interaction effect among the ***R*** matrix, complete or missing data, and the sample size (η_p^2 = 0.249), the interaction effect among the ***R*** matrix, complete or missing data, and the number of time points (η_p^2 = 0.410), the interaction effect among the ***R*** matrix, complete or missing data, and the ***G*** matrix (η_p^2 = 0.379), the interaction effect among the ***R*** matrix, the sample size, and the number of time points (η_p^2 = 0.279), the interaction effect among the ***R*** matrix, the sample size, and the ***G*** matrix (η_p^2 = 0.152), and the interaction effect among the ***R*** matrix, the number of time points, and the ***G*** matrix (η_p^2 = 0.111). There were also five two-way interaction effects including the interaction effect between the ***R*** matrix and complete or missing data (η_p^2 = 0.902), the interaction effect between the ***R*** matrix and the sample size (η_p^2 = 0.165), the interaction effect between the ***R*** matrix and the number of time points (η_p^2 = 0.331), the interaction effect between the ***R*** matrix and the ***G*** matrix (η_p^2 = 0.347), and the interaction effect between the sample size and the number of time points (η_p^2 = 0.112). The ***R*** matrix used in the analysis also had large effects (η_p^2 = 0.887). Figures 5, 6, 7, 8, 9, and 10 showed the three-way interaction effect patterns. The estimations of standard errors of the growth rate for the complete data were unbiased across all the conditions and were close to the correct model. For the missing data conditions, CS, AR(1) and TOEP(2) matrices had larger biases. For these three R matrices, the biases were larger for the medium G matrix (vs small), 7 time points (vs 4) and 500 subjects (vs 2000).

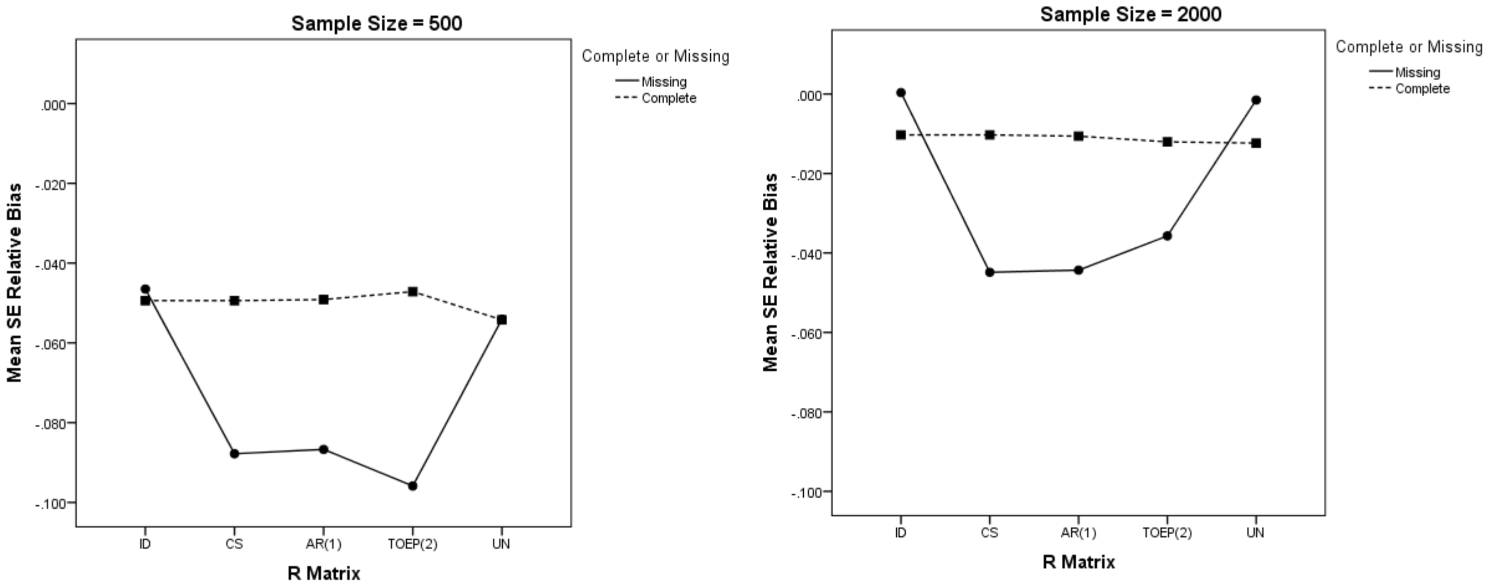

Figure 5. Mean standard error bias of the growth rate as a function of the sample size, complete or missing data, and ***R*** matrix in study 1

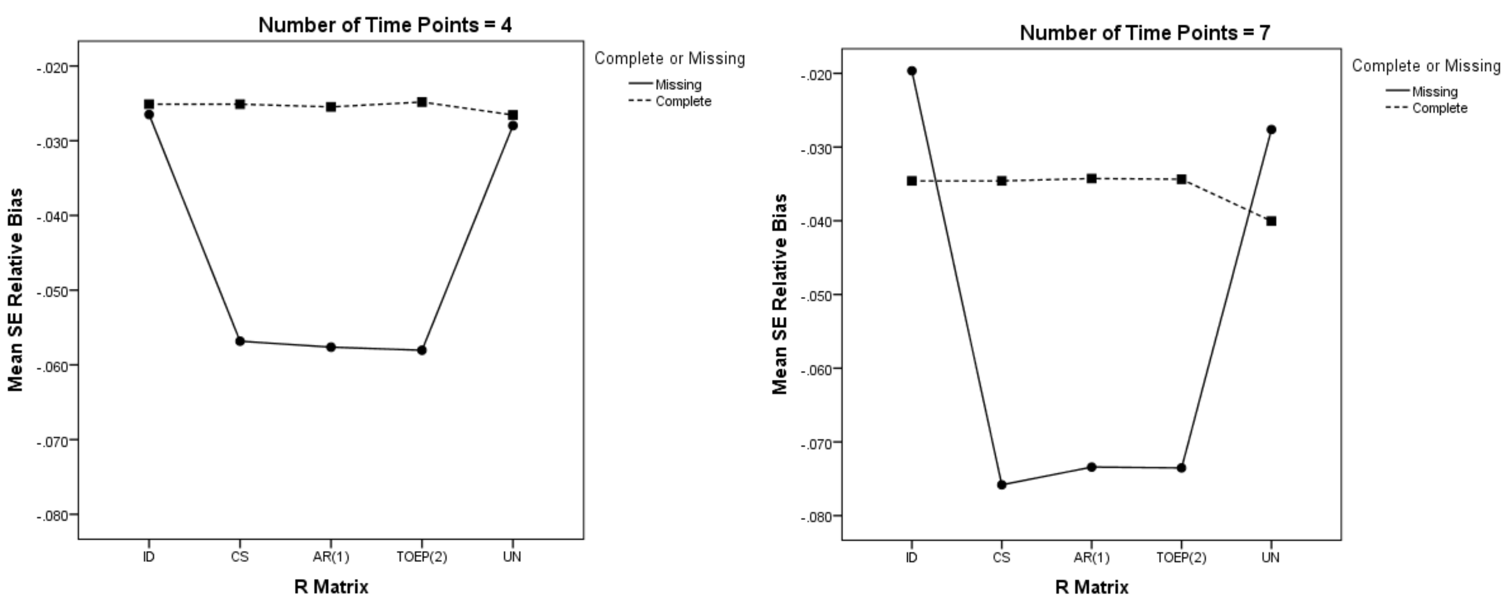

Figure 6. Mean standard error bias of the growth rate as a function of the number of time points, complete or missing data, and ***R*** matrix in study 1

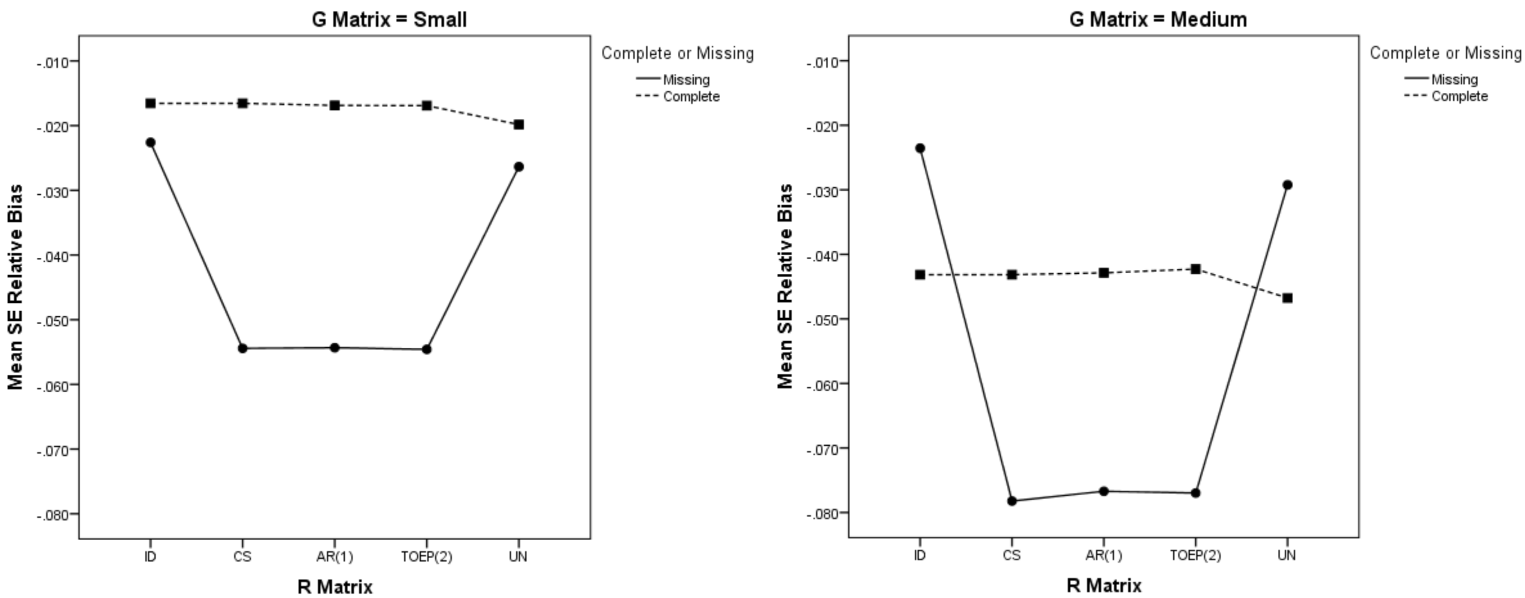

Figure 7. Mean standard error bias of the growth rate as a function of the ***G*** matrix, complete or missing data, and ***R*** matrix in study 1

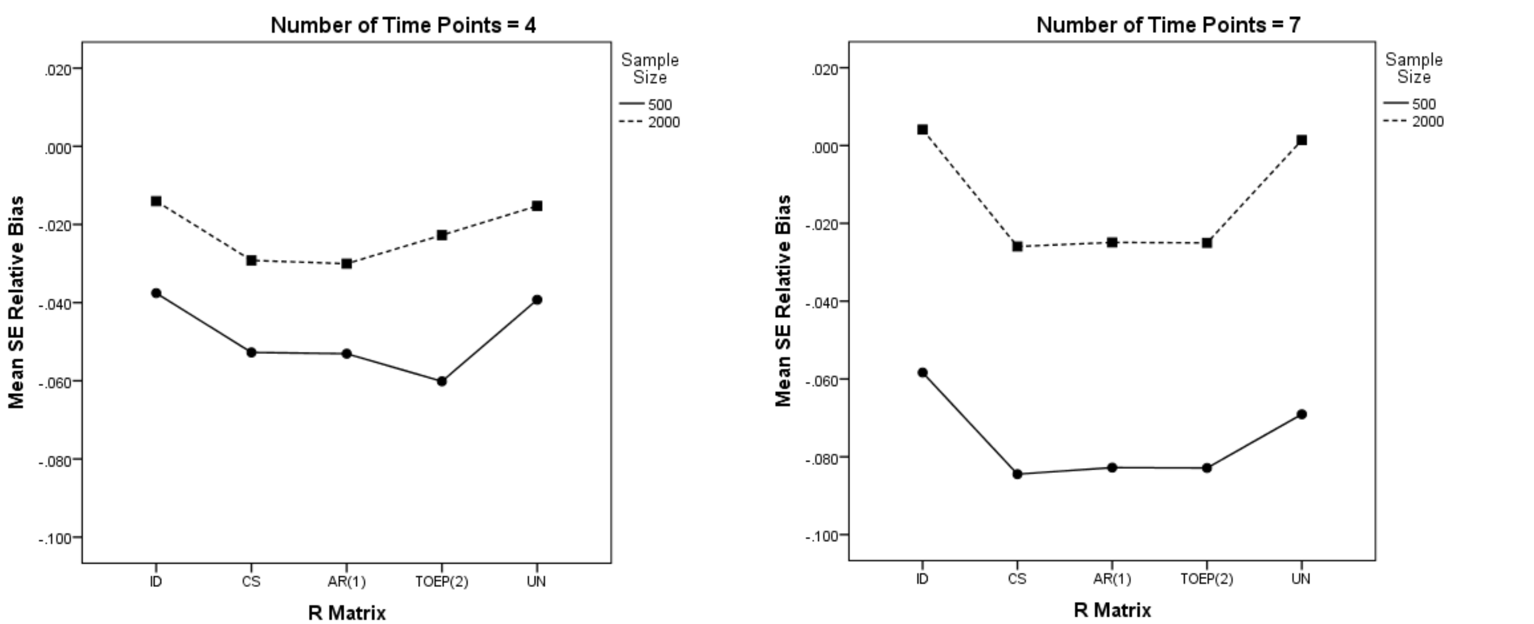

Figure 8. Mean standard error bias of the growth rate as a function of the number of time points, sample size, and *R* matrix in study 1

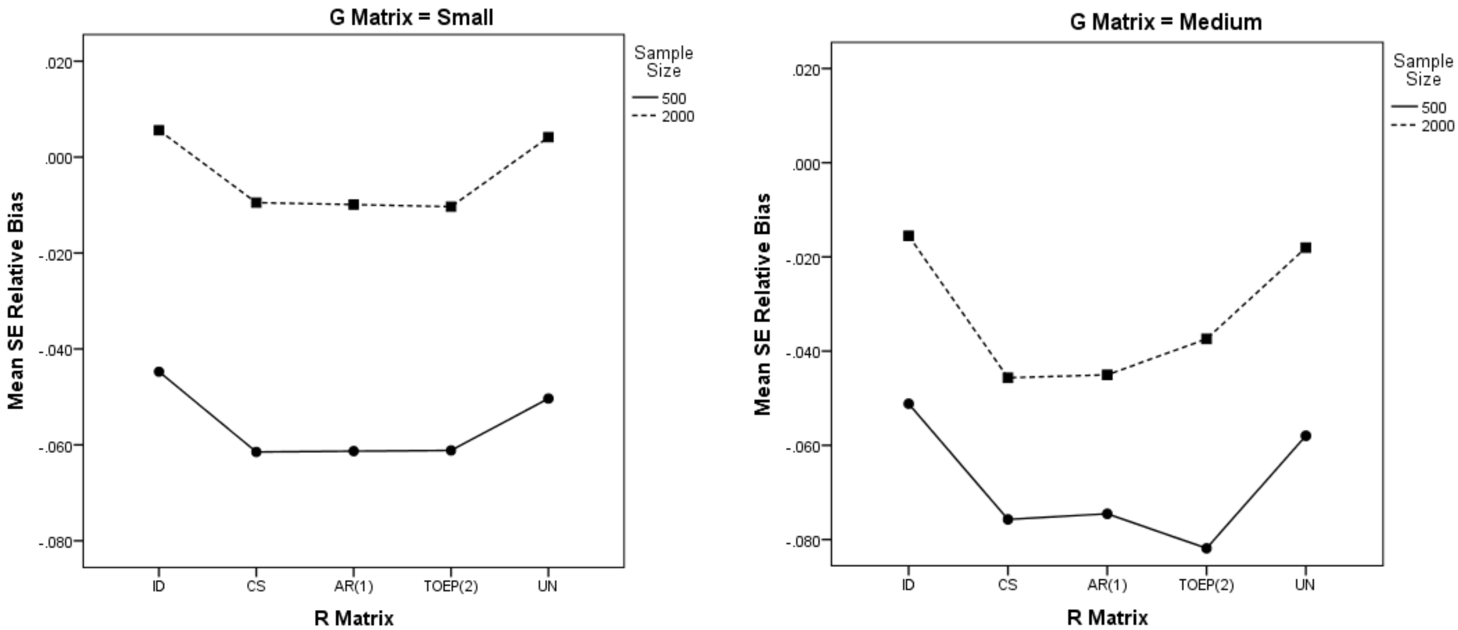

Figure 9. Mean standard error bias of the growth rate as a function of the ***G*** matrix, sample size, and ***R*** matrix in study 1

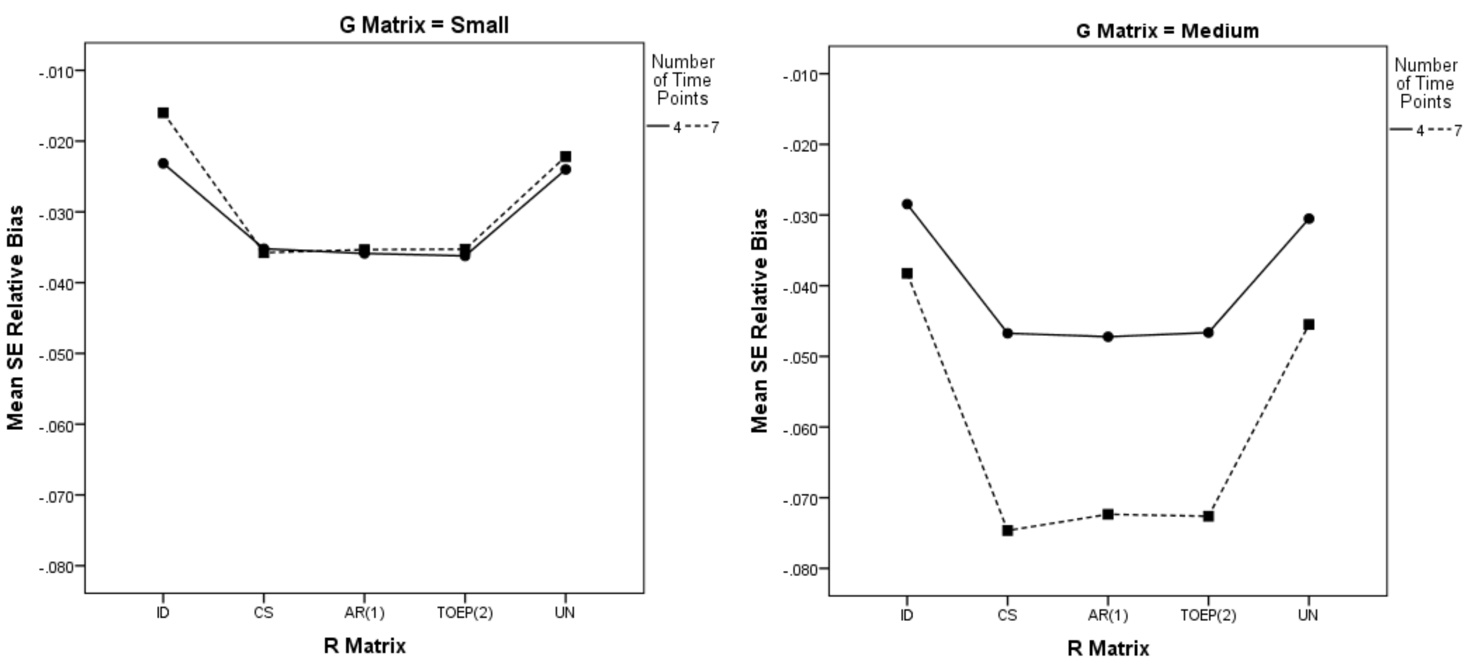

Figure 10. Mean standard error bias of the growth rate as a function of the ***G*** matrix, number of time points, and ***R*** matrix in study 1

Overall mean of the acceleration rate (β_{20}). The estimations of the standard errors of β_{20} were under-estimated for all the conditions.

According to the ANOVA results, there were two three-way and five two-way interaction effects. The three-way interaction effects included the interaction effect among the ***R*** matrix, complete or missing data, and the number of time points (η_p^2 = 0.183), and the interaction effect among the ***R*** matrix, the number of time points, and the ***G*** matrix (η_p^2 = 0.195). The five two-way interaction effects included the interaction between the ***R*** matrix and complete or missing data (η_p^2 = 0.159), the interaction between the ***R*** matrix and the number of time points (η_p^2 = 0.798), the interaction effect between the ***R*** matrix and the ***G*** matrix (η_p^2 = 0.717), and the interaction effect between the sample size and the ***G*** matrix (η_p^2 = 0.170), and the interaction effect between the number of time points and the ***G*** matrix (η_p^2 = 0.165). The ***R*** matrix, the effect size of ***G*** matrix, and the number of time points had large effects (η_p^2 = 0.985, 0.666, and 0.516). Figures 11 and 12 showed the three-way interaction effect patterns. All conditions with ID or UN as the ***R*** matrix had close to zero bias values, while conditions with the other ***R*** matrices (CS, AR(1), TOEP(2)) had significantly larger biases. For these three ***R*** matrices, conditions with the larger ***G*** matrix had larger biases than those with smaller ***G*** matrix, while such differences increased for more time points. The biases were similar for complete or missing data. Figures 13 presented the two-way interaction effect between the sample size and the ***G*** matrix. The larger the ***G*** matrix, the higher the relative biases were. For the larger ***G*** matrix, the relative biases were smaller for the smaller sample size, while the relative biases were larger for the smaller sample size when the ***G*** matrix was small.

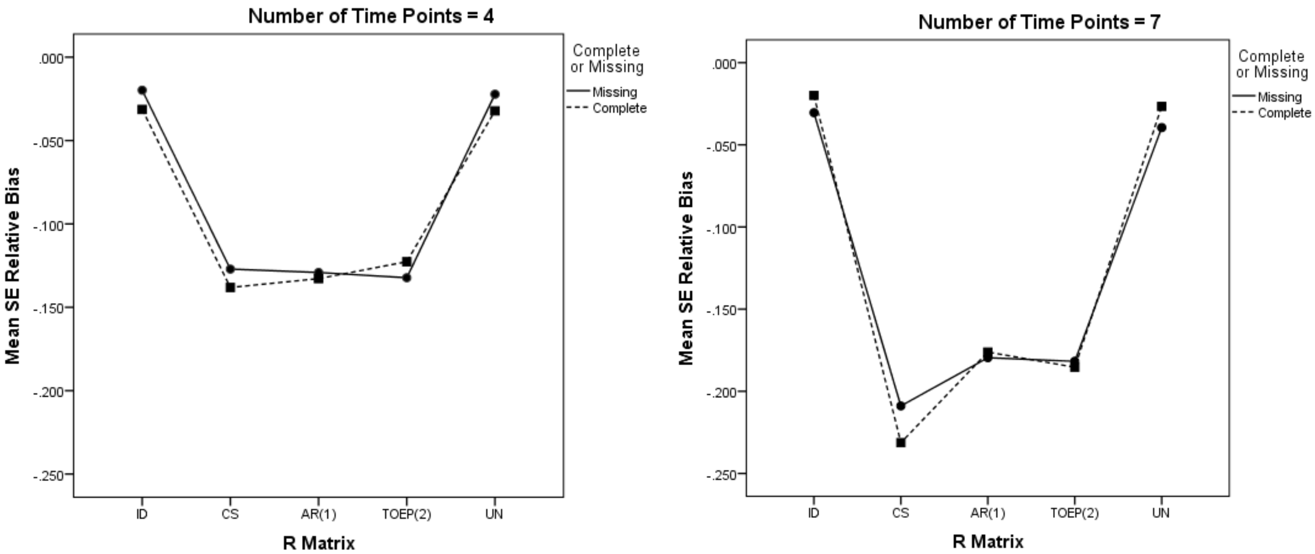

Figure 11. Mean standard error bias of the acceleration rate as a function of the number of time points, complete or missing data, and ***R*** matrix in study 1

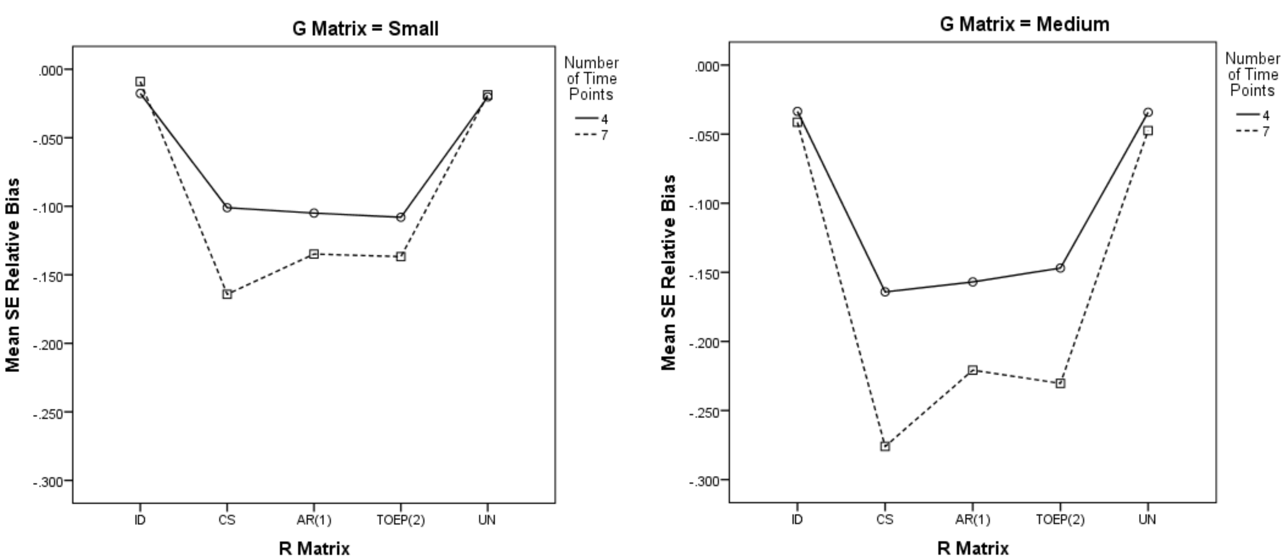

Figure 12. Mean standard error bias of the acceleration rate as a function of the ***G*** matrix, number of time points, and ***R*** matrix in study 1

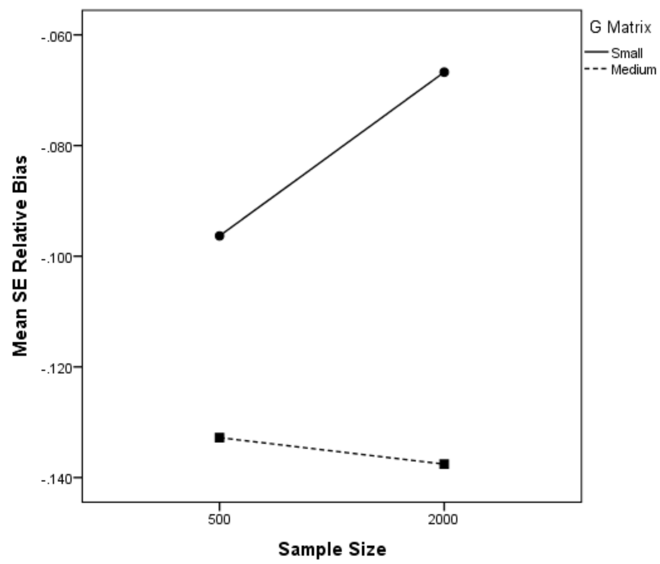

Figure 13. Mean standard error bias of the acceleration rate as a function of the ***G*** matrix and sample size in study 1

Effect of W on the initial status (β_{01}). The relative biases of standard errors of β_{01} were overestimated for all the conditions (see Table 16).

According to the ANOVA results in Table 17, one three-way interaction effect was present among the ***R*** matrix, the number of time points, and ***G*** matrix (η_p^2 = 0.224). Three two-way interaction effects were also substantial, including the interaction effect between the ***R*** matrix and complete or missing data (η_p^2 = 0.545), the interaction between the ***R*** matrix and the number of time points (η_p^2 = 0.357), and the interaction effect between the ***R*** matrix and ***G*** matrix (η_p^2 = 0.688). The ***R*** matrix was the largest effect (η_p^2 = 0.988). Figure 14 showed the three-way interaction effect pattern. All conditions with ID or UN as the ***R*** matrix had close to zero bias values, while conditions with the other ***R*** matrices (CS, AR(1), TOEP(2)) had significantly larger biases. For these three ***R*** matrices, conditions with larger ***G*** matrix had larger biases than those with smaller ***G*** matrix, while such differences decreased for more time points. Figures 15 presented the two-way interaction effect between the ***R*** matrix and complete or missing data and suggested that conditions with complete data had larger biases than those with missing data.

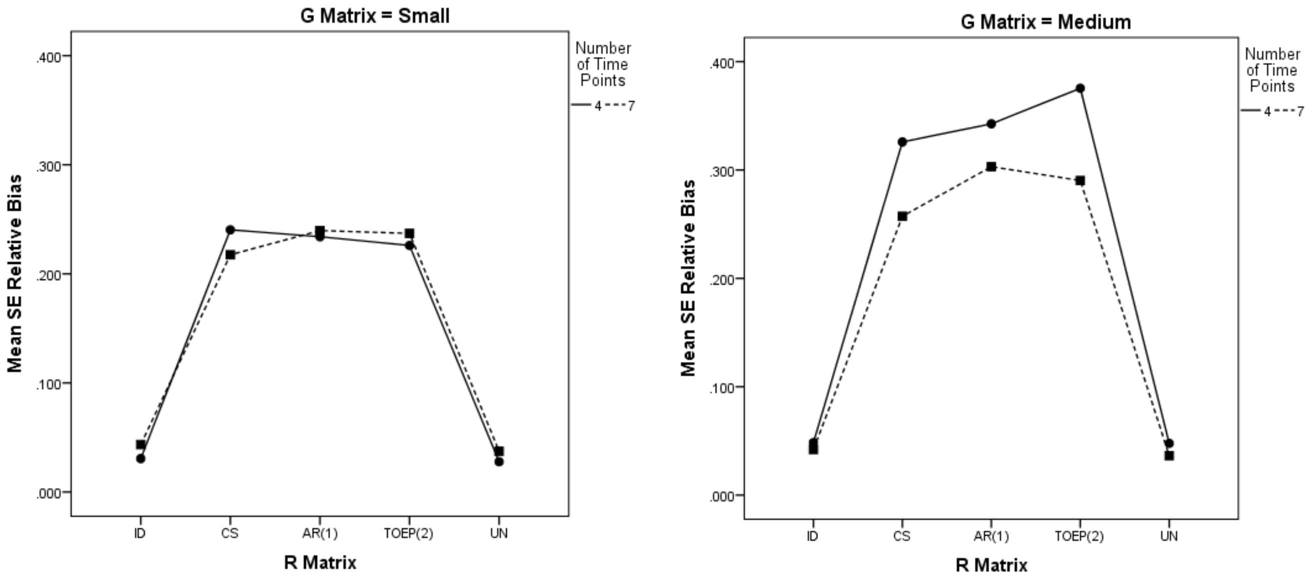

Figure 14. Mean standard error bias of $\boldsymbol{\beta_{01}}$ as a function of the $\boldsymbol{G}$ matrix, number of time points, and $\boldsymbol{R}$ matrix in study 1

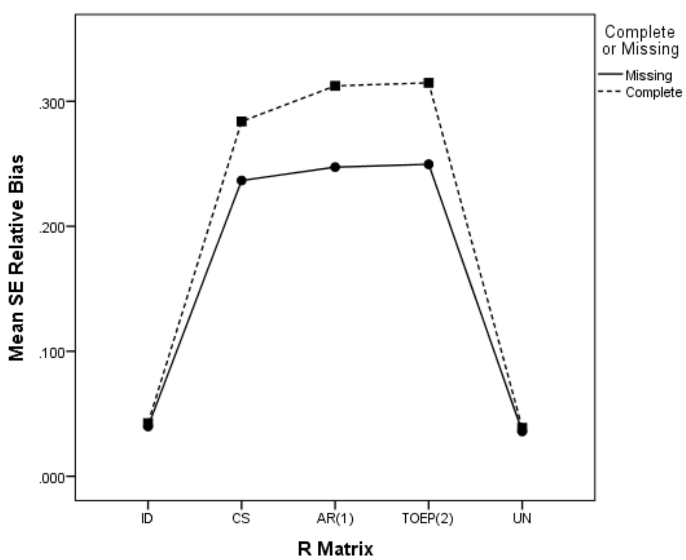

Figure 15. Mean standard error bias of $\boldsymbol{\beta_{01}}$ as a function of the complete or missing data and $\boldsymbol{R}$ matrix in study 1

Effect of W on the growth rate of the linear change (β_{11}). The relative biases of the standard error of β_{11} were slightly over-estimated, which were smaller than the estimations of the other parameters and were within the acceptable range. The estimations of the standard error of β_{11} were unbiased. Figure 16 just shows the pattern of the differences among the ***R*** matrix, complete or missing data, and the number of time points.

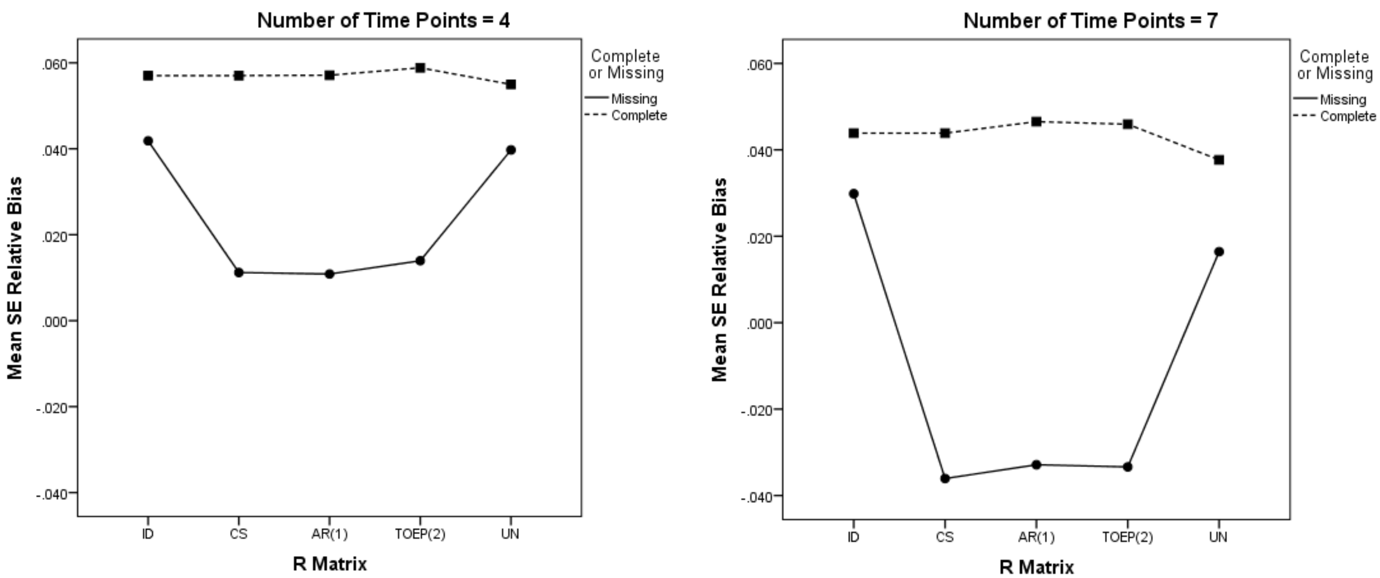

Figure 16. Mean standard error bias of $\boldsymbol{\beta_{11}}$ as a function of the number of time points, complete or missing data, and ***R*** matrix in study 1

Effect of W on the acceleration rate of the quadratic slope (β_{21}). The relative biases of standard errors of β_{21} were under-estimated when CS, AR(1) and TOEP(2) were used as the ***R*** matrix in the analysis, while they were unbiased when ID and UN were used as the ***R*** matrix in the analysis.

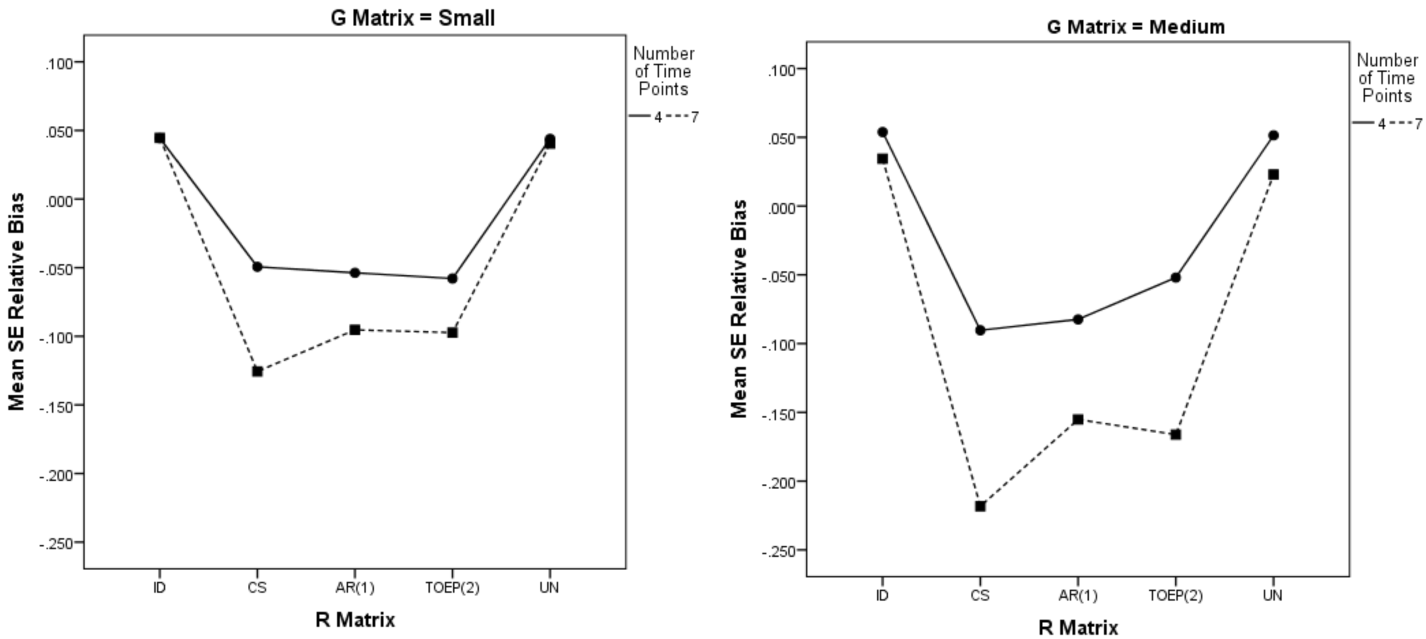

Figure 17. Mean standard error bias of $\boldsymbol{\beta_{21}}$ as a function of the $\boldsymbol{G}$ matrix, number of time points, and $\boldsymbol{R}$ matrix in study 1

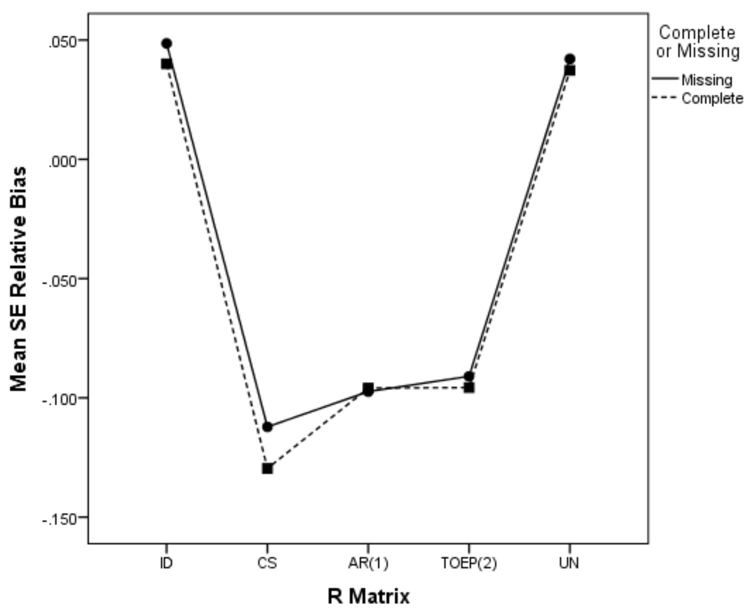

Figure 18. Mean standard error bias of $\boldsymbol{\beta_{21}}$ as a function of the complete or missing data and $\boldsymbol{R}$ matrix in study 1

According to the ANOVA results in Table 17, there was a three-way interaction effect that was among the ***R*** matrix used in the analysis, the ***G*** matrix, and the number of time points (η_p^2 = 0.240). Three two-way interaction effects were also noticeable that were the interaction between the ***R*** matrix and complete or missing data (η_p^2 = 0.105), the interaction between the ***R*** matrix and the number of time points (η_p^2 = 0.792), and the interaction between the ***R*** matrix used in the analysis and the ***G*** matrix (η_p^2 = 0.652). The ***R*** matrix was the largest effect (η_p^2 = 0.984). Figure 17 showed the three-way interaction effect and suggested that the relative biases were larger for more time points, while the larger ***G*** matrix increased the differences. Figure 18 shows the two-way interaction effect between complete or missing data and the ***R*** matrix. The relative biases were smaller in missing data than those in complete data. When a CS was used as the ***R*** matrix, such differences increased.

4.1.3.3 Summary of influences on fixed effects in simulation study 1

The under-specification of the ***G*** matrix and the over-specification of the ***R*** matrix resulted in biased standard error estimates of fixed effects, but not the estimates of fixed effects. The standard errors of the intercept were over-estimated, and the standard errors of the linear and quadratic slopes were under-estimated. The standard errors of the effects of W on the intercept and linear slope were over-estimated. The standard errors of the effect of W on the quadratic slope were under-estimated.

4.1.4 Random effects

In simulation study 1, the random effects of the intercept (τ_{00}), growth rate (τ_{11}), quadratic growth rate (τ_{22}), and their associated covariances were present in the generated data.

However, only the random effects of the intercept and growth rate were considered in the analysis. Therefore, there were totally four parameters related to the random effects including one first-level residual variance (σ^2) and three second-level variance and covariance which were the variances of the random intercept (τ_{00}) and the random growth rate (τ_{11}), and their covariance (τ_{10}). The relative biases for each condition were calculated by equation 37 and were reported in Table 18.

Mixed ANOVA models were also performed on relative biases of variance components. The same five factors were considered as in the analysis for the standard errors of fixed effects. The four between-subject factors included the sample size, the number of time points, complete or missing data, and the effect size of ***G*** matrix. One within-subject factor was the ***R*** matrix used in the analysis. The ANOVA results were reported in Table 19.

4.1.4.1 Relative bias of the first-level residual variance

The relative biases of the first-level residual variance for each condition were presented in Tables 18 when the ***R*** matrix was over-specified and the ***G*** matrix was under-specified. They were over-estimated for all designed factors.

The ANOVA results in Table 19, showed that there were two three-way and four two-way interaction effects. The three-way interaction effects were the interaction among the ***R*** matrix, complete or missing data, and the number of time points (η_p^2 = 0.103), and the interaction among the ***R*** matrix, the number of time points, and the ***G*** matrix (η_p^2 = 0.287). The two-way interaction effects were the interaction between the ***R*** matrix and complete or missing data (η_p^2 = 0.268), the interaction between the ***R*** matrix and the number of time points (η_p^2 = 0.430), the interaction between the ***R*** matrix and the ***G*** matrix (η_p^2 = 0.714), and the interaction between the number of time points and the ***G*** matrix (η_p^2 = 0.327). The ***R*** matrix (η_p^2 = 0.923), complete or missing data (η_p^2 = 0.342), number of time points (η_p^2 = 0.579), and the ***G*** matrix (η_p^2 = 0.817) had large effects on the relative bias of the first-level residual variance. Figures 19 and 20 show the three-way interaction effect patterns. The biases were larger for complete data (vs. missing data) and the larger ***G*** matrix, while such difference decreased for more time points.

Table 18. Relative bias of random effect for each condition in study 1

Complete or missing data	**Sample size**	**Time point**	***G* matrix**	***R* matrix**	σ^2	τ_{00}	τ_{10}	τ_{11}
Complete	500	4	Small	ID	0.003	0.004	0.003	-0.005
Complete	500	4	Small	CS	0.250	0.760	0.628	-0.204
Complete	500	4	Small	AR(1)	0.249	0.760	0.628	-0.202
Complete	500	4	Small	TOEP(2)	0.243	0.767	0.626	-0.195
Complete	500	4	Medium	ID	-0.003	0.003	-0.004	0.002
Complete	500	4	Medium	CS	0.494	0.756	0.616	-0.197
Complete	500	4	Medium	AR(1)	0.619	0.716	0.639	-0.270
Complete	500	4	Medium	TOEP(2)	0.754	0.674	0.659	-0.349
Complete	500	7	Small	ID	-0.000	0.000	-0.000	-0.001
Complete	500	7	Small	CS	0.130	0.612	0.507	-0.075
Complete	500	7	Small	AR(1)	0.194	0.568	0.526	-0.184
Complete	500	7	Small	TOEP(2)	0.183	0.575	0.522	-0.168
Complete	500	7	Medium	ID	0.002	-0.002	0.005	-0.001
Complete	500	7	Medium	CS	0.261	0.609	0.502	-0.075
Complete	500	7	Medium	AR(1)	0.440	0.579	0.545	-0.214
Complete	500	7	Medium	TOEP(2)	0.374	0.592	0.529	-0.170
Complete	2000	4	Small	ID	0.001	-0.006	0.004	-0.001
Complete	2000	4	Small	CS	0.250	0.765	0.629	-0.200
Complete	2000	4	Small	AR(1)	0.246	0.769	0.628	-0.194
Complete	2000	4	Small	TOEP(2)	0.239	0.775	0.626	-0.186
Complete	2000	4	Medium	ID	0.000	0.002	0.005	0.001
Complete	2000	4	Medium	CS	0.501	0.766	0.627	-0.200
Complete	2000	4	Medium	AR(1)	0.621	0.728	0.649	-0.270
Complete	2000	4	Medium	TOEP(2)	0.755	0.692	0.672	-0.347

Table 18 (continued)

Complete or missing data	Sample size	Time point	*G* matrix	*R* matrix	σ^2	τ_{00}	τ_{10}	τ_{11}
Complete	2000	7	Small	ID	-0.000	-0.003	-0.001	-0.002
Complete	2000	7	Small	CS	0.132	0.612	0.504	-0.077
Complete	2000	7	Small	AR(1)	0.196	0.568	0.523	-0.184
Complete	2000	7	Small	TOEP(2)	0.185	0.576	0.519	-0.169
Complete	2000	7	Medium	ID	0.000	0.002	0.004	0.002
Complete	2000	7	Medium	CS	0.262	0.614	0.503	-0.073
Complete	2000	7	Medium	AR(1)	0.442	0.584	0.546	-0.213
Complete	2000	7	Medium	TOEP(2)	0.375	0.597	0.531	-0.168
Missing	500	4	Small	ID	0.001	0.004	0.000	-0.009
Missing	500	4	Small	CS	0.216	0.794	0.428	-0.183
Missing	500	4	Small	AR(1)	0.173	0.780	0.426	-0.127
Missing	500	4	Small	TOEP(2)	0.117	0.836	0.422	-0.057
Missing	500	4	Medium	ID	-0.003	0.003	-0.002	0.002
Missing	500	4	Medium	CS	0.439	0.803	0.368	-0.194
Missing	500	4	Medium	AR(1)	0.474	0.700	0.370	-0.215
Missing	500	4	Medium	TOEP(2)	0.521	0.669	0.357	-0.249
Missing	500	7	Small	ID	0.001	-0.002	-0.008	-0.004
Missing	500	7	Small	CS	0.101	0.585	0.075	-0.109
Missing	500	7	Small	AR(1)	0.141	0.493	0.073	-0.179
Missing	500	7	Small	TOEP(2)	0.139	0.496	0.074	-0.176
Missing	500	7	Medium	ID	0.000	-0.002	0.017	-0.001
Missing	500	7	Medium	CS	0.208	0.597	0.032	-0.119
Missing	500	7	Medium	AR(1)	0.334	0.469	0.034	-0.227
Missing	500	7	Medium	TOEP(2)	0.305	0.480	0.035	-0.206

Table 18 (continued)

Complete or missing data	**Sample size**	**Time point**	***G* matrix**	***R* matrix**	σ^2	τ_{00}	τ_{10}	τ_{11}
Missing	2000	4	Small	ID	0.001	-0.003	0.007	-0.003
Missing	2000	4	Small	CS	0.215	0.798	0.425	-0.178
Missing	2000	4	Small	AR(1)	0.167	0.789	0.422	-0.116
Missing	2000	4	Small	TOEP(2)	0.107	0.849	0.418	-0.041
Missing	2000	4	Medium	ID	-0.000	0.002	0.007	0.002
Missing	2000	4	Medium	CS	0.442	0.809	0.374	-0.194
Missing	2000	4	Medium	AR(1)	0.474	0.712	0.377	-0.213
Missing	2000	4	Medium	TOEP(2)	0.491	0.696	0.367	-0.223
Missing	2000	7	Small	ID	-0.000	-0.004	0.001	-0.002
Missing	2000	7	Small	CS	0.101	0.585	0.076	-0.105
Missing	2000	7	Small	AR(1)	0.140	0.497	0.075	-0.173
Missing	2000	7	Small	TOEP(2)	0.138	0.499	0.075	-0.170
Missing	2000	7	Medium	ID	-0.000	0.004	0.009	0.003
Missing	2000	7	Medium	CS	0.208	0.601	0.025	-0.115
Missing	2000	7	Medium	AR(1)	0.333	0.474	0.027	-0.221
Missing	2000	7	Medium	TOEP(2)	0.305	0.484	0.028	-0.201

Table 19. ANOVA results for the relative biases of random effects in study 1

Factors	σ^2	τ_{00}	τ_{11}	τ_{10}
R matrix (R)	**0.923**	**0.970**	**0.844**	**0.922**
Complete or missing data (CM)	**0.342**	0.016	0.013	**0.528**
Sample size (SS)	–	0.001	0.001	–
Number of time point (T)	**0.579**	**0.542**	0.045	**0.307**
Effect size of ***G*** matrix (G)	**0.817**	0.028	0.060	0.003
R*CM	**0.268**	0.047	**0.129**	**0.702**
R*SS	0.001	0.003	0.001	–
R*T	**0.430**	**0.421**	**0.257**	**0.496**
R*G	**0.714**	0.070	**0.257**	0.013
CM*SS	–	–	–	–
CM*T	0.049	0.058	0.040	0.099
CM*G	0.043	0.006	0.003	0.009
SS*T	–	–	–	–
SS*G	–	–	–	–
T*G	**0.327**	0.032	0.027	–
R*CM*SS	0.001	–	–	–
R*CM*T	**0.103**	0.053	**0.131**	**0.200**
R*CM*G	0.032	0.017	0.007	0.023
R*SS*T	0.001	0.002	0.001	–
R*SS*G	–	–	–	–
R*T*G	**0.287**	0.061	**0.178**	0.002
CM*SS*T	–	–	–	–
CM*SS*G	–	–	–	–
CM*T*G	0.005	0.001	–	0.001
SS*T*G	–	–	–	–

Note: Partial Eta-Square ($\eta_p{}^2$) is reported in the table.

–: indicates that the $\eta_p{}^2$<0.001

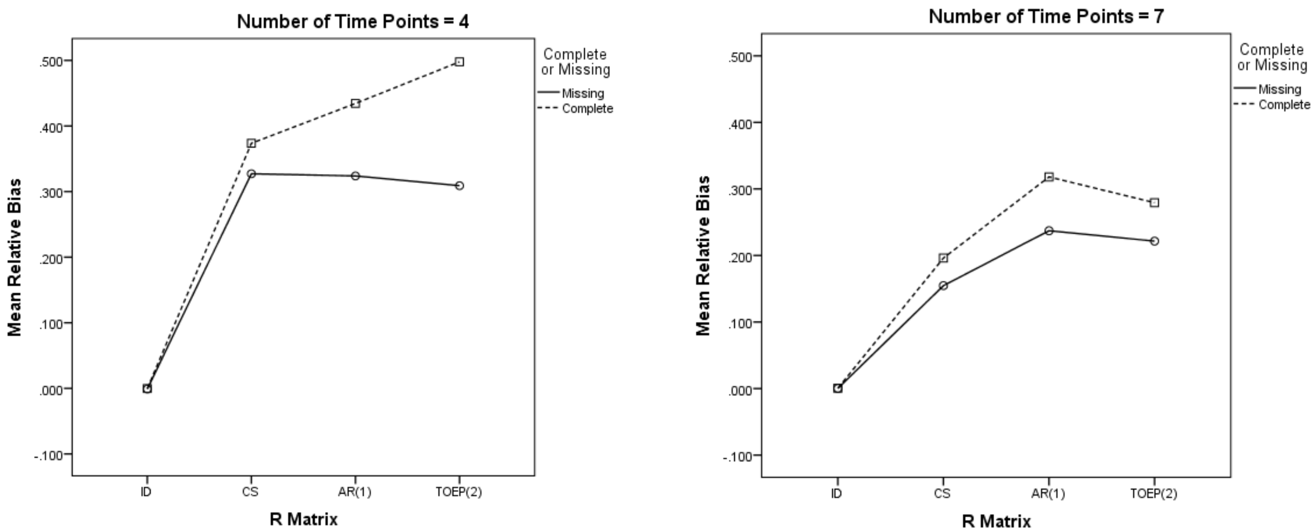

Figure 19. Mean relative bias of $\boldsymbol{\sigma}^2$ as a function of the number of time points, complete or missing data, and ***R*** matrix in study 1

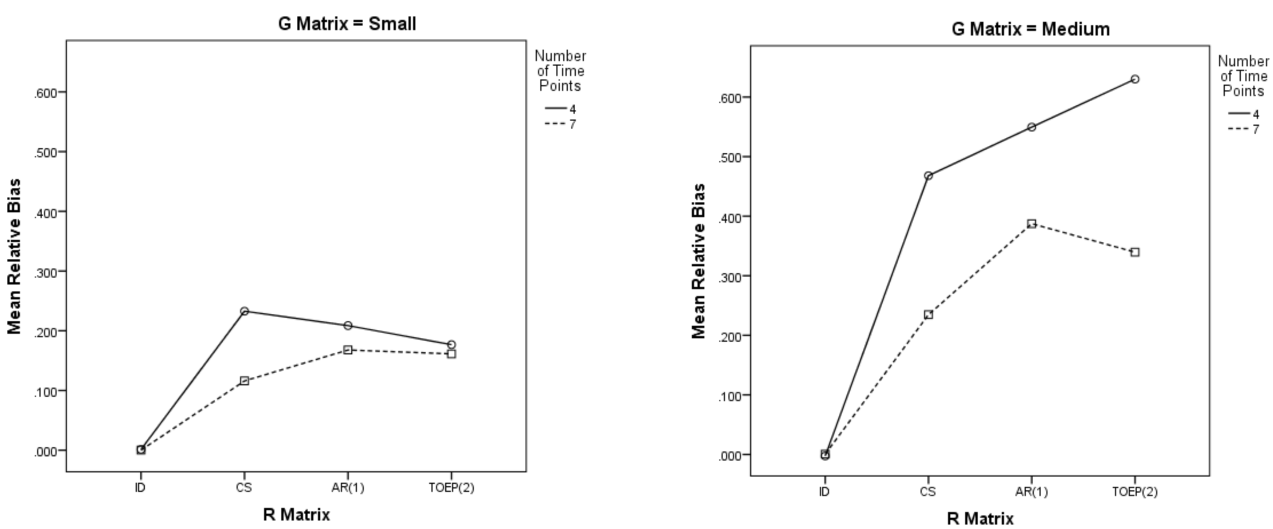

Figure 20. Mean relative bias of $\boldsymbol{\sigma}^2$ as a function of the ***G*** matrix, number of time points, and ***R*** matrix in study 1

4.1.4.2 Relative bias of the second-level random effects

The relative biases of the second-level random effects for each condition were presented in Tables 18 when the ***R*** matrix was over-specified and the ***G*** matrix was under-specified. The results of an ID being used as the ***R*** matrix were presented in the Table as the correct model. When a UN was used as the ***R*** matrix, the random effects were null. The results from mixed ANOVA models were presented in Table 19.

Random effect of intercept (τ_{00}). The relative biases of random effects of the intercept were biased. They were smaller in the 7 waves' analysis than those in the 4 waves' analysis. All the τ_{00} were over-estimated in all designed conditions. The relative bias of τ_{00} was slightly smaller when AR(1) was used as the ***R*** matrix than CS and TOEP(2) were used.

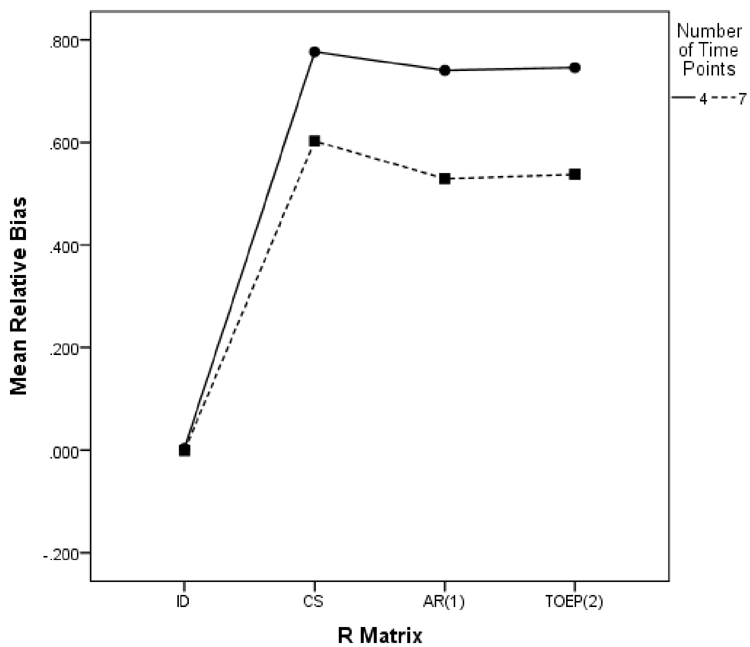

Figure 21. Mean relative bias of $\boldsymbol{\tau_{00}}$ as a function of the number of time points and ***R*** matrix in study 1

According to the ANOVA results, the following conditions had the appreciable effects on the relative bias for estimates of τ_{00}: the ***R*** matrix used in the analysis (η_p^2 = 0.970), then number of time points (η_p^2 = 0.542), and a two-way interaction between the ***R*** matrix and the number of time points (η_p^2 = 0.421). The results were consistent with the relative biases of τ_{00} for each condition. The results suggested that the estimations of τ_{00} were biased when the random effects of the accelerate rate was omitted even a more complex ***R*** matrix was used instead. The relative biases were much higher than the correct model when using CS, AR(1), and TOEP(2) as the ***R*** matrix in the analysis. Figure 21 presented the two-way interaction effects and suggested that relative biases were smaller for more time points.

Random effect of the growth rate (τ_{11}). The relative biases of the random effect of the growth rate were negative values (see Table 18) that meant all the τ_{11}were under-estimated in all designed conditions except the correct models (ID).

The ANOVA results showed that there were two three-way interaction effects and three two-way interaction effects. The three-way interaction effects were the interaction among the ***R*** matrix, the ***G*** matrix, and the number of time points (η_p^2 = 0.178) and the interaction among the ***R*** matrix, complete or missing data, and the number of time points (η_p^2 = 0.131). The three two-way interaction effects included the interaction effect between the ***R*** matrix and the complete or missing data (η_p^2 = 0.129), the interaction between the ***R*** matrix and the number of time points (η_p^2 = 0.257), and the interaction between the ***R*** matrix and ***G*** matrix (η_p^2 = 0.257). The ***R*** matrix used in the analysis had large effects on the relative bias of τ_{11}(η_p^2 = 0.844). The relative biases of τ_{11} were -0.144, -0.200, and -0.189 for CS, AR(1), and TOEP(2) as the ***R*** matrix, respectively. Figures 22 and 23 illustrated the three-way interaction effect patterns and suggested that the relative biases for missing data were smaller in less time points, which were larger in more time points. And also the larger the ***G*** matrix, the higher the relative biases were, and the differences decreased in more time points.

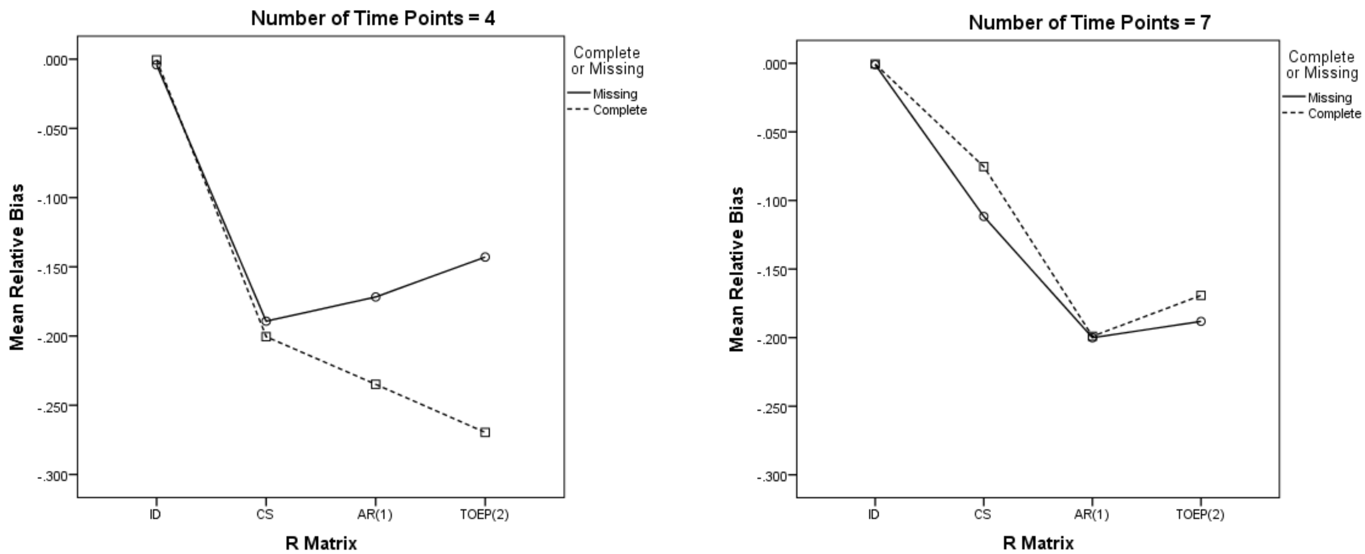

Figure 22. Mean relative bias of $\boldsymbol{\tau_{11}}$ as a function of the number of time points, complete or missing data, and ***R*** matrix in study 1

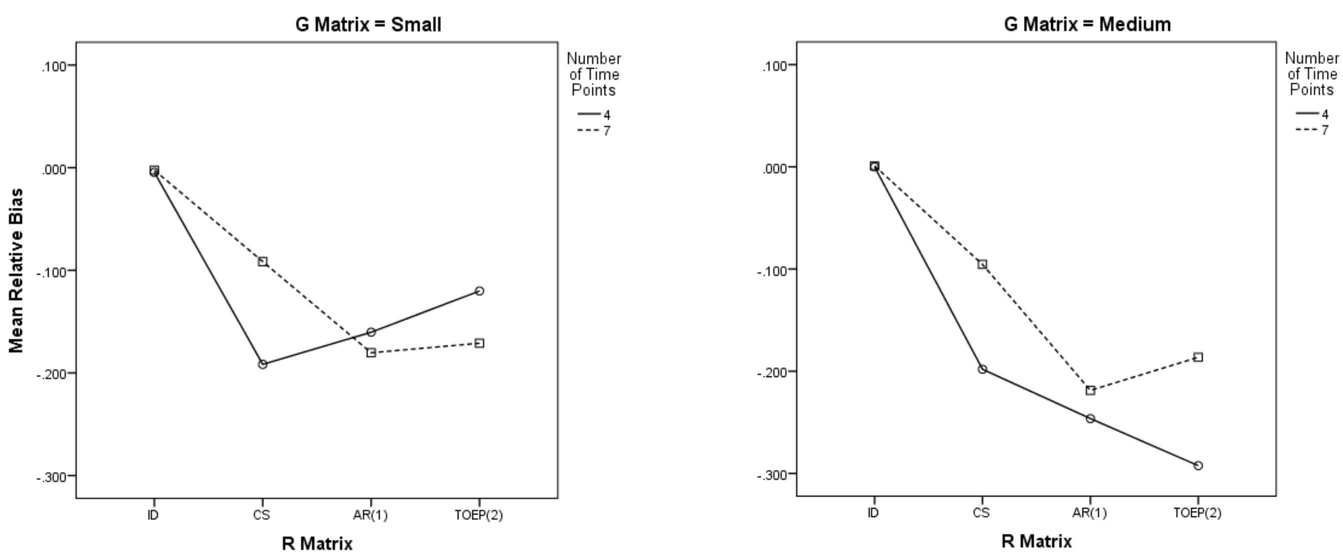

Figure 23. Mean relative bias of $\boldsymbol{\tau_{11}}$as a function of the ***G*** matrix, number of time points, and ***R*** matrix in study

Covariance between the random intercept and the linear slope (τ_{10}). The covariance of τ_{10} were over-estimated for all the conditions and the relative biases were similar across all the conditions.

According to the ANOVA results in Table 19, a three-way interaction effect and two two-way interaction effects were noticeable. The three-way interaction effect was among the ***R*** matrix, complete or missing data, and the number of time points (η_p^2 = 0.200). The two two-way interaction effects were the interaction between the ***R*** matrix used in the analysis, complete or missing data (η_p^2 = 0.702), and the interaction between the ***R*** matrix and the number of time points (η_p^2 = 0.496). The ***R*** matrix used in the analysis had the largest effects on the relative bias of τ_{10} (η_p^2 = 0.992). The complete or missing data and the number of time points also had effects on the relative bias of τ_{10} (η_p^2 = 0.528 and η_p^2 = 0.307). The three-way interaction effects was illustrated in Figure 24. The results suggested that the relative biases with missing data were smaller than those with complete data, while such differences increased for more time points.

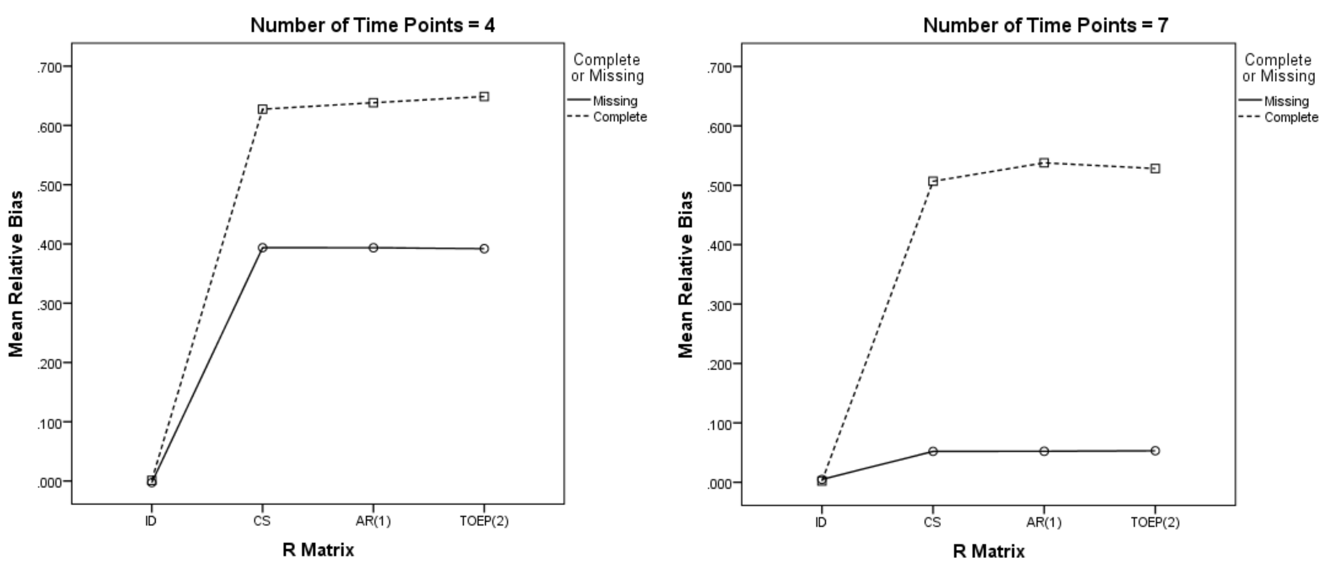

Figure 24. Mean relative bias of $\boldsymbol{\tau_{10}}$ as a function of the number of time points, complete or missing data, and ***R*** matrix in study 1

4.1.4.3 Summary of influences on random effects in simulation study 1

There were no influences on the fixed effect in simulation study 1. However, the random effects were influenced by the over-specification of the ***R*** matrix and the under-specification of the ***G*** matrix. The first level residual variance and the variance of the random intercept were over-estimated, and the variance of the random linear slope was under-estimated. The covariance between the random intercept and the random linear slope was also over-estimated.

4.1.5 Type I error rate

The Type I error rate was examined for those conditions in which the true parameter values of the growth rate (β_{10}), the acceleration rate (β_{20}), effect of *W* on the initial status (β_{01}), effect of *W* on the growth rate of the linear change (β_{11}), and effect of *W* on the acceleration rate of the quadratic slope (β_{21}) were equal to zero under the over-specification of the ***R*** matrix and the under-specification of the ***G*** matrix. The results are presented in Tables 20.

Table 20 shows the Type I error rates by the number of time points, the ***G*** matrix, and the ***R*** matrix used in the analysis. The Type I error rates of β_{01} and β_{11} were smaller or close to the nominal Type I error rate of .05. For the other parameters, the Type I error rates were inflated for most conditions due to the under-estimations of their associated standard errors. In the 4 waves' analysis, the Type I error rates of β_{10} were lower than those in the 7 waves' analysis when the ***R*** matrix was CS, AR(1), and TOEP(2). The Type I error rates of β_{20} were relatively higher with the range of 4.5% to 9.4% in the 4 waves' analysis and 4.95% to 11.45% in the 7 waves' analysis. In the 4 waves' analysis, the Type I error rates of β_{20} were lower than those in the 7 waves' analysis except when the ***R*** matrix was UN. The Type I error rates of β_{01} were low in which the Type I error rates were ranged from 1.45% to 4.95%. The Type I error rates of β_{11}

were relatively lower, and lower than 5% in most of the conditions. The Type I error of β_{21} had the similar pattern as Type I rates of β_{20} that were relatively higher. When UN was used as the ***R*** matrix in the analysis, the Type I error rates were always lower than those when the other ***R*** matrices were used. The highest Type I rate was the one when the CS was used as the ***R*** matrix and the ***G*** matrix was medium.

Table 20. Type I error rates by number of time points, ***G*** matrix and ***R*** matrix in study 1

Time points	***G*** matrix	***R*** matrix	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
4	Small	Correct (%)	4.55	4.60	4.30	4.50	4.65
		CS (%)	4.70	7.15	1.45	4.85	6.95
		AR(1) (%)	4.85	7.30	1.50	4.80	7.05
		TOEP(2) (%)	4.90	7.35	1.50	4.85	7.10
		UN (%)	4.40	4.50	4.60	4.50	4.80
	Medium	Correct (%)	4.00	5.80	4.85	3.50	4.45
		CS (%)	5.10	9.40	1.90	3.85	8.50
		AR(1) (%)	5.20	9.30	1.80	3.80	8.20
		TOEP(2) (%)	4.99	9.07	1.62	3.82	7.32
		UN (%)	3.95	5.85	4.95	3.30	4.40
7	Small	Correct (%)	4.00	4.90	5.15	4.60	3.55
		CS (%)	4.50	9.35	2.55	5.40	7.80
		AR(1) (%)	4.60	8.40	2.15	5.25	6.55
		TOEP(2) (%)	4.60	8.45	2.15	5.25	6.65
		UN (%)	4.25	5.30	5.30	5.00	3.65
	Medium	Correct (%)	4.10	4.65	5.15	3.95	4.45
		CS (%)	5.15	14.36	2.10	5.05	13.06
		AR(1) (%)	5.00	10.95	1.75	4.80	10.35
		TOEP(2) (%)	5.10	11.45	2.10	4.80	10.85
		UN (%)	4.10	4.95	5.45	4.40	4.75

4.1.6 Singularity rate

When quadratic HLMs are used to estimate the coefficients, the inverse of the matrix product ***X'X*** matrix has to be calculated first. If this product is singular, an infinity of solutions exists, especially for a large number of time points in longitudinal studies. Therefore, when the product is singular, the generalized inverse is used. For the analysis with missing data, the singularity happened more frequently and then the estimated ***R*** matrix was a reduced matrix. Tables 21 shows the frequencies of singular matrix happened and the reduced dimension of the ***R*** matrix by the number of time points and the effect sizes of the ***G*** matrix.

Table 21 shows the frequencies of dimension of the reduced ***R*** matrix had a similar pattern for small and medium ***G*** matrices. In the 4 waves' analysis, there were about 60% of missing data sets had the solution of the matrix product, about 32% and 8% of missing data sets had a reduced ***R*** matrix with dimensions of 3 and 2, respectively. In the 7 waves' analysis, there were only about 26% of estimated ***R*** matrices having the dimensions of 7 and 74% of results with a reduced ***R*** matrix.

Table 21. Dimension of reduced R matrix by the number of time points and ***G*** matrix size in study 1

Dimension of reduced R matrix	*G* matrix = small		*G* matrix = medium	
	Time point		Time point	
N (Col Pct)	**4**	**7**	**4**	**7**
7		2592 (25.92%)		2620 (26.20%)
6		1868 (18.68%)		1872 (18.72%)
5		2724 (27.24%)		2596 (25.96%)
4	5995 (59.96%)	1928 (19.28%)	5678 (61.68%)	2107 (21.07%)
3	3256 (32.57%)	768 (7.68%)	2778 (30.18%)	624 (6.24%)
2	747 (7.47%)	120 (1.20%)	750 (8.15%)	180 (1.80%)

4.2 SIMULATION STUDY 2

In simulation study 2, the data generation was based on a simple ***G*** matrix and a complex ***R*** matrix. In the generated ***G*** matrix, the correlation between random effects was 0.4 and there were random effects of the intercept and linear slope. The ***R*** matrix was generated as CS, AR(1), and TOEP(2). In the analysis, the random effects of the intercept, the linear slope, and the quadratic slope in the ***G*** matrix were considered and the ID as the ***R*** matrix were performed in the analyses. To compare the results, the correct models were also performed. The results showed the influences of the under-specification of the ***R*** matrix and the over-specification of the ***G*** matrix on the fixed and their corresponding standard errors, and random effects. The methods of specification of an optimal covariance structure were compared under the condition of the under-specification of the ***R*** matrix and the over-specification of the ***G*** matrix. In the tables of this section, the models were the correct models when the designed ***R*** matrix was the same as the ***R*** matrix used in the analysis.

4.2.1 Convergence rate

Table 22 shows the convergence rates of the under-specification of the ***R*** matrix and the over-specification of the ***G*** matrix in simulation study 2. The convergence rate was about 100%. Only two cases did not converge out of 48,000 cases when CS was used as the ***R*** matrix, which were the correct models.

Table 22. Convergence rates in simulation study 2

Converged	R matrix used in analysis				Total
	CS	AR(1)	TOEP(2)	ID	
Yes	7998 (99.98%)	8000 (100%)	8000 (100%)	24000 (100%)	47998 (100%)
No	2 (0.03%)	0 (0.00%)	0 (0.00%)	0 (0.00%)	2 (0.00%)

4.2.2 Standardized Root Mean square Residual (SRMR)

The AIC, AICC, BIC, and SRMR were compared on the specification of the optimal ***R*** matrix when the ***R*** matrix was under-specified and the ***G*** matrix was over-specified. Table 23 shows the results across all the conditions. BIC was the best method in selecting the optimal covariance matrix. The lowest correct rate of selection was 98.16% when the designed ***R*** matrix was a CS. The correct rates in selecting the optimal covariance structures by AIC and AICC were similar that were better than those by SRMR. SRMR tended to select the most complex covariance structure. However, the correct rates were low that were 55.34% and 73.46% when the ***R*** matrix used in simulation was CS and AR(1) structures, respectively. When the designed ***R*** matrix was TOEP(2), the correct rate by SRMR was 92.05%. The specification patterns in searching the optimal covariance matrix were similar among the number of time points, complete or missing data, effect sizes of growth parameters, and the sample size.

Table 23. Selection rates in simulation study 2

R matrix used in simulation	Selected models	AIC	AICC	BIC	SRMR
CS	Correct model	5451 (68.14%)	5463 (68.29%)	7853 (98.16%)	4427 (55.34%)
	R matrix = ID	2549 (31.86%)	2537 (31.71%)	147 (1.84%)	3573 (44.66%)
AR(1)	Correct model	7696 (96.20%)	7704 (96.30%)	7997 (99.96%)	5877 (73.46%)
	R matrix = ID	304 (3.8%)	296 (3.70%)	3 (0.04%)	2123 (26.54 %)
TOEP(2)	Correct model	7994 (99.93%)	7994 (99.93%)	8000 (100%)	7364 (92.05%)
	R matrix = ID	6 (0.08%)	6 (0.08%)	0 (0.00%)	636 (7.95%)

4.2.3 Fixed effects

The fixed effects included the intercept (β_{00}), the effect of W on the initial status (β_{01}), the overall mean of the growth rate (β_{10}), the effect of W on the growth rate of the linear change (β_{11}), the overall mean of the acceleration rate (β_{20}), and the effect of W on the acceleration rate of the quadratic slope (β_{21}) in equation 28, in which W is a level-2 continuous variable. The results of the relative bias of fixed effects and their corresponding standard errors are addressed in this section when the ***R*** matrix was under-specified and the ***G*** matrix was over-specified.

4.2.3.1 Relative bias of parameter estimates

The relative bias of parameters for each condition was calculated by the equation 37 and presented in Tables 24.

Intercept (β_{00}). The relative biases of the intercept for each condition were very small and close to 0 across all the conditions with the range from -0.0002 to 0.0003.

Overall mean of the growth rate (β_{10})*.* The relative biases of β_{10} for each condition were small with the range from -0.004 to 0.005.

Overall mean of the acceleration rate (β_{20})*.* The relative biases of β_{20} for each condition were small with the range from -0.002 to 0.001.

Effect of W on the initial status (β_{01})*.* The relative biases of β_{01} for each condition were small across all the conditions with the range from -0.004 to 0.013. The largest relative biases of β_{01} were present when the designed ***R*** matrix was TOEP(2). However, they were in the acceptable range.

Effect of W on the growth rate of the linear change (β_{11})*.* The relative biases of β_{11} for each condition were very small with the range from -0.011 to 0.002. The largest relative biases of β_{11} were present when the designed ***R*** matrix was a TOEP(2) and they were also in the acceptable range.

Effect of W on the acceleration rate of the quadratic slope (β_{21})*.* The relative biases of β_{21} for each condition were small with the range from -0.006 to 0.005.

In summary, the relative biases of fixed effects were very small, which were not impacted by the under-specification of the ***R*** matrix and the over-specification of the ***G*** matrix. Therefore, the estimation of the fixed effects was unbiased across all the designed factors under the under-specification of the ***R*** matrix and over-specification of the ***G*** matrix.

Table 24. Relative bias of parameter for each condition in study 2

Complete or missing	Sample size	Time point	*R* matrix in data generation	*R* matrix	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Complete	500	4	CS	CS	0.000	-0.002	0.000	0.005	0.000	0.002
Complete	500	4	CS	ID	0.000	-0.002	0.000	0.005	0.000	0.002
Complete	500	4	AR(1)	AR(1)	0.000	0.004	-0.000	0.007	-0.002	0.001
Complete	500	4	AR(1)	ID	0.000	0.003	-0.000	0.007	-0.002	0.001
Complete	500	4	TOEP(2)	TOEP(2)	0.000	-0.001	0.000	0.011	-0.008	-0.005
Complete	500	4	TOEP(2)	ID	0.000	-0.001	0.000	0.011	-0.010	-0.005
Complete	500	7	CS	CS	0.000	-0.001	0.001	0.004	0.002	0.002
Complete	500	7	CS	ID	0.000	-0.001	0.001	0.004	0.002	0.002
Complete	500	7	AR(1)	AR(1)	0.000	0.004	-0.001	0.007	-0.002	0.001
Complete	500	7	AR(1)	ID	0.000	0.003	-0.000	0.007	-0.001	0.001
Complete	500	7	TOEP(2)	TOEP(2)	0.000	-0.001	0.001	-0.002	-0.007	0.002
Complete	500	7	TOEP(2)	ID	0.000	-0.001	0.001	-0.004	-0.009	0.005
Complete	2000	4	CS	CS	-0.000	0.002	-0.000	0.005	-0.001	0.001
Complete	2000	4	CS	ID	-0.000	0.002	-0.000	0.005	-0.001	0.001
Complete	2000	4	AR(1)	AR(1)	-0.000	0.001	-0.001	-0.000	-0.003	0.001
Complete	2000	4	AR(1)	ID	-0.000	0.001	-0.001	-0.000	-0.003	0.001
Complete	2000	4	TOEP(2)	TOEP(2)	-0.000	0.001	0.001	0.004	-0.001	0.001
Complete	2000	4	TOEP(2)	ID	-0.000	-0.000	0.001	0.004	-0.002	0.001

Table 24 (continued)

Complete or missing	Sample size	Time point	*R* matrix in data generation	*R* matrix	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Complete	2000	7	CS	CS	-0.000	0.002	-0.001	0.005	0.001	0.002
Complete	2000	7	CS	ID	-0.000	0.002	-0.001	0.005	0.001	0.002
Complete	2000	7	AR(1)	AR(1)	-0.000	0.001	-0.000	-0.001	-0.004	0.001
Complete	2000	7	AR(1)	ID	-0.000	0.001	0.000	-0.001	-0.004	0.001
Complete	2000	7	TOEP(2)	TOEP(2)	-0.000	0.000	0.000	0.003	-0.001	0.001
Complete	2000	7	TOEP(2)	ID	-0.000	-0.000	-0.000	0.002	-0.001	0.002
Missing	500	4	CS	CS	0.000	-0.003	-0.001	0.006	0.001	0.002
Missing	500	4	CS	ID	0.000	-0.003	-0.001	0.006	0.001	0.002
Missing	500	4	AR(1)	AR(1)	0.000	0.005	0.000	0.006	-0.002	0.001
Missing	500	4	AR(1)	ID	0.000	0.004	0.000	0.006	-0.002	0.001
Missing	500	4	TOEP(2)	TOEP(2)	0.000	-0.004	-0.001	0.013	-0.009	-0.006
Missing	500	4	TOEP(2)	ID	0.000	-0.003	-0.001	0.013	-0.011	-0.006
Missing	500	7	CS	CS	0.000	-0.003	-0.000	0.005	0.001	0.002
Missing	500	7	CS	ID	0.000	-0.003	-0.000	0.005	0.000	0.002
Missing	500	7	AR(1)	AR(1)	0.000	0.001	-0.002	0.007	0.000	0.002
Missing	500	7	AR(1)	ID	0.000	0.002	-0.002	0.006	0.002	0.003
Missing	500	7	TOEP(2)	TOEP(2)	0.000	-0.002	0.001	-0.002	-0.004	0.004
Missing	500	7	TOEP(2)	ID	0.000	-0.002	0.001	-0.003	-0.008	0.004

Table 24 (continued)

Complete or missing	Sample size	Time point	R matrix in data generation	R matrix	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Missing	2000	4	CS	CS	-0.000	0.001	-0.001	0.004	-0.001	0.002
Missing	2000	4	CS	ID	-0.000	0.001	-0.001	0.004	-0.001	0.002
Missing	2000	4	AR(1)	AR(1)	-0.000	0.002	-0.000	0.000	-0.003	0.001
Missing	2000	4	AR(1)	ID	-0.000	0.002	-0.000	0.000	-0.003	0.001
Missing	2000	4	TOEP(2)	TOEP(2)	-0.000	-0.000	0.000	0.005	-0.002	-0.000
Missing	2000	4	TOEP(2)	ID	-0.000	-0.001	0.000	0.005	-0.003	-0.000
Missing	2000	7	CS	CS	-0.000	0.002	0.000	0.005	0.002	0.002
Missing	2000	7	CS	ID	-0.000	0.002	0.000	0.005	0.002	0.002
Missing	2000	7	AR(1)	AR(1)	-0.000	-0.001	-0.001	-0.001	-0.003	0.001
Missing	2000	7	AR(1)	ID	-0.000	-0.001	-0.001	-0.001	-0.003	0.001
Missing	2000	7	TOEP(2)	TOEP(2)	-0.000	0.000	0.001	0.002	-0.001	0.002
Missing	2000	7	TOEP(2)	ID	-0.000	0.000	0.001	0.002	-0.001	0.002

4.2.3.2 Relative bias of standard errors of fixed effects

The relative bias of standard errors of the fixed effects was calculated by equation 38. Table 25 shows the relative biases of standard errors of the fixed effects for each condition. The estimations of standard errors of fixed effects were unbiased for most conditions. There were only four conditions under which the estimations of standard errors of β_{01} and β_{21} were biased, respectively. A series of mixed ANOVAs were performed to test the effects of simulation factors on the relative bias of standard errors of fixed effects due to the under-specification of the ***R*** matrix and the over-specification of the ***G*** matrix. The ANOVAs tested the five designed factors and their two-way and three-way interaction effects. The four between-subject factors included the sample size, the number of time points, complete or missing data, and the ***R*** matrix in data generation. The within-subject factor was the ***R*** matrix used in the analysis. For each generated dataset, the relative biases of standard errors of fixed effects in the true models were compared to those in the models with an ID as the ***R*** matrix in the analysis. Only the effects with partial $\eta_p{}^2$ greater than 0.1 were further interpreted. The ANOVA results were presented in Table 26.

Intercept (β_{00}). The relative biases of standard errors of the intercept were smaller than 0.1 for all conditions in Table 25. They were ranged from -0.066 to 0.048, indicating the estimations of standard errors of the intercept were not biased.

The mixed ANOVA models were performed and the results were presented in Table 26. The two-way interaction effect was detected between the sample size and the ***R*** matrix used in data generation ($\eta_p{}^2$ = 0.187). Figure 25 showed the interaction effect and suggested the biases were within the acceptable range. The relative biases were larger when the ***R*** matrix used in data generation was CS or TOEP(2) when the sample size was 500. There were no any differences between the correct model and an ID as the ***R*** matrix in the analysis.

Table 25. Relative bias of standard errors of fixed effects for each condition in study 2

Complete or missing	Sample size	Time point	*R* matrix in data generation	*R* matrix	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Complete	500	4	CS	CS	0.015	-0.025	-0.039	0.046	0.046	0.064
Complete	500	4	CS	ID	0.016	-0.025	-0.030	0.048	0.046	0.073
Complete	500	4	AR(1)	AR(1)	-0.008	-0.034	-0.004	0.129	0.043	0.065
Complete	500	4	AR(1)	ID	-0.007	-0.034	0.000	0.130	0.043	0.070
Complete	500	4	TOEP(2)	TOEP(2)	0.045	-0.002	0.041	-0.026	0.017	0.031
Complete	500	4	TOEP(2)	ID	0.043	0.014	0.040	-0.028	0.038	0.030
Complete	500	7	CS	CS	0.014	-0.025	0.024	0.054	0.060	-0.004
Complete	500	7	CS	ID	0.014	-0.025	0.035	0.055	0.060	0.006
Complete	500	7	AR(1)	AR(1)	-0.020	-0.057	-0.028	0.117	0.044	0.054
Complete	500	7	AR(1)	ID	-0.025	-0.054	-0.035	0.115	0.029	0.055
Complete	500	7	TOEP(2)	TOEP(2)	0.020	-0.013	-0.002	-0.007	0.031	0.031
Complete	500	7	TOEP(2)	ID	0.023	-0.004	-0.003	0.002	0.042	0.042
Complete	2000	4	CS	CS	-0.056	0.004	-0.001	0.006	0.044	0.008
Complete	2000	4	CS	ID	-0.056	0.004	0.002	0.006	0.044	0.012
Complete	2000	4	AR(1)	AR(1)	-0.049	-0.023	0.015	0.088	0.043	0.049
Complete	2000	4	AR(1)	ID	-0.049	-0.019	0.016	0.088	0.039	0.050
Complete	2000	4	TOEP(2)	TOEP(2)	-0.054	-0.038	0.046	0.033	0.024	0.051
Complete	2000	4	TOEP(2)	ID	-0.055	-0.033	0.047	0.031	0.034	0.051

Table 25 (continued)

Complete or missing	Sample size	Time point	R matrix in data generation	R matrix	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Complete	2000	7	CS	CS	-0.057	-0.002	-0.008	0.035	0.029	0.064
Complete	2000	7	CS	ID	-0.057	-0.002	-0.003	0.035	0.029	0.069
Complete	2000	7	AR(1)	AR(1)	-0.051	-0.010	-0.026	0.065	0.045	0.009
Complete	2000	7	AR(1)	ID	-0.054	-0.009	-0.020	0.064	0.050	-0.007
Complete	2000	7	TOEP(2)	TOEP(2)	-0.059	-0.023	-0.019	-0.007	0.082	0.001
Complete	2000	7	TOEP(2)	ID	-0.048	-0.026	0.005	-0.011	0.077	0.012
Missing	500	4	CS	CS	0.011	-0.015	-0.060	0.056	0.037	0.058
Missing	500	4	CS	ID	0.013	-0.016	-0.052	0.059	0.036	0.068
Missing	500	4	AR(1)	AR(1)	-0.017	-0.007	-0.024	0.131	0.051	0.036
Missing	500	4	AR(1)	ID	-0.015	-0.011	-0.019	0.132	0.052	0.044
Missing	500	4	TOEP(2)	TOEP(2)	0.048	0.022	0.047	-0.007	0.007	0.021
Missing	500	4	TOEP(2)	ID	0.047	0.024	0.049	-0.008	0.028	0.023
Missing	500	7	CS	CS	0.027	-0.051	-0.011	0.053	0.064	-0.003
Missing	500	7	CS	ID	0.028	-0.051	-0.003	0.053	0.066	0.007
Missing	500	7	AR(1)	AR(1)	-0.019	-0.070	-0.057	0.127	0.013	0.041
Missing	500	7	AR(1)	ID	-0.019	-0.062	-0.043	0.124	-0.000	0.031
Missing	500	7	TOEP(2)	TOEP(2)	0.005	-0.006	-0.031	-0.002	0.036	0.089
Missing	500	7	TOEP(2)	ID	0.011	0.015	-0.024	-0.006	0.050	0.110

Table 25 (continued)

Complete or missing	Sample size	Time point	R matrix in data generation	R matrix	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
Missing	2000	4	CS	CS	-0.056	-0.021	0.027	-0.008	0.025	0.011
Missing	2000	4	CS	ID	-0.056	-0.022	0.031	-0.007	0.026	0.016
Missing	2000	4	AR(1)	AR(1)	-0.052	-0.020	0.039	0.084	0.028	0.025
Missing	2000	4	AR(1)	ID	-0.052	-0.017	0.038	0.084	0.024	0.026
Missing	2000	4	TOEP(2)	TOEP(2)	-0.066	-0.051	0.022	0.015	0.032	0.008
Missing	2000	4	TOEP(2)	ID	-0.066	-0.049	0.021	0.017	0.040	0.005
Missing	2000	7	CS	CS	-0.035	0.025	0.018	0.021	0.029	0.036
Missing	2000	7	CS	ID	-0.035	0.025	0.022	0.021	0.029	0.042
Missing	2000	7	AR(1)	AR(1)	-0.048	0.003	-0.020	0.062	0.033	0.040
Missing	2000	7	AR(1)	ID	-0.049	0.007	-0.018	0.061	0.040	0.028
Missing	2000	7	TOEP(2)	TOEP(2)	-0.051	0.011	0.036	0.003	0.066	0.079
Missing	2000	7	TOEP(2)	ID	-0.044	0.005	0.036	-0.000	0.053	0.036

Table 26. ANOVA results for the relative biases of standard errors of fixed effects in study 2

Factors	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
R matrix in data generation (RG)	**0.139**	0.075	**0.284**	**0.566**	0.005	0.006
Complete or missing data (CM)	0.001	0.012	0.001	–	0.009	–
Sample size (SS)	**0.663**	0.037	**0.223**	0.094	–	0.034
Number of time point (T)	0.003	–	**0.152**	0.001	0.013	–
R matrix in data analysis (RA)	0.007	**0.129**	0.073	–	0.061	0.008
RA*CM	0.001	0.001	–	0.001	–	0.014
RA*SS	–	0.058	0.001	0.003	0.041	0.073
RA*T	0.003	0.003	0.011	0.003	**0.106**	0.012
RA*RG	0.016	**0.103**	0.008	0.002	**0.287**	0.062
CM*SS	0.001	–	**0.154**	0.008	0.001	–
CM*T	0.012	0.004	–	–	–	0.057
CM*RG	0.012	0.019	0.001	0.002	0.002	0.024
SS*T	0.037	**0.198**	0.028	0.004	0.004	0.016
SS*RG	**0.187**	**0.263**	0.043	**0.157**	0.045	0.015
T*RG	0.032	0.027	**0.338**	0.032	0.037	0.053
RA*CM*SS	0.001	–	0.025	0.004	0.004	0.017
RA*CM*T	–	0.053	–	0.005	–	0.018
RA*CM* RG	0.002	0.009	0.009	0.002	0.011	0.024
RA*SS*T	0.002	0.069	0.006	0.001	0.021	0.025
RA*SS* RG	0.006	**0.150**	0.013	0.002	**0.310**	0.022
RA*T* RG	0.039	0.014	0.008	0.002	**0.140**	0.035
CM*SS*T	0.004	0.090	0.033	0.004	–	0.002
CM*SS* RG	–	0.004	0.035	0.001	–	0.023
CM*T* RG	0.008	0.019	0.022	0.001	0.009	0.071
SS*T* RG	0.033	0.006	**0.205**	0.036	0.030	**0.161**

Note: Partial Eta-Square (η_p^2) is reported in the table.

–: indicates that the η_p^2<0.001

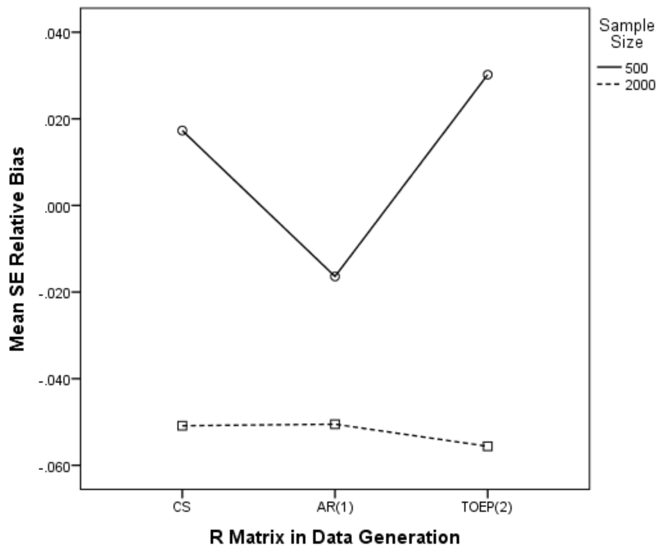

Figure 25. Mean standard error bias of the intercept as a function of the sample size and ***R*** matrix in data generation in study 2

Overall mean of the growth rate (β_{10}). The relative biases of standard errors of β_{10} were small and were in the acceptable range for all the conditions, which had the range from -0.070 to 0.025.

According to the ANOVA results, a three-way interaction effect and three two-way interaction effects were present in the analysis. The three-way interaction was among the ***R*** matrix in data generation, the sample size, and the ***R*** matrix used in the analysis (η_p^2 = 0.150). The two-way interaction effects included the interaction between the ***R*** matrix in the data generation and the ***R*** matrix used in the analysis (η_p^2 = 0.103), the interaction between the sample size and the ***R*** matrix in the data generation (η_p^2 = 0.263), and the interaction between the sample size and the number of time points (η_p^2 = 0.198). Figures 26 illustrated the three-way interaction effect pattern and suggested that correct models were close to an ID as the ***R*** matrix in the analysis.

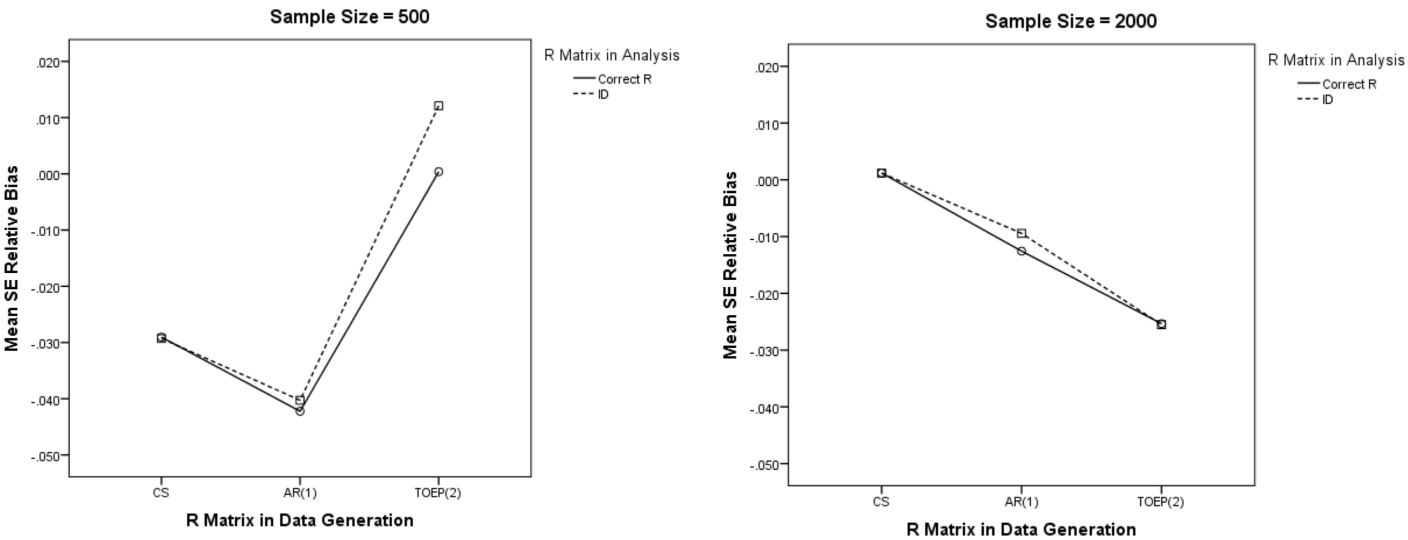

Figure 26. Mean standard error bias of the growth rate as a function of the sample size, ***R*** matrix in the analysis, and ***R*** matrix in data generation in study 2

Overall mean of the acceleration rate (β_{20}). The relative biases of standard errors of β_{20} were small within the acceptable range from -0.060 to 0.049. The estimations of the standard errors of β_{20} was unbiased for all conditions.

According to the ANOVA results, there were one three-way and two two-way interaction effects. The three-way interaction effect was among the ***R*** matrix in the data generation, the sample size, and the number of time points (η_p^2 = 0.205). The two-way interaction effects included the interaction between the ***R*** matrix in data generation and the number of time points (η_p^2 = 0.338), and the interaction between the sample size and complete or missing data (η_p^2 = 0.154). The three-way interaction effect patterns were illustrated in Figure 27 and suggested that the relative biases were smaller for the larger sample size and more time points.

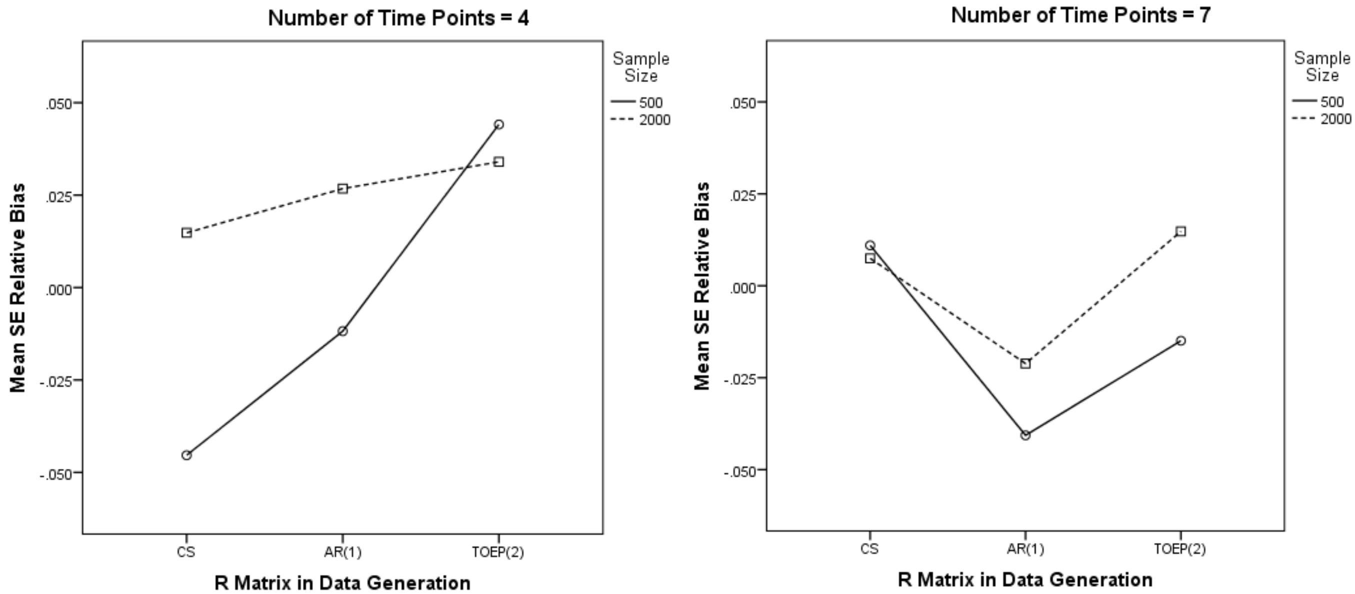

Figure 27. Mean standard error bias of the acceleration rate as a function of the number of time points, sample size, and ***R*** matrix in study 2

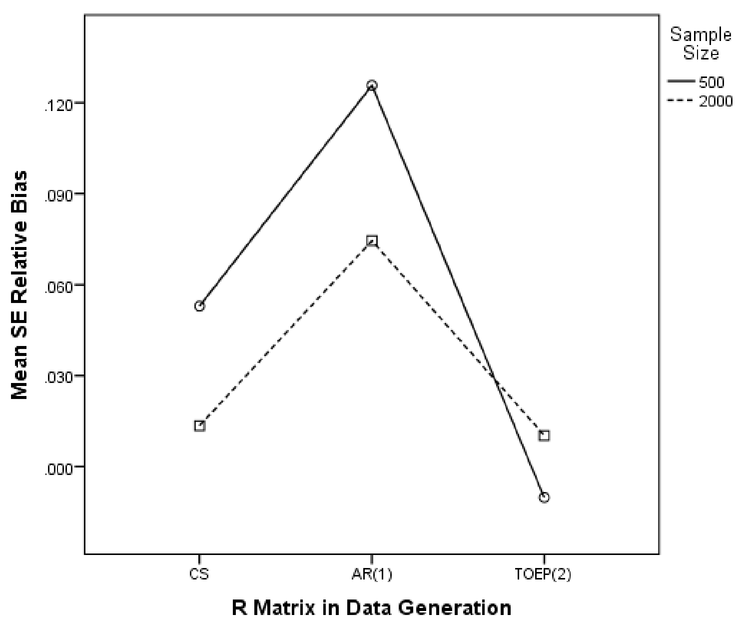

Figure 28. Mean standard error bias of $\boldsymbol{\beta_{01}}$ as a function of the sample size and *R* matrix in data generation in study 2

Effect of W on the initial status (β_{01}). The relative biases of standard errors of β_{01} were small in most of the conditions (see Table 25) with the range from -0.028 to 0.132. Under four of the conditions, the estimations of the standard errors of β_{01} were biased and over-estimated.

According to the ANOVA results in Table 26, one two-way interaction effect was present between the ***R*** matrix in data generation and the sample size (η_p^2 = 0.157). Figure 28 showed the interaction effects and suggested that the relative biases were larger for the smaller sample size and AR(1) as the ***R*** matrix in data generation.

Effect of W on the growth rate of the linear change (β_{11}). The relative biases of the standard error of β_{11} were slightly over-estimated, which were within the acceptable range from -0.000 to 0.082. The estimations of the standard error of β_{11} were unbiased.

According to the ANOVA results in Table 26, two three-way interaction effects and two two-way interaction effects were noticeable. The three-way interaction effects included the interaction among the ***R*** matrix in data generation, the sample size, and the ***R*** matrix used in the analysis (η_p^2 = 0.310), and interaction among the ***R*** matrix in data generation, the number of time points, and the ***R*** matrix in the analysis (η_p^2 = 0.140). The two-way interaction effects included the interaction between the ***R*** matrix in the analysis and the number of time points (η_p^2 = 0.106), and the interaction between the ***R*** matrix in data generation and the ***R*** matrix used in the analysis (η_p^2 = 0.287). Figures 29 and 30 showed the pattern of the three-way interaction effects and suggested that the biases were larger for 500 subjects (vs 2000) and 7 time points (vs 4) .

Effect of W on the acceleration rate of the quadratic slope (β_{21}). The relative biases of the standard errors of β_{21} were very small for most of the conditions, except the condition of the sample size 500, TOEP(2) as the ***R*** matrix in data generation in 7 waves' analysis with missing data. The relative biases were ranged from -0.007 to 0.110.

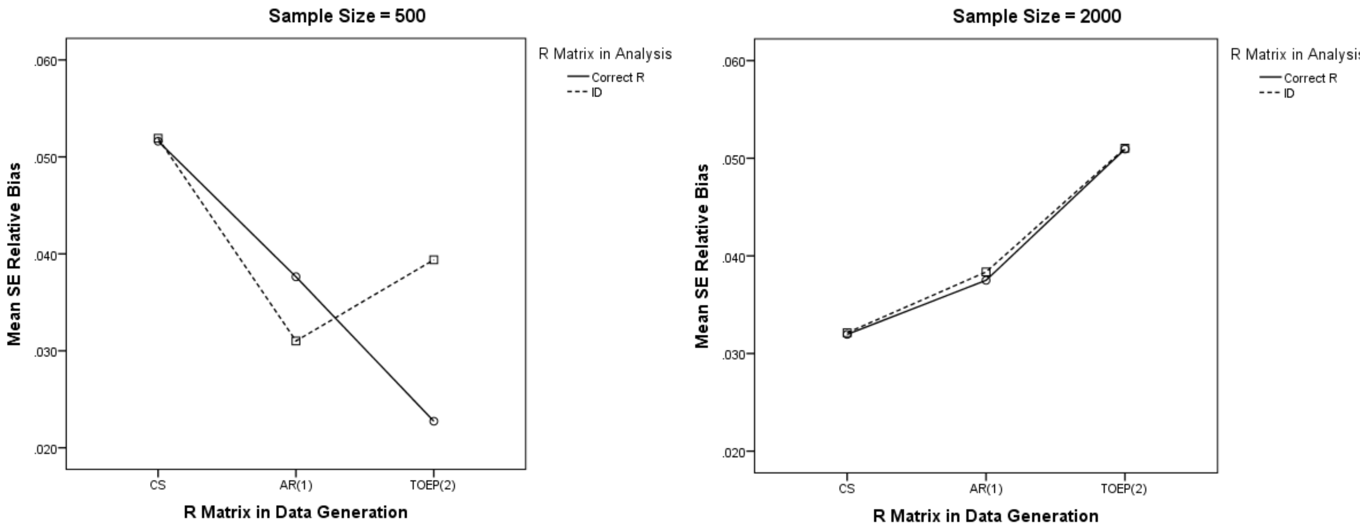

Figure 29. Mean standard error bias of $\boldsymbol{\beta_{11}}$ as a function of the sample size, *R* matrix used in analysis, and *R* matrix in data generation in study 2

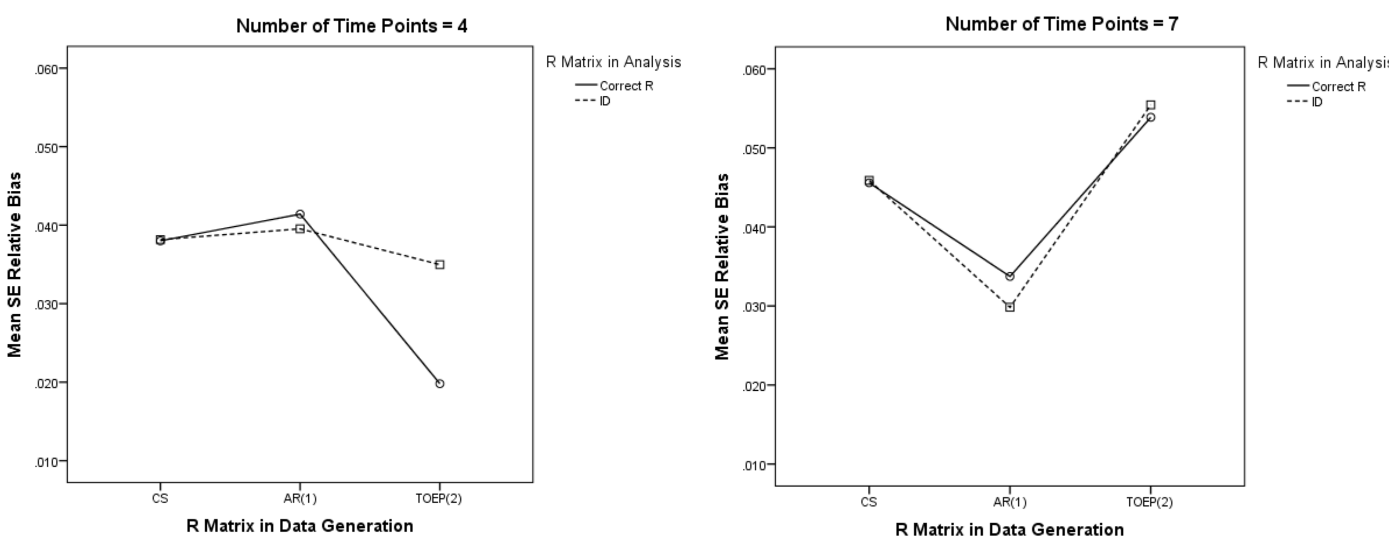

Figure 30. Mean standard error bias of $\boldsymbol{\beta_{11}}$ as a function of the number of time points, *R* matrix used in analysis, and *R* matrix in data generation in study 2

According to the ANOVA results in Table 26, there was a three-way interaction effect that was among the ***R*** matrix in data generation, the sample size, and the number of time points (η_p^2 = 0.161). Figure 31 showed the three-way interaction effect and suggested that the relative biases were larger for 500 subjects (vs 2000), and biases with AR(1) as the ***R*** matrix in data generation were in between those with CS and TOEP (2) as the ***R*** matrix in data generation.

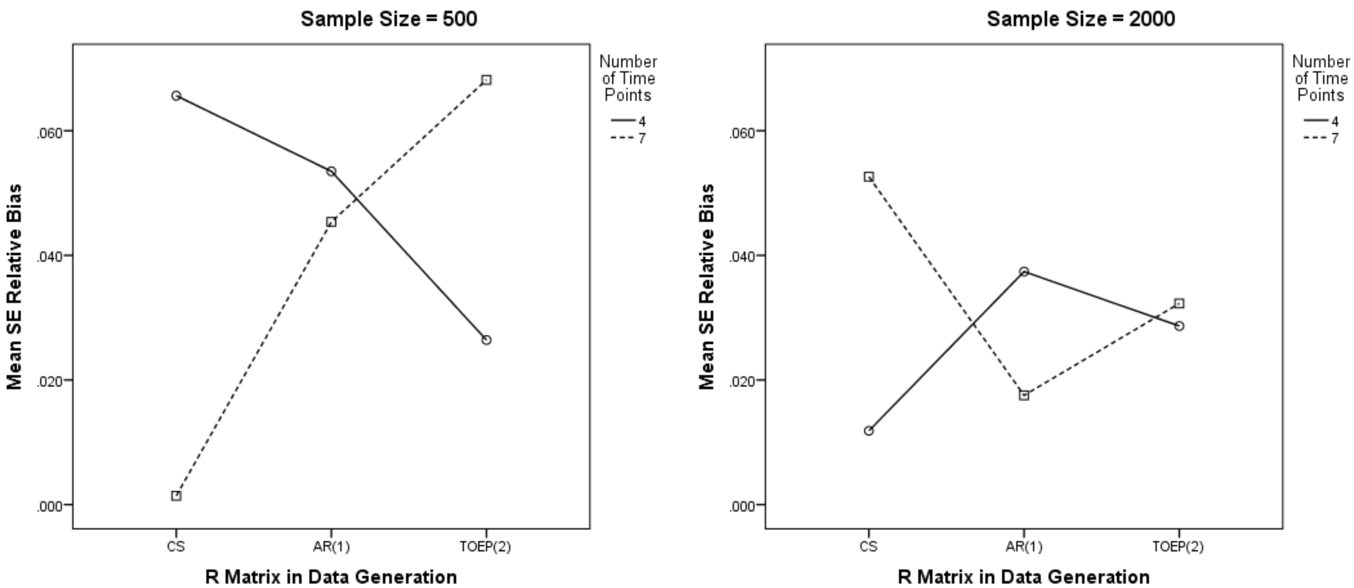

Figure 31. Mean standard error bias of $\boldsymbol{\beta_{21}}$ as a function of the sample size, number of time points, and *R* matrix in data generation in study 2

4.2.3.3 Summary of influences on fixed effects in simulation study 2

The estimation of the fixed effects were not impacted by the over-specification of the ***G*** matrix and the under-specification of the ***R*** matrix. The estimations of the standard errors of some fixed effects were not impacted by the over-specification of the ***G*** matrix and under-specification of the ***R*** matrix for most of the conditions. Some were slightly over-estimated and some were slightly under-estimated based on the certain conditions.

4.2.4 Random effects

In simulation study 2, the random effects of the intercept (τ_{00}) and the growth rate (τ_{11}) were present in the generated data. To examine the influence of over-specification of the ***G*** matrix and under-specification of the ***R*** matrix, the random effects of the intercept, growth rate, and quadratic growth rate (τ_{22}) were considered in the analysis. Therefore, there were totally four parameters related to the random effects including one first-level residual variance (σ^2) and three second-level variance and covariance including the variances of the random intercept (τ_{00}) and the random growth rate (τ_{11}), and their covariance (τ_{10}). The relative biases of these four parameters for each condition were calculated by equation 37 and were reported in Table 27.

Mixed ANOVA models were also performed on relative biases of variance components. The same five factors were considered as in the analysis for the standard errors of fixed effects. The four between-subject factors included the sample size, the number of time points, complete or missing data, and the ***R*** matrix in data generation. One within-subject factor was the ***R*** matrix used in the analysis. The ANOVA results were reported in Table 28.

4.2.4.1 Relative bias of the first-level residual variance

The relative bias of the first-levels residual variance random effects for each condition were presented in Tables 27 when the ***G*** matrix was over-specified and the ***R*** matrix was under-specified. They were under-estimated for all designed factors.

The ANOVA results in Table 28, showed that there was one two-way interaction effect between the ***R*** matrix used in the analysis and the ***R*** matrix in data generation (η_p^2 = 0.685). The variance of the first-level residual was under-estimated when the ***R*** matrix was under-specified and the ***G*** matrix was over-specified. The ***R*** matrix in data generation and the ***R*** matrix in data analysis also had large effects on the first-level residual variance (η_p^2 = 0.793 and η_p^2 = 0.294). Figure 32 showed the two-way interaction effect and suggested that the biases were smaller for the correct model (vs ID as the ***R*** matrix in the analysis). However, the relative biases were the same for both correct model and an ID as the ***R*** matrix in the analysis when CS as the ***R*** matrix in the data generation.

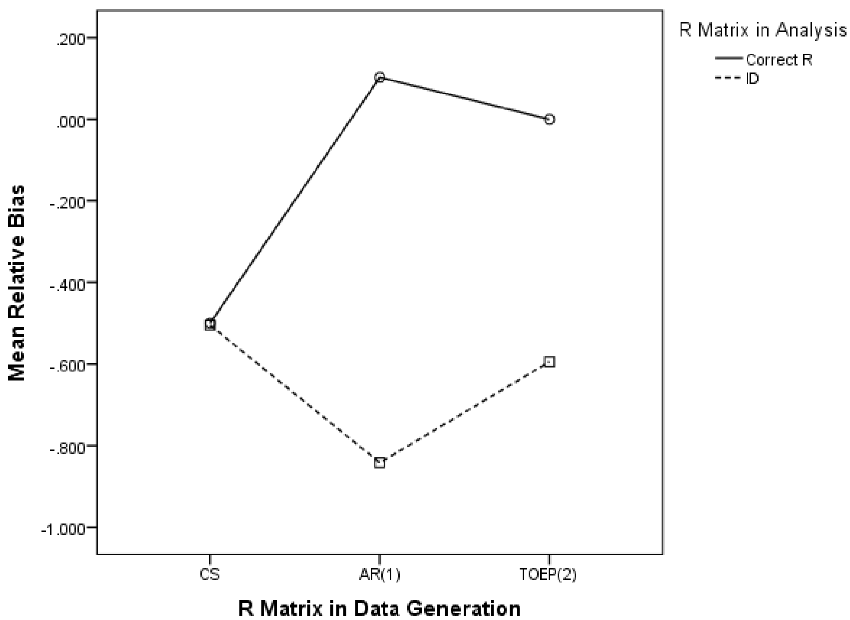

Figure 32. Mean relative bias of σ^2 as a function of the *R* matrix in data generation and *R* matrix in the analysis in study 2

Table 27. Relative bias of random effects for each condition in study 2

Complete or missing	Sample size	Time point	R matrix in data generation	R matrix	σ^2	τ_{00}	τ_{10}	τ_{11}
Complete	500	4	CS	CS	-0.499	0.498	0.001	-0.001
Complete	500	4	CS	ID	-0.508	0.510	0.003	0.002
Complete	500	4	AR(1)	AR(1)	0.196	-0.203	0.002	0.003
Complete	500	4	AR(1)	ID	-0.868	0.859	0.000	0.170
Complete	500	4	TOEP(2)	TOEP(2)	0.001	0.003	0.011	-0.004
Complete	500	4	TOEP(2)	ID	-0.750	0.727	0.015	0.399
Complete	500	7	CS	CS	-0.500	0.500	0.005	0.001
Complete	500	7	CS	ID	-0.503	0.502	0.003	0.001
Complete	500	7	AR(1)	AR(1)	0.054	-0.056	0.008	0.001
Complete	500	7	AR(1)	ID	-0.813	0.793	0.008	0.305
Complete	500	7	TOEP(2)	TOEP(2)	-0.002	0.005	0.007	-0.003
Complete	500	7	TOEP(2)	ID	-0.430	0.393	0.005	0.281
Complete	2000	4	CS	CS	-0.500	0.500	0.001	0.001
Complete	2000	4	CS	ID	-0.504	0.502	0.001	0.003
Complete	2000	4	AR(1)	AR(1)	0.121	-0.123	0.002	0.003
Complete	2000	4	AR(1)	ID	-0.867	0.862	0.003	0.171
Complete	2000	4	TOEP(2)	TOEP(2)	-0.000	-0.000	0.003	-0.000
Complete	2000	4	TOEP(2)	ID	-0.750	0.723	0.007	0.400
Complete	2000	7	CS	CS	-0.500	0.500	0.000	-0.000
Complete	2000	7	CS	ID	-0.502	0.500	-0.000	-0.000
Complete	2000	7	AR(1)	AR(1)	0.019	-0.018	0.006	0.003
Complete	2000	7	AR(1)	ID	-0.813	0.798	0.005	0.308
Complete	2000	7	TOEP(2)	TOEP(2)	-0.000	-0.001	0.001	0.000
Complete	2000	7	TOEP(2)	ID	-0.429	0.388	0.001	0.285

Table 27 (continued)

Complete or missing	Sample size	Time point	R matrix in data generation	R matrix	σ^2	τ_{00}	τ_{10}	τ_{11}
Missing	500	4	CS	CS	-0.500	0.505	0.002	-0.001
Missing	500	4	CS	ID	-0.510	0.513	0.000	0.002
Missing	500	4	AR(1)	AR(1)	0.182	-0.191	0.006	0.008
Missing	500	4	AR(1)	ID	-0.867	0.859	-0.003	0.173
Missing	500	4	TOEP(2)	TOEP(2)	0.000	0.002	0.008	-0.003
Missing	500	4	TOEP(2)	ID	-0.744	0.725	-0.020	0.426
Missing	500	7	CS	CS	-0.499	0.486	0.002	-0.001
Missing	500	7	CS	ID	-0.503	0.503	-0.002	-0.001
Missing	500	7	AR(1)	AR(1)	0.079	-0.080	0.014	0.005
Missing	500	7	AR(1)	ID	-0.820	0.801	-0.022	0.355
Missing	500	7	TOEP(2)	TOEP(2)	-0.002	0.005	0.008	-0.003
Missing	500	7	TOEP(2)	ID	-0.455	0.424	-0.071	0.365
Missing	2000	4	CS	CS	-0.501	0.504	0.001	-0.000
Missing	2000	4	CS	ID	-0.506	0.505	0.002	0.001
Missing	2000	4	AR(1)	AR(1)	0.129	-0.132	0.003	0.005
Missing	2000	4	AR(1)	ID	-0.867	0.862	-0.003	0.175
Missing	2000	4	TOEP(2)	TOEP(2)	-0.000	-0.000	0.003	0.001
Missing	2000	4	TOEP(2)	ID	-0.745	0.722	-0.027	0.427
Missing	2000	7	CS	CS	-0.500	0.499	-0.000	-0.001
Missing	2000	7	CS	ID	-0.502	0.501	-0.001	-0.001
Missing	2000	7	AR(1)	AR(1)	0.042	-0.039	0.008	0.002
Missing	2000	7	AR(1)	ID	-0.820	0.808	-0.032	0.356
Missing	2000	7	TOEP(2)	TOEP(2)	-0.000	-0.001	-0.001	-0.001
Missing	2000	7	TOEP(2)	ID	-0.453	0.419	-0.077	0.365

Table 28. ANOVA results for relative biases of random effects in study 2

Factors	σ^2	τ_{00}	τ_{10}	τ_{11}
R matrix in data generation (RG)	**0.294**	**0.322**	0.002	**0.709**
Complete or missing data (CM)	–	–	0.004	0.019
Sample size (SS)	0.001	0.001	–	–
Number of time point (T)	0.025	0.030	0.001	0.013
R matrix in data analysis (RA)	**0.793**	**0.774**	0.045	**0.970**
RA*CM	–	–	0.049	**0.114**
RA*SS	0.001	0.001	–	–
RA*T	0.082	0.085	0.015	0.095
RA*RG	**0.685**	**0.665**	0.032	**0.948**
CM*SS	–	–	–	–
CM*T	–	–	0.001	0.007
CM*RG	–	–	0.003	0.014
SS*T	–	–	–	–
SS*RG	0.002	0.003	–	–
T*RG	0.083	0.087	0.001	**0.213**
RA*CM*SS	–	–	–	–
RA*CM*T	–	0.001	0.011	0.054
RA*CM* RG	–	–	0.035	0.087
RA*SS*T	–	–	–	–
RA*SS* RG	0.002	0.002	–	0.001
RA*T* RG	0.052	0.054	0.007	**0.674**
CM*SS*T	–	–	–	–
CM*SS* RG	–	–	–	–
CM*T* RG	–	–	–	0.004
SS*T* RG	–	–	–	–

Note: Partial Eta-Square (η_p^2) is reported in the table.

–: indicates that the η_p^2<0.001

4.2.4.2 Relative bias of the second-level random effects

The relative biases of the second-level random effects for each condition were presented in Tables 27 when the ***G*** matrix was over-specified and the ***R*** matrix was under-specified. The results from mixed ANOVA models were presented in Table 28.

Random effect of intercept (τ_{00}). The relative biases of the random effect of the intercept were out of the acceptable range. All τ_{00} were over-estimated in all designed conditions.

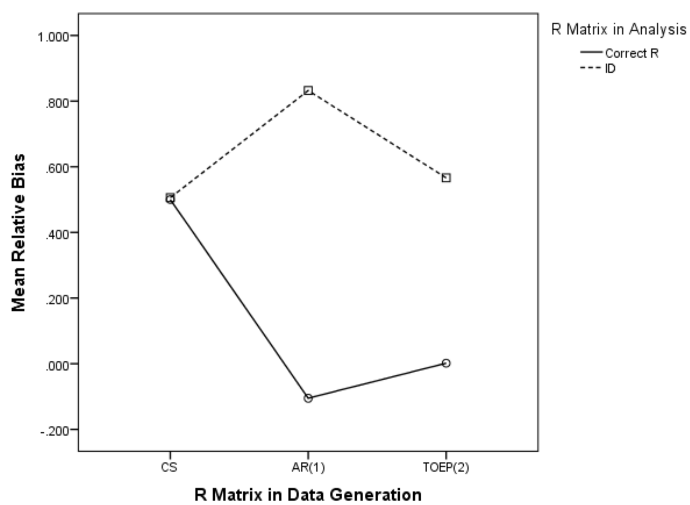

Figure 33. Mean relative bias of $\boldsymbol{\tau_{00}}$ as a function of the ***R*** matrix in data generation and analysis for study 2

According to ANOVA results, the following conditions had the appreciable effects on the relative bias for estimates of τ_{00}: the ***R*** matrix used in the analysis (η_p^2 = 0.774), the ***R*** matrix in data generation (η_p^2 = 0.322), and a two-way interaction effect between the ***R*** matrix used in the analysis and the ***R*** matrix in data generation (η_p^2 = 0.665). Figure 33 presented the two-way interaction effect and suggested that the biases were smaller using the correct model, while they were larger when the AR(1) was the ***R*** matrix in data generation.

Random effect of the growth rate (τ_{11}). The relative biases of random effect of the growth rate were out of the acceptable range for most of the conditions (see Table 27). The random effects of the growth rate were over-estimated in all designed conditions.

The ANOVA results showed that there were one three-way interaction effect and three two-way interaction effects. The three-way interaction effect was among the ***R*** matrix used in the analysis, the ***R*** matrix in data generation, and the number of time points (η_p^2 = 0.674). The three two-way interaction effects included the interaction effect between the ***R*** matrix used in the analysis and the complete or missing data (η_p^2 = 0.114), the interaction between the ***R*** matrix used in the analysis and the ***R*** matrix in data generation (η_p^2 = 0.948), and the interaction between the ***R*** matrix in data generation and the number of time points (η_p^2 = 0.213). The two-way interaction effect between the ***R*** matrix used in the analysis and complete or missing data can be observed in Figures 34. The ***R*** matrices in data generation and in data analysis also had large effects on the variance of the random linear slope (η_p^2 = 0.709 and η_p^2 = 0.970). Figure 34 illustrated the three-way interaction effect and suggested that the biases were larger when the ***R*** matrix in the analysis was under-specified as ID. However, when CS was the ***R*** matrix in the data generation, the biases was the same for both correct models and an ID as the ***R*** matrix.

Covariance between the random intercept and linear slope (τ_{10}). The covariance τ_{10} were slightly under+-estimated for most of the conditions and the relative biases of τ_{10} were within an acceptable range from -0.077 to 0.015.

According to the ANOVA results in Table 28, the results were consistent with the relative bias of τ_{10} for each condition. There were no any significant effects on the relative bias of τ_{10}.

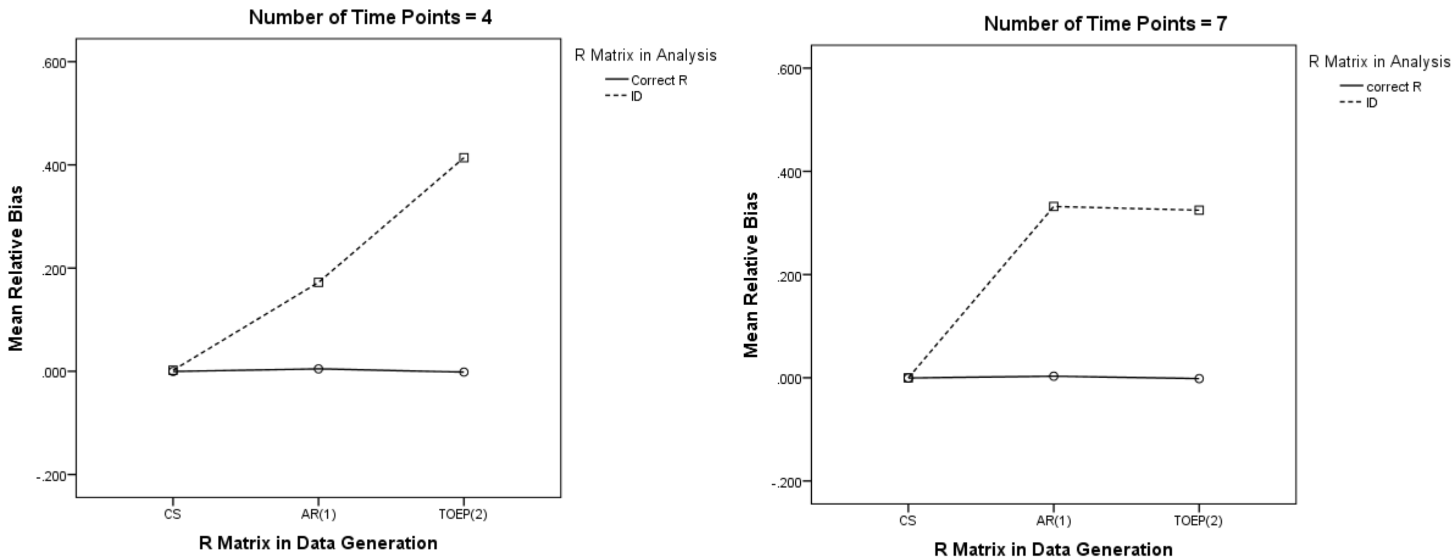

Figure 34. Mean relative bias of $\boldsymbol{\tau_{11}}$as a function of the number of time points, *R* matrix in data generation, and *R* matrix in analysis in study 2

4.2.4.3 Summary of influences on random effects in simulation study

There were no influences on the fixed effects and the standard errors of the fixed effects by the under-specification of the ***R*** matrix and over-specification of the ***G*** matrix in simulation study 2. The random effects were influenced by the under-specification of the ***R*** matrix and over-specification of the ***G*** matrix. The first-level residual variance was under-estimated. The variances of the random intercept and linear slope were over-estimated. The covariance between the random intercept and the random linear slope was unbiased.

4.2.5 Type I error rate

The Type I error rates were examined for the conditions that the values of true parameters were equal to zero under the under-specification of the ***R*** matrix and over-specification of the ***G*** matrix. The examined parameters included the fixed effects and random effects. The fixed effects included the overall mean of the growth rate (β_{10}), the overall mean of the acceleration rate (β_{20}), the effect of *W* on the initial status (β_{01}), the effect of *W* on the growth rate of the linear change (β_{11}), the effect of W on the acceleration rate of the quadratic slope (β_{21}). The random effects included the random effect of the quadratic growth rate (τ_{22}), then the covariance between the random intercept and the random quadratic slope (τ_{20}), and the covariance between the random linear slope and the random quadratic slope (τ_{21}). The results are presented in Tables 29 and 30 for fixed and random effects, respectively.

4.2.5.1 Type I error for fixed effects

Table 29 shows the Type I error rates for the fixed effects by the number of time points, complete data or missing data, and the sample size.

Type I error rates by the number of time points: In the 4 waves' analysis, the Type I error rates of β_{10} were higher than those in the 7 waves' analysis when the designed ***R*** matrix was CS and AR(1). The rates were higher in the 7 waves' analysis when the designed ***R*** matrix was TOEP(2). The Type I error rates of β_{20} were relatively higher with the range of 4.35% to 5.25% in the 4 waves' analysis and 4.75% to 6.40% in the 7 waves' analysis. In the 7 waves' analysis, the Type I error rates of β_{20} were higher than 5% when the designed ***R*** matrix was AR(1) and TOEP(2). The Type I error rates of β_{01} were the highest when the designed ***R*** matrix was AR(1) in the 7 waves' analysis and when the designed ***R*** matrix was TOEP(2) in the 4 waves' analysis. The Type I error rates of β_{11} were the highest in both the 4 and 7 waves' analyses when the designed ***R*** matrix was CS. When the designed ***R*** matrix was TOEP(2), the Type I error of β_{21} was the highest one in the 4 waves' analysis and lowest one in the 7 waves' analysis

Table 29. Type I error rates for fixed effects in study 2

Factors	Levels	R matrix in simulated data	R matrix in analysis	Time (β_{10}) (%)	Time^2 (β_{20}) (%)	Wi (β_{01}) (%)	Time × Wi (β_{11}) (%)	Time^2 × Wi (β_{21}) (%)
Time point	4	CS	Correct	4.85	4.95	4.50	4.45	4.95
			ID	4.90	4.80	4.60	4.45	4.70
		AR(1)	Correct	4.95	4.45	5.15	3.95	4.45
			ID	4.80	4.35	5.20	4.00	4.50
		TOEP(2)	Correct	4.85	5.45	6.25	3.95	5.40
			ID	4.55	5.25	6.35	3.20	5.35
	7	CS	Correct	4.25	4.75	4.85	5.05	3.90
			ID	4.15	4.75	4.90	5.05	3.85
		AR(1)	Correct	5.00	6.65	5.15	3.70	5.40
			ID	4.40	6.40	5.10	3.35	4.85
		TOEP(2)	Correct	4.55	5.25	5.20	4.05	4.50
			ID	4.65	5.20	4.55	3.95	3.65
Complete or missing data	Missing	CS	Correct	4.45	4.60	4.65	4.45	4.55
			ID	4.40	4.60	4.80	4.45	4.40
		AR(1)	Correct	4.85	5.55	5.00	3.90	5.25
			ID	4.40	5.25	5.00	3.85	5.00
		TOEP(2)	Correct	4.65	5.55	5.80	3.90	4.60
			ID	4.85	5.45	5.45	3.70	4.20
	Complete	CS	Correct	4.65	5.10	4.70	5.05	4.30
			ID	4.65	4.95	4.70	5.05	4.15
		AR(1)	Correct	5.10	5.55	5.30	3.75	4.60
			ID	4.80	5.50	5.30	3.50	4.35
		TOEP(2)	Correct	4.75	5.15	5.65	4.10	5.30
			ID	4.35	5.00	5.45	3.45	4.80
Sample size	500	CS	Correct	4.45	4.70	5.36	3.80	3.85
			ID	4.30	4.65	5.35	3.80	3.65
		AR(1)	Correct	4.65	5.55	6.25	3.85	5.65
			ID	4.15	5.05	6.20	3.95	5.30
		TOEP(2)	Correct	3.85	5.25	5.30	3.90	5.30
			ID	3.95	4.85	5.25	3.30	4.45
	2000	CS	Correct	4.65	5.00	4.00	5.70	5.00
			ID	4.75	4.90	4.15	5.70	4.90
		AR(1)	Correct	5.30	5.55	4.05	3.80	4.20
			ID	5.05	5.70	4.10	3.40	4.05
		TOEP(2)	Correct	5.55	5.45	6.15	4.10	4.60
			ID	5.25	5.60	5.65	3.85	4.55

Type I error by complete and missing data: In the analysis with missing data, the Type I error rates of β_{10} were higher than those in the analysis with the complete data in average, which were smaller than 5% for all the conditions. The Type I error rates of β_{20} and β_{21} were higher than 5% when the designed ***R*** matrix was AR(1) and TOEP(2) in both the complete and missing data. The Type I error rates of β_{01} were relatively higher than the others, especially when the designed ***R*** matrix was TOEP(2). The Type I error rates of β_{11} were relatively lower in which they were smaller than 5% for the most of the conditions. The Type I error rates of β_{21} were lower than 5% except the correct models.

Type I error by the sample size: The Type I error rates of β_{10} were lower for the sample size of 500 than those for the sample size of 2000 on average. The Type I error rates of β_{20} and β_{01} were relatively higher. The Type I error rates of β_{11} were lower than the others. The Type I error rates of β_{21} were lower than 5% for most of the conditions.

4.2.5.2 Type I error for random effects

Table 30 shows the Type I error rates of the random effects (τ_{20}, τ_{21}, and τ_{22}) by the number of time points, complete data or missing data, and the sample size.

The Type I error rates of τ_{20} and τ_{22} were very high and close to 100% when the designed ***R*** matrix was AR(1) and TOEP(2). The Type I rates of τ_{21} were lower than the Type I error rates of τ_{20} and τ_{22} when the designed ***R*** matrix was AR(1) and TOEP(2) that were higher than 5% for most of the conditions. The Type I error rates were close to 5% when the designed ***R*** matrix was CS across all the conditions.

Table 30. Type I error rates for random effects in study 2

Factors	Levels	***R*** matrix	τ_{20} (%)	τ_{21} (%)	τ_{22} (%)
Time point	4	CS	5.10	4.90	4.95
		AR(1)	98.33	6.43	99.75
		TOEP(2)	100	8.80	100
	7	CS	4.88	4.95	3.93
		AR(1)	100	26.23	100
		TOEP(2)	99.98	27.23	100
Complete and missing data	Missing	CS	5.03	4.85	4.63
		AR(1)	98.50	27.40	99.75
		TOEP(2)	99.98	31.95	100
	Complete	CS	4.95	5.00	4.25
		AR(1)	99.83	5.25	100
		TOEP(2)	100	4.08	100
Sample size	500	CS	4.50	4.50	4.15
		AR(1)	98.33	9.58	99.75
		TOEP(2)	99.98	9.98	100
	2000	CS	5.23	5.35	4.73
		AR(1)	100	23.08	100
		TOEP(2)	100	26.05	100

4.2.6 Singularity rate

Table 31 shows the dimension frequencies of the reduced ***R*** matrix had a similar pattern for the designed ***R*** matrices. In the 4 waves' analysis, there were about 50% of the missing data sets had the solution for the matrix product, about 40% and 10% of the missing data sets had the reduced ***R*** matrix with the dimensions of 3 and 2, respectively. In the 7 waves' analysis, there were only about 7% of the estimated ***R*** matrices having the dimension of 7 and about 93% of the results having the reduced ***R*** matrices.

Table 31. Singularity rate by the number of time points and generated R matrix in study 2

Dimension of reduced ***R*** matrix	***R*** matrix = CS		***R*** matrix = AR(1)		***R*** matrix = TOEP(2)	
	Time point		Time point		Time point	
N (Col Pct)	4	7	4	7	4	7
7		296 (7.40%)		310 (7.75%)		246 (6.15%)
6		933 (23.33%)		936 (23.40%)		930 (23.25%)
5		1362 (34.04%)		1298 (32.45%)		1452 (36.30%)
4	1997 (49.94%)	964 (24.11%)	2038 (50.95%)	1054 (26.35%)	1990 (49.75%)	968 (24.20%)
3	1628 (40.71%)	384 (9.6%)	1540 (38.55%)	312 (7.8%)	1628 (40.70%)	356 (8.9%)
2	374 (9.35%)	60 (1.5%)	422 (10.55%)	90 (2.25%)	382 (9.55%)	48 (1.2%)

4.3 SUMMARY OF THE RESULTS

The results from two simulation studies showed that there were no influences on the fixed effects even the ***R*** matrix and the ***G*** matrix were misspecified. However and the standard errors of the fixed effects and random effects were influenced by the misspecification of the ***R*** matrix and the ***G*** matrix. Table 32 and Table 33 show the impact on the standard errors of fixed effects and random effects, respectively.

Table 32. The influence on estimations of standard errors of fixed effects

Simulation	Misspecification of		Standard error of fixed effects		
	R matrix	*G* matrix	Intercept (β_{00})	Time (β_{10})	Time^2 (β_{20})
1	Unstructured	Null	Underestimates Similar to correct model	Underestimates Similar to correct model	Underestimates Similar to correct model
	Over-specification	Under-specification	<u>Overestimates</u>	Underestimates *Similar to correct model*	<u>Underestimates</u>
2	Under-specification	Over-specification	*Underestimates* Similar to correct model	*Underestimates* Similar to correct model	Overestimates Similar to correct model
Simulation	*R* matrix	*G* matrix	Wi (β_{01})	Time × Wi (β_{11})	Time^2 × Wi (β_{21})
1	Unstructured	Null	Overestimates Similar to correct model	Overestimates Similar to correct model	Overestimates Similar to correct model
	Over-specification	Under-specification	<u>Overestimates</u>	Overestimates Similar to correct model	<u>Underestimates</u>
2	Under-specification	Over-specification	<u>Overestimates</u>	Overestimates Similar to correct model	Overestimates Similar to correct model

Table 33. The influence on estimations of random effects

Misspecification of		First-level	Second-level Random effects		
R matrix	***G*** matrix	σ^2	τ_{00}	τ_{10}	τ_{11}
Over-specification	Under-specification	<u>Overestimates</u>	<u>Overestimates</u>	<u>Overestimates</u>	<u>Underestimates</u>
Under-specification	Over-specification	<u>*Underestimates*</u>	<u>Overestimates</u>	Underestimates Similar to correct model	<u>Overestimates</u>

In the tables 32 and 33, underlined cells were biased estimations, the cells with italic disagreed with previous studies, the cells with highlighted background were new findings from the study. The comparisons with previous studies in detail were discussed in the discussion section.

5.0 DISCUSSION

The purpose of this dissertation is to investigate the influence on the fixed and random effects in two-level hierarchical quadratic growth models due to the misspecification of the within-subject and between-subject covariance structures through two simulations. The estimations of the growth parameters, their corresponding standard errors, and variance/covariance components of random effects were examined. Selecting the optimal covariance structure by the standardized root mean square was compared with information criteria methods. This section summarizes the major findings, states the study limitations, and provides the future research directions.

5.1 SUMMARY OF MAJOR FINDINGS

Two simulation studies are designed to examine the compensation of covariances due to the under-specification at one level with the over-specification at another level. The findings answer the three main research questions, and also provide practical guidance for selecting the optimal covariance structure and proper models.

Question 1: If the within-subject covariance structure is simple and the between-subject covariance structure is complex, once the between-subject covariance structure is under-specified, will the complex within-subject covariance structure recover the overall covariance structure? What is the impact on the fixed and random effects?

Question 2: If the within-subject covariance structure is complex and the between-subject covariance structure is simple, once the within-subject covariance structure matrix is under-specified, will the complex between-subject covariance structure recover the overall covariance structure? What is the impact on the fixed and random effects?

Question 3: Does the standardized root mean square residual provide improvement over information criteria methods in searching for the optimal covariance structure using hierarchical quadratic growth models?

Simulation study 1 aims to answer the research question 1, simulation study 2 aims to answer the research question 2, and the two simulation studies together aim to answer the research question 3.

5.1.1 Simulation study 1

Simulation study 1 investigated whether the under-specification of the second-level covariance structure (***G*** matrix) can be compensated by the over-specification of the first-level covariance structure (***R*** matrix). To answer the research question 1, a two-level hierarchical quadratic growth model was considered with a level-2 variable (*W*) predicting the level-1 intercept, the linear slope and the quadratic slope. Five simulation design factors were considered, including the sample size (500 and 2000), the number of time points (4 and 7), missing or balanced data (complete and missing data), the effect sizes of the ***G*** matrix (small and medium), and the ***R*** matrix (CS, AR(1), TOEP(2), and UN) in the analyses. To compare the relative biases of fixed and random effects, the correct models with ID as the ***R*** matrix were also performed. In addition, the Type I error rates for the fixed effects were examined for which the data generation model had all fixed effects (except intercept) set at zero value.

The estimates of the fixed effects were unbiased in all conditions when the ***G*** matrix was under-specified and the ***R*** matrix was over-specified. This finding was consistent with the previous research when the covariance structures were misspecified (Ferron et al., 2002; Kasim & Raudenbush, 1998; Kwok et al., 2007; Lange & Laird, 1989; Lee, 2010; Murphy & Pituch, 2009).

The estimates of the standard errors of the fixed effects were biased. When the ***R*** matrix was UN, the standard errors of the intercept (β_{00}) and the effect of *W* on the initial status (β_{01}) were slightly under-estimated and over-estimated, respectively, and there were very close to the correct model with ID as the R matrix. The findings for the intercept is consistent with the previous studies (Ferron et al., 2002; Kwok et al., 2007; Lee, 2010) in which UN was the ***R*** matrix in the analysis. The standard errors of the intercept (β_{00}) and the effect of *W* on the initial status (β_{01}) were significantly over-estimated when the ***R*** matrix used in the analysis was CS, AR(1), and TOEP(2), which is consistent with Lee's (2010) results on the intercept, but also extend to the effect of the second-level variable on the initial status.

The standard errors of the linear slope (β_{10}) and quadratic slopes (β_{20}) were under-estimated for all the conditions, which agreed with the previous researches (Ferron et al., 2002; Kwok et al., 2007; Lee, 2010). The relative biases of the standard errors of β_{10} were smaller than those of β_{20} in magnitude. The relative biases of the standard errors of β_{10} were less than .1 (considered unbiased) for all conditions except the three conditions with R matrix as CS, AR(1), and TOEP(2) for missing data, 500 subjects, 7 time points, and medium G matrix. However, the relative biases of the standard errors of β_{20} were greater than .1 for all conditions except the conditions with the R matrix as ID and UN, and the conditions with the ***R*** matrix as CS, AR(1), and TOEP(2) for 2000 subjects, 4 time points, and small G matrix. If the ***R*** matrix was CS, AR(1), and TOEP(2), the magnitude of the relative biases of the standard errors of β_{10} were almost the same for different ***R*** matrices used in the analysis when the other factors were at the same level.

The relative biases of the standard errors of the effect of *W* on the linear change rate (β_{11}) were smaller than .1 in all conditions. However, the effect of *W* on the quadratic slope (β_{21}) had negatively biased standard errors except in the conditions with UN and ID (the correct model) as the ***R*** matrix. When the ***R*** matrix was CS, AR(1), and TOEP(2), the standard error of (β_{21}) has larger bias in magnitude for more time points and larger G matrix.

The estimates of random effect variances/covariance were also biased when the ***R*** matrix was over-specified and the ***G*** matrix was under-specified. The first-level residual variances were over-estimated, which agreed with the previous study by Kwok et al. (2007). This study extends the findings to more general condition when the ***G*** matrix dimensions were underspecified.

The estimates of the variance of the intercept (τ_{00}) were over-estimated for all the conditions, which agreed with the previous research (Kwok et al., 2007). However, the estimates of the variance of the growth rate (τ_{11}) were under-estimated for all the conditions, which differs from the study by Kwok et al. (2007) that had over-estimation. In their study, the ***R*** matrix was over-specified, but the ***G*** matrix was the correct covariance structure that was UN. In the current study, the ***G*** matrix was under-specified. The estimates of covariance (τ_{10}) between the intercept and linear slope were over-estimated.

When the ***R*** matrix was over-specified and the ***G*** matrix was under-specified, the estimates of the fixed effects were unbiased, but the standard error of the fixed effects were biased. The resulted under-estimation of standard errors of the quadratic growth parameters (quadratic slope and the effect of level-2 variable on the quadratic slope), which in turn, resulted in higher Type I error rates, especially when the ***G*** matrix was large. These results, along with the resulted biased variance components, suggest that the over-specification of the first-level covariance structure cannot compensate the under-specification of the second-level covariance structure, especially for the fixed effects related to the quadratic slopes, and variance components of linear slopes. When the second-level covariance structure has to be under-specified, we recommend to use UN as the level-1 covariance structure so that the fixed effects and their standard errors will be unbiasedly estimated given that applied researchers are more interested in hypothesis testing of fixed effects.

5.1.2 Simulation study 2

Simulation study 2 investigated whether the under-specification of the first-level covariance structure (***R*** matrix) can be compensated by the over-specification of the second-level covariance structure (***G*** matrix). To answer the research question 2, four factors were considered. There were two levels of the sample size (500 and 2000), two levels of the number of time points (4 and 7), two levels of missing or balanced data (complete and missing data), and three levels of the ***R*** matrix (CS, AR(1), and TOEP(2)) in the data generation. In addition, a continuous level-2 variable was added in two-level hierarchical quadratic growth models.

The estimates of the fixed effects were unbiased. This finding is consistent with the previous researches when the covariance structures were misspecified (Ferron et al., 2002; Kasim & Raudenbush, 1998; Kwok et al., 2007; Lange & Laird, 1989; Lee, 2010; Murphy & Pituch, 2009).

The estimations of the standard errors of fixed effects were unbiased for almost all the conditions (only one condition has bias slightly greater than .1 for three parameters). The finding is not totally consistent with the previous studies (Kwok et al., 2007; Lee, 2010). This was because in the study by Kwok et al. (2007), the ***G*** matrix used in the model was correct and the same as the data generation model; in Lee's study (2010), the designed ***G*** matrix was a 2×2 matrix with only random effects of the intercept and linear slope and the covariance between the intercept and linear slope was zero. The ***G*** matrix used in the analysis was UN in Lee's study. It was not clear whether the ***G*** matrix was over-specified or it was the correct matrix in Lee's study. However, the results that the relative bias of the standard errors of the fixed effects were close to the correct model, were consistent with the previous studies. Also the concept of the over-specification of the ***G*** matrix in the current study was different from Lee's study. In Lee's study, only the covariance structure changed with a more complex matrix. But in this study, the modeled ***G*** matrix had higher dimensions, which accounted for a small portion of the total covariance structure of the repeated measures.

Under the under-specification of the ***R*** matrix and the over-specification of the ***G*** matrix, the standard errors of the effect of W on the initial status (β_{01}) were slightly over-estimated, which extends the over-estimates of the intercept in Lee's study (2010). The relative biases of the standard errors of the effect of W on the growth rate of the linear change (β_{11}) were smaller than those of the quadratic slope (β_{21}), and they both were close to the correct model. They were slightly over-estimated, which extends the relative biases on the growth rate in Lee's study (2010).

The estimates of random effects were also biased when the ***R*** matrix was under-specified and the ***G*** matrix was over-specified. The first-level residual variance was under-estimated, which is not consistent with the previous study by Kwok et al. (2007). This may be due to the ***G*** matrix in the previous study was correctly specified.

The estimates of the random intercept variance (τ_{00}) and the linear growth rate variance (τ_{11}) were over-estimated for all the conditions, which agreed with the previous research (Kwok et al., 2007). In their study, the ***R*** matrix was over-specified and the ***G*** matrix was UN, which had similar models and setting of covariance structures. The estimates of the covariance between random intercept and linear slope were slightly under-estimated and close to the correct models.

When the ***R*** matrix was under-specified and the ***G*** matrix was over-specified, the estimates of fixed effects and their standard errors were unbiased, but variance/covariance of the random effects were biased. Therefore, the over-specification of the second-level covariance structure does not impact fixed effects but neither can it compensate the total covariance structure due to the under-specification of the first-level covariance.

5.1.3 Standardized Root Mean square Residual in selecting the optimal covariance structure

Based on the results from the two simulations studies, SRMR has the correct rates for searching the optimal covariance structure at 39.9% and 73.6% on average for two studies, respectively. When the ***R*** matrix was over-specified and the ***G*** matrix was under-specified in the simulation study 1, BIC was the best method in selection of an optimal covariance structure at the correct rate of 100% under the designed conditions. The correct rates for AIC and AICC were close at about 94%. When the ***R*** matrix was under-specified and the ***G*** matrix was over-specified in simulation 2, BIC, AIC, and AICC had the correct rates for searching the optimal covariance structure at 99.4%, 88.1%, and 88.2%, respectively. The results from the two studies were consistent that SRMR tended to choose a more complex ***R*** matrix.

The results are somewhat not consistent with the study by Lee (2010), in which the correct rate for searching the correct covariance structure at about 81% across all the conditions, much higher than the rates that SRMR had in the current study. In addition, AIC and BIC had lower rates of correctly selecting the covariance structure in Lee's study. We conclude that SRMR does not provide improvement over information criteria methods in searching for the optimal covariance structure in hierarchical quadratic growth models under the designed conditions in both studies. SRMR was calculated based on the differences of total variance/covariance matrix between the model based variance/covariance structure and the correct data covariance structure. Due to the misspecification of the ***G*** and ***R*** matrices, the estimation of model based covariance matrix was biased, which made the SRMR method working poorly in identifying the optimal covariance structure.

We found that BIC performed better than AIC. In comparison to AIC, BIC penalizes the number of parameters more strongly depending on the relative magnitude of sample size and number of parameters. The superiority of BIC over AIC was consistent with prior studies in linear mixed models (Ferron et al., 2002; Liu et al., 2012; Ye, 2005).

5.1.4 Conclusion and Recommendation

The convergence rates were very high in the study when the sample size at the second-level was greater than 500. When the ***R*** matrix was over-specified and the ***G*** matrix was under-specified in simulation study 1, the convergence rates were slightly lower than in simulation study 2 when the ***R*** matrix was under-specified and the ***G*** matrix was over-specified.

There were no biases on the estimations of fixed effects even when the ***R*** matrix and ***G*** matrix were misspecified. When using the longitudinal data to run hierarchical quadratic growth models, the analysis results are reliable if only the magnitude of growth parameters is of interest. There were no impacts on the fixed effects due to the misspecification of between-subject and within-subject covariance structures in hierarchical quadratic growth models.

The estimation of the standard errors of the fixed effects was biased when the within-subject and between-subject covariance structures were misspecified. In simulation study 1, when the ***R*** matrix was over-specified and the ***G*** matrix was under-specified, the relative biases of standard errors of fixed effects were larger in magnitude than those in simulation study 2 when the ***R*** matrix was under-specified and the ***G*** matrix was over-specified. When using the inferential statistics, the test results for fixed effects should be checked carefully since the Type I error rate may be inflated due to the under-estimation of the standard error of the fixed effects associated with the underspecified quadratic slope in the ***G*** matrix in Study 1. When random slopes of quadratic change cannot be modeled, e.g., due to limited sample size, we recommend to use unspecified ***R*** matrix so that fixed effects and their standard errors can be estimated bias free. However, over-specified ***G*** matrix has little impact on fixed effects and their standard errors.

In applied studies, UN was recommended as the ***R*** matrix when the ***G*** matrix had to be under-specified if researchers are interested in only fixed effects. On the other hand, when researchers are interested in the random effects of level-1 coefficients, it is possible that the fixed effects have biased standard errors with these random effects underspecified. We recommend that the researchers also examine the fixed effects with UN covariance structure in addition to the random effect model of interest. When the results of fixed effects are similar between the model with random effects and the model with UN covariance structure, more confidence is built in the fixed effect results. When the results are different, researchers can explore the other ***R*** and ***G*** covariance structures to obtain results close to those with UN structure.

There are biased estimations of random effects due to the misspecification of within-subject and between-subject covariance structures, especially when CS was used as the ***R*** matrix. If the random effects are of interest, different ***R*** matrices and ***G*** matrices should be examined to compare the differences among the different covariance structure. If there are large differences among the results when using different ***R*** matrix, the results should be interpreted carefully.

When hierarchical quadratic growth models are used in longitudinal studies, it is common that only lower dimensions of ***R*** matrix can be estimated for unbalanced data, especially for the data with more time points. However, there is no impact on the fixed effects.

5.2 LIMITATIONS AND FUTURE RESEARCH DIRECTIONS

Hierarchical growth models are widely used in longitudinal studies. This study used two Monte Carlo simulations to address the proposed research questions in a two-level hierarchical growth model. Though the factors and conditions were carefully selected, the results may not be generalized to other situations. Therefore, the conclusions and recommendations should be considered in light of the limitations of the simulation studies.

First, the model used in the study is a two-level hierarchical quadratic growth model. The fixed effects, including the intercept, linear and quadratic growth parameters, the effect of a second-level variable and it’s interaction with linear and quadratic growth parameters, and the random effects of the intercept, linear and quadratic growth parameters were considered. It is unknown whether the influences of misspecification of covariance structures on the fixed and random effects are the same in three or higher level hierarchical growth models.

Second, the simulation studies only considered two levels of number of time points (4 and 7). Based on the literature review, a wide range of the number of time points in previous studies were from 2 to 14. More time points could be considered in the future study. In addition, as the number of time points is increased, other higher order growth parameters (such as piece-wise growth) could be considered.

Finally, the misspecification of the covariance structures impacted the estimation of the standard error of the fixed effects and random effects, which in turn inflated the Type I error rates or increased the statistical power for the growth parameters. The study results showed BIC was a very good tool to select the optimal covariance structure when the ***R*** matrix was over-specified and the ***G*** matrix was under-specified. However, when the ***R*** matrix was under-specified and the ***G*** matrix was over-specified, AIC, BIC and SRMR all did not work very well, and the correct rates for selecting the optimal covariance structure were very low. More work is needed to search for more accurate and efficient methods for selecting the optimal covariance structure.

APPENDIX A. SAS CODE FOR SIMULATION STUDY 1

```
*MACRO OF GENERATING THE DATA AND CALL TO RUN MODELS;
%let  attrate = 0.10;

%let vc_ID_4 = {1  0  0  0,
               0  1  0  0,
               0  0  1  0,
               0  0  0  1};

%let vc_ID_7 = {1  0  0  0  0  0  0,
               0  1  0  0  0  0  0,
               0  0  1  0  0  0  0,
               0  0  0  1  0  0  0,
               0  0  0  0  1  0  0,
               0  0  0  0  0  1  0,
               0  0  0  0  0  0  1};

%let Z_matrix_4 = {1  -1.5  2.25,
                  1  -0.5  0.25,
                  1   0.5  0.25,
                  1   1.5  2.25};

%let Z_matrix_7 = {1  -1.5  2.25,
                  1  -1    1,
                  1  -0.5  0.25,
                  1   0    0,
                  1   0.5  0.25,
                  1   1    1,
                  1   1.5  2.25};

%let small_stu = {0.5     0.141    0.1,
                 0.141   0.25   0.071,
                 0.1     0.071  0.125};

%let medium_stu = {1       0.283     0.2,
                  0.283    0.5    0.141,
                  0.2      0.141    0.25};
```

```
/*correlation = 0.4*/
%macro simple_R_complex_G;
 %let varcov4 = &vc_ID_4;
 %let varcov7 = &vc_ID_7;
 %let Wi_numbers = 1;

                proc iml;
                        reset print;
                        e4 = &varcov4;
                        create randomerror4 from e4;
                        append from e4;

                        e_mean4 = {0};
                        create e_means4 from e_mean4;
                        append from e_mean4;

                        e7 = &varcov7;
                        create randomerror7 from e7;
                        append from e7;

                        e_mean7 = {0};
                        create e_means7 from e_mean7;
                        append from e_mean7;
                quit;

%do rep = 1 %to &Nrep;
 %do samplesize = 1 %to 2;
        %if &samplesize = 1 %then %let Nstu = 500;
        %else %if &samplesize = 2 %then %let Nstu = 2000;

        %do G_effectsize = 1 %to 2;
          %if &G_effectsize = 1 %then %do;
            %let cov_stu = &small_stu;
                %let tuo_00 = 0.5;
                %let tuo_11 = 0.25;
                %let tuo_22 = 0.125;
     %end;
          %else %if &G_effectsize = 2 %then %do;
       %let cov_stu = &medium_stu;
                %let tuo_00 = 1;
                %let tuo_11 = 0.5;
                %let tuo_22 = 0.25;
          %end;

/*creates means & cov structure of student's level random effect to be used to create their
values in the MVN macro; */
```

```
                        proc iml;
                        cov=&cov_stu;
                         mean={0,0,0}; /*means of student's random effect*/
                        create stu_varcov from cov;
                        append from cov;
                        create stu_means from mean;
                        append from mean;
                        quit;

          %do coefficient_effectsize = 1 %to 2;
            %if &coefficient_effectsize = 1 %then %do;
              %let b00 = 10; /*intercept*/
              %let b01 = 0; /*W*/
              %let b10 = 0; /*time*/
              %let b11 = 0; /*W*time*/
              %let b20 = 0; /*time2: time squared*/
              %let b21 = 0; /*W*time2*/
                 %end;
            %if &coefficient_effectsize = 2 %then %do;
              %let b00 = 10; /*intercept*/
              %let b01 = 0.5*sqrt(&tuo_00); /*W*/
              %let b10 = 0.5*sqrt(&tuo_11); /*time*/
              %let b11 = 0.5*sqrt(&tuo_11); /*W*time*/
           %let b20 = 0.5*sqrt(&tuo_22); /*time2: time squared*/
              %let b21 = 0.5*sqrt(&tuo_22); /*W*time2*/
                 %end;


%let seed1 = 1234567 + &rep*1000+&samplesize*100
                       +&G_effectsize*10+ &coefficient_effectsize;
              /*Create the first level residual*/
  %mvn(varcov = randomerror4, means = e_means4, n = &Nstu,
                   seed = &seed1, sample = overallerror4);
  %mvn(varcov = randomerror7, means = e_means7, n = &Nstu,
                   seed = &seed1, sample = overallerror7);

                        data overallerror4;
                        set overallerror4;
                        rename col1-col4 = e1-e4;
                        run;

                        data overallerror7;
                        set overallerror7;
                        rename col1-col7 = e1-e7;
                        run;
```

```
/*randomstudent is the dataset containing the r0ij and r1ii values;*/
        %let seed2 = 7654321 + &rep+&samplesize*10+&G_effectsize*100
                        +&coefficient_effectsize*1000;
        %MVN(varcov=stu_varcov, means=stu_means, n=&Nstu,
                seed=&seed2,sample=randomstudent);

                        data randomstudent;
                        set randomstudent;
                        rename      col1 = u0i
                        col2 = u1i
                        col3 = u2i;
                        run;


            *create student level (second level) variable;
                        data stu_effect;
                            do stu_ID = 1 to &Nstu;
                             Wi = &Wi_numbers*rannor(&seed1+1000);
                             output;
                            end;
                        run;

                        *create student membership at time1;
                        data student1;
                            merge stu_effect randomstudent;
                        run;

                        *create student in five time point;
                        data student1_4;
                                set student1;
                                time1 = -1.5;
                                time2 = -0.5;
                                time3 = 0.5;
                                time4 = 1.5;
                        run;

                        *Create student file in nine time point;
                        data student1_7;
                                set student1;
                                time1 = -1.5;
                                time2 = -1;
                                time3 = -0.5;
                                time4 = 0;
                                time5 = 0.5;
                                time6 = 1;
                                time7 = 1.5;
```

```
run;

*transpose data;
data student4;
	set student1_4;
	array timevar [4] time1 - time4;
	do i = 1 to 4;
		time=timevar[i];
		output;
	end;
	drop i time1-time4;
run;

data student7;
	set student1_7;
	array timevar [7] time1 - time7;
	do i = 1 to 7;
		time=timevar[i];
		output;
	end;
	drop i time1-time7;
run;

*restructures the e values to a column vector;
data evalues4;
	set overallerror4;
	array e[4] e1-e4;
	do i = 1 to 4;
		eti = e[i];
		output;
	end;
	keep eti;
run;

data evalues7;
	set overallerror7;
	array e[7] e1-e7;
	do i = 1 to 7;
		eti = e[i];
		output;
	end;
	keep eti;
run;

*generates the dependent variable;
*This is the complete dataset;
```

```
data complete4;
        replication = &rep;
        merge student4 evalues4;
        time2 = time*time;
y = &b00 +&b01*Wi + &b10*time + &b11*Wi*time
     +&b20*time2+&b21*Wi*time2+ u0i +u1i*time +u2i*time2+eti;
      run;

data complete7;
        replication = &rep;
        merge student7 evalues7;
        time2 = time*time;

y = &b00 +&b01*Wi + &b10*time + &b11*Wi*time
     +&b20*time2+&b21*Wi*time2+ u0i +u1i*time +u2i*time2+eti;
        run;


/******* generate the other datasets with missing values ******/
data indicator4;
        set student1_4(drop = Wi--u2i);
        x0 = 0;
        x1 = ranbin(&seed1, 1, &attrate);
        x2 = ranbin(&seed1+1, 1, 2*&attrate);
        x3 = ranbin(&seed1+2, 1, 3*&attrate);
run;

*transpose data;
data student1_4Long;
                set indicator4;
                array timevar [4] time1 - time4;
                array xs[4] x0 - x3;
                do i = 1 to 4;
                        time=timevar[i];
                        missing_indicator = xs[i];
                        output;
                end;
                drop i time1-time4 x0-x3;
run;

data indicator7;
                set student1_7;
                x0 = 0;
                x1 = ranbin(&seed1, 1, &attrate);
                x2 = ranbin(&seed1+1, 1, 2*&attrate);
                x3 = ranbin(&seed1+2, 1, 3*&attrate);
```

```
                x4 = ranbin(&seed1+3, 1, 4*&attrate);
                x5 = ranbin(&seed1+4, 1, 5*&attrate);
                x6 = ranbin(&seed1+5, 1, 6*&attrate);
            run;


        *transpose data;
            data student1_7Long;
                set indicator7;
                array timevar [7] time1 - time7;
                array xs[7] x0 - x6;

                do i = 1 to 7;
                    time=timevar[i];
                    missing_indicator = xs[i];
                    output;
                end;
                drop i time1-time7 x0-x6;
            run;

            data missing4;
            merge complete4 student1_4Long;
            by stu_ID time;
            if missing_indicator = 1 then y = .;
            run;

            data missing7;
            merge complete7 student1_7Long;
            by stu_ID time;
            if missing_indicator = 1 then y = .;
            run;

*Call for analysis;
*datatype = 1 for complete data, datatype = 0 for missing data;
    %HLManalysis_4(inputdata = complete4, datatype = 1,
                sample = &rep, outdata = results_4);

    %HLManalysis_4(inputdata = missing4, datatype = 0,
                sample = &rep, outdata = results_missing_4);

    %HLManalysis_7(inputdata = complete7, datatype = 1,
                 sample = &rep, outdata = results_7);

    %HLManalysis_7(inputdata = missing7, datatype = 0,
                sample = &rep, outdata = results_missing_7);
            %end;
```

```
            %end;
          %end;
  %end;
  %mend simple_R_complex_G;


*MACRO OF RUNNING THE ANALYSIS;

%macro HLManalysis_4(inputdata=, datatype=, sample=, outdata=);
	*Calculate the correct total variance first;
	proc corr data = Overallerror4 cov;
	var e1-e4;
	ods output cov = e_cov4;
	run;

	proc corr data = Randomstudent cov;
	var u0i u1i u2i;
	ods output cov = u_cov4;
	run;

	proc iml;
		use e_cov4;
		read all into within_cov_matrix [colname=varname];

		use u_cov4;
		read all into Tau;

		ZGZ = &Z_matrix_4*Tau*&Z_matrix_4`;
		Total_variance1 = ZGZ + within_cov_matrix;

		Total_variance = shape(total_variance1, 1, 16);

		create Total_covariance_correct4 from Total_variance;
		append from Total_variance;

		variance_of_stu1=shape(Tau,1,9);

		create random_effect_generate from variance_of_stu1;
		append from variance_of_stu1;
	quit;

	data random_effect_generate;
	fit_covariance = 1;
	set random_effect_generate;
	drop col2 col3 col6;
	rename col1 = random_UN_1_1_
```

```
                col4 = random_UN_2_1_
                col5 = random_UN_2_2_
                 col7 = random_UN_3_1_
                 col8 = random_UN_3_2_
                 col9 = random_UN_3_3_;
        run;

        data total_covariance_correct4;
        fit_covariance = 1;
        set total_covariance_correct4;
        drop col2-col4 col7-col8 col12;
        rename  col1 = Total_variance_UN_1_1_
                 col5 = Total_variance_UN_2_1_
                 col6 = Total_variance_UN_2_2_
                 col9 = Total_variance_UN_3_1_
                 col10 = Total_variance_UN_3_2_
                 col11 = Total_variance_UN_3_3_
                 col13 = Total_variance_UN_4_1_
                 col14 = Total_variance_UN_4_2_
                 col15 = Total_variance_UN_4_3_
                 col16 = Total_variance_UN_4_4_;
        run;

        data coefficient_generated;
        fit_covariance = 1;
        beta_intercept = &b00;
        beta_time = &b10;
        beta_time2 = &b20;
        beta_Wi = &b01;
        beta_time_Wi = &b11;
        beta_time2_Wi = &b21;
        run;
          /*This is the correct model*/
proc mixed data = &inputdata noclprint covtest method = reml;
class stu_id;
model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
random intercept time time2/subject = stu_id type = un v;
       ods output v = v_correct_ID CovParms = Covariance_correct_ID
         solutionF = Coefficient_correct_ID
         ConvergenceStatus=Convergen_correct_ID
         fitstatistics= AIC_correct_ID;
        *correct_ID means correct model(time,and time-square)with ID R-matrix;
        run;

/*Fit with time2, but time2 is fixed effect, no random effect*/
proc mixed data = &inputdata noclprint covtest method = reml;
           class stu_id;
```

```
model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
            random intercept time/subject = stu_id type = un v;
            repeated /subject = stu_id type = CS;
            ods output v = v_t2fixed_CS CovParms = Covariance_t2fixed_CS
                solutionF = Coefficient_t2fixed_CS
                ConvergenceStatus=Convergen_t2fixed_CS
                fitstatistics= AIC_t2fixed_CS;
         run;

         /*Fit with time2, but time2 is fixed effect only, no random effect*/
proc mixed data = &inputdata noclprint covtest method = reml;
            class stu_id;
model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
            random intercept time/subject = stu_id type = un v;
            repeated /subject = stu_id type = AR(1);
        ods output v = v_t2fixed_AR CovParms = Covariance_t2fixed_AR
                solutionF = Coefficient_t2fixed_AR
                ConvergenceStatus=Convergen_t2fixed_AR
                fitstatistics= AIC_t2fixed_AR;
         run;

/*Fit with time2, but time2 is fixed effect only, no random effect*/
proc mixed data = &inputdata noclprint covtest method = reml;
            class stu_id;
model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
            random intercept time/subject = stu_id type = un v;
            repeated /subject = stu_id type = TOEP(2);
ods output v = v_t2fixed_TOEP CovParms =Covariance_t2fixed_TOEP
                solutionF = Coefficient_t2fixed_TOEP
                ConvergenceStatus=Convergen_t2fixed_TOEP
                fitstatistics= AIC_t2fixed_TOEP;
         run;

proc mixed data = &inputdata noclprint covtest method = reml;
            class stu_id;
model y = time time2 Wi Wi*time Wi*time2/solution ddfm = satterth;
            repeated /subject = stu_id type = UN R;
        ods output CovParms = Covariance_t2fixed_UN R = R_t2fixed_UN
                solutionF = Coefficient_t2fixed_UN
                ConvergenceStatus=Convergen_t2fixed_UN
                fitstatistics= AIC_t2fixed_UN;
         run;

         %mend HLManalysis_4;
```

```
%macro HLManalysis_7(inputdata = , datatype = , sample = , outdata=);
	proc corr data = Overallerror7 cov;
	var e1-e7;
	ods output cov = e_cov7;
	run;

	proc corr data = Randomstudent cov;
	var u0i u1i u2i;
	ods output cov = u_cov7;
	run;

	proc iml;
		use e_cov7;
		read all into within_cov_matrix [colname=varname];

		use u_cov7;
		read all into Tau;

		ZGZ = &Z_matrix_7*Tau*&Z_matrix_7`;
		Total_variance1 = ZGZ + within_cov_matrix;

		 Total_variance = shape(total_variance1, 1, 49);

	    create Total_covariance_correct7 from Total_variance;
		 append from Total_variance;

	quit;

	data total_covariance_correct7;
	fit_covariance = 1;
	set total_covariance_correct7;
	drop col2-col7 col10-col14 col18-col21 col26-col28 col34 col35 col42;
	rename			col1 = Total_variance_UN_1_1_
				col8 = Total_variance_UN_2_1_
				col9 = Total_variance_UN_2_2_
				col15 = Total_variance_UN_3_1_
				col16 = Total_variance_UN_3_2_
				col17 = Total_variance_UN_3_3_
				col22 = Total_variance_UN_4_1_
				col23 = Total_variance_UN_4_2_
				col24 = Total_variance_UN_4_3_
				col25 = Total_variance_UN_4_4_
				col29 = Total_variance_UN_5_1_
				col30 = Total_variance_UN_5_2_
				col31 = Total_variance_UN_5_3_
				col32 = Total_variance_UN_5_4_
				col33 = Total_variance_UN_5_5_
```

```
                              col36 = Total_variance_UN_6_1_
                              col37 = Total_variance_UN_6_2_
                              col38 = Total_variance_UN_6_3_
                              col39 = Total_variance_UN_6_4_
                              col40 = Total_variance_UN_6_5_
                              col41 = Total_variance_UN_6_6_
                              col43 = Total_variance_UN_7_1_
                              col44 = Total_variance_UN_7_2_
                              col45 = Total_variance_UN_7_3_
                              col46 = Total_variance_UN_7_4_
                              col47 = Total_variance_UN_7_5_
                              col48 = Total_variance_UN_7_6_
                              col49 = Total_variance_UN_7_7_;
     run;


                    /*This is the correct model*/
proc mixed data = &inputdata noclprint covtest method = reml;
       class stu_id;
       model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
       random intercept time time2/subject = stu_id type = un v;
    ods output v = v_correct_ID CovParms = Covariance_correct_ID
         solutionF = Coefficient_correct_ID
         ConvergenceStatus=Convergen_correct_ID
         fitstatistics= AIC_correct_ID;
     run;


     /*Fit with time2, but time2 is fixed effect only, no random effect*/
proc mixed data = &inputdata noclprint covtest method = reml;
       class stu_id;
       model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
       random intercept time/subject = stu_id type = un v;
       repeated /subject = stu_id type = CS;
    ods output v = v_t2fixed_CS CovParms = Covariance_t2fixed_CS
         solutionF = Coefficient_t2fixed_CS
         ConvergenceStatus=Convergen_t2fixed_CS
         fitstatistics= AIC_t2fixed_CS;
     run;


     /*Fit with time2, but time2 is fixed effect only, no random effect*/
proc mixed data = &inputdata noclprint covtest method = reml;
       class stu_id;
       model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
       random intercept time/subject = stu_id type = un v;
```

```
        repeated /subject = stu_id type = AR(1);
    ods output v = v_t2fixed_AR CovParms = Covariance_t2fixed_AR
          solutionF = Coefficient_t2fixed_AR
          ConvergenceStatus=Convergen_t2fixed_AR
          fitstatistics= AIC_t2fixed_AR;
     run;


     /*Fit with time2, but time2 is fixed effect only, no random effect*/
proc mixed data = &inputdata noclprint covtest method = reml;
        class stu_id;
        model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
        random intercept time/subject = stu_id type = un v;
        repeated /subject = stu_id type = TOEP(2);
    ods output v = v_t2fixed_TOEP CovParms = Covariance_t2fixed_TOEP
          solutionF = Coefficient_t2fixed_TOEP
          ConvergenceStatus=Convergen_t2fixed_TOEP
          fitstatistics= AIC_t2fixed_TOEP;
     run;

proc mixed data = &inputdata noclprint covtest method = reml;
        class stu_id;
        model y = time time2 Wi Wi*time Wi*time2/solution ddfm = satterth;
        repeated /subject = stu_id type = UN r;
    ods output CovParms = Covariance_t2fixed_UN R = R_t2fixed_UN
          solutionF = Coefficient_t2fixed_UN
          ConvergenceStatus=Convergen_t2fixed_UN
          fitstatistics= AIC_t2fixed_UN;
     run;

     %mend HLManalysis_7;
```

APPENDIX B. SAS CODE FOR SIMULATION STUDY 2

```
*MACRO OF GENERATING THE DATA AND CALLING THE MACRO TO RUN THE ANALYSIS;
%let  attrate = 0.10;

%let vc_CS_4 = {1     0.5   0.5   0.5,
                0.5   1     0.5   0.5,
                0.5   0.5   1     0.5,
                0.5   0.5   0.5   1};

%let vc_CS_7 = {1    0.5  0.5  0.5  0.5  0.5  0.5,
                0.5  1    0.5  0.5  0.5  0.5  0.5,
                0.5  0.5  1    0.5  0.5  0.5  0.5,
                0.5  0.5  0.5  1    0.5  0.5  0.5,
                0.5  0.5  0.5  0.5  1    0.5  0.5,
                0.5  0.5  0.5  0.5  0.5  1    0.5,
                0.5  0.5  0.5  0.5  0.5  0.5  1};

/*rou = 0.8*/
%let vc_AR_4 = {1       0.8     0.64 0.512,
                0.8     1       0.8  0.64,
                0.64    0.8     1    0.8,
                0.512   0.64    0.8  1};


%let vc_AR_7 = {1          0.8        0.64     0.512   0.4096  0.32768   0.262144,
                0.8        1          0.8      0.64    0.512   0.4096    0.32768,
                0.64       0.8        1        0.8     0.64    0.512     0.4096,
                0.512      0.64       0.8      1       0.8     0.64      0.512,
                0.4096     0.512      0.64     0.8     1       0.8       0.64,
                0.32768    0.4096     0.512    0.64    0.8     1         0.8,
                0.262144   0.32768    0.4096   0.512   0.64    0.8       1};

%let vc_TOEP_4 = {1    0.5   0     0,
                  0.5  1     0.5   0,
                  0    0.5   1     0.5,
                  0    0     0.5   1};
```

```
%let vc_TOEP_7 = {1    0.5    0    0     0     0     0,
                  0.5  1      0.5  0     0     0     0,
                  0    0.5    1    0.5   0     0     0,
                  0    0      0.5  1     0.5   0     0,
                  0    0      0    0.5   1     0.5   0,
                  0    0      0    0     0.5   1     0.5,
                  0    0      0    0     0     0.5   1};


%let Z_matrix_4 = {1  -1.5  2.25,
                   1  -0.5  0.25,
                   1   0.5  0.25,
                   1   1.5  2.25};

%let Z_matrix_7 = {1  -1.5  2.25,
                   1  -1     1,
                   1  -0.5  0.25,
                   1   0     0,
                   1   0.5  0.25,
                   1   1     1,
                   1   1.5  2.25};

%let medium_stu = {1       0.283  0,
                   0.283  0.5     0,
                   0       0       0};

/*correlation = 0.4*/

%macro complex_R_simple_G(result1, result2, result3, result4);
    %let Wi_numbers = 1;
    %let tuo_00 = 1;
    %let tuo_11 = 0.5;
    %let cov_stu = &medium_stu;

/*creates means & cov structure of student's level random effect
    to be used to create their values in the MVN macro; */
        proc iml;
        cov=&cov_stu;
        mean={0,0,0}; /*means of student's random effect;  */
        create stu_varcov from cov;
        append from cov;
        create stu_means from mean;
        append from mean;
        quit;

    %do rep = 1 %to &Nrep;
```

```
%do samplesize = 1 %to 2;
        %if &samplesize = 1 %then %let Nstu = 500;
        %else %if &samplesize = 2 %then %let Nstu = 2000;

          %do coefficient_effectsize = 1 %to 2;
            %if &coefficient_effectsize = 1 %then %do;
              %let b00 = 10; /*intercept*/
              %let b01 = 0; /*W*/
              %let b10 = 0; /*time*/
              %let b11 = 0; /*W*time*/
              %let b20 = 0; /*time2: time squared*/
              %let b21 = 0; /*W*time2*/
                  %end;
            %if &coefficient_effectsize = 2 %then %do;
              %let b00 = 10; /*intercept*/
              %let b01 = 0.5*sqrt(&tuo_00); /*W*/
              %let b10 = 0.5*sqrt(&tuo_11); /*time*/
              %let b11 = 0.5*sqrt(&tuo_11); /*W*time*/
              %let b20 = 0.5; /*time2: time squared*/
              %let b21 = 0.5; /*W*time2*/
                  %end;

        %do R_effectsize = 1 %to 3;
          %if &R_effectsize = 1 %then %do;
            %let varcov4 = &vc_CS_4;
            %let varcov7 = &vc_CS_7;
    %end;
          %else %if &R_effectsize = 2 %then %do;
            %let varcov4 = &vc_AR_4;
            %let varcov7 = &vc_AR_7;
          %end;
          %else %if &R_effectsize = 3 %then %do;
            %let varcov4 = &vc_TOEP_4;
           %let varcov7 = &vc_TOEP_7;
          %end;


                  proc iml;
                        reset print;
                        e4 = &varcov4;
                        create randomerror4 from e4;
                        append from e4;

                        e_mean4 = {0};
                        create e_means4 from e_mean4;
                        append from e_mean4;
```

```
                    e7 = &varcov7;
                    create randomerror7 from e7;
                    append from e7;

                    e_mean7 = {0};
                    create e_means7 from e_mean7;
                    append from e_mean7;
               quit;


    %let seed1 = 1234567 + &rep*1000 + &samplesize*100
               + &R_effectsize*10 + &coefficient_effectsize;


                    /*Create the first level residual*/
    %mvn(varcov = randomerror4, means = e_means4, n = &Nstu,
      seed = &seed1, sample = overallerror4);
    %mvn(varcov = randomerror7, means = e_means7, n = &Nstu,
      seed = &seed1, sample = overallerror7);

                    data overallerror4;
                    set overallerror4;
                    rename col1-col4 = e1-e4;
                    run;

                    data overallerror7;
                    set overallerror7;
                    rename col1-col7 = e1-e7;
                    run;

*randomstudent is the dataset containing the r0ij and r1ii values;
%let seed2 = 7654321 + &rep+&samplesize*10
          + &R_effectsize*100 + &coefficient_effectsize*1000;


    %MVN(varcov=stu_varcov, means=stu_means, n=&Nstu,
      seed=&seed2, sample=randomstudent);

                    data randomstudent;
                    set randomstudent;
                    rename      col1 = u0i
                    col2 = u1i
                    col3 = u2i;
                    run;

          *create student level (second level) variable;
```

```
data stu_effect;
	do stu_ID = 1 to &Nstu;
	  Wi = &Wi_numbers*rannor(&seed1+1000);
	  output;
	end;
run;

*create student membership at time1;
data student1;
	merge stu_effect randomstudent;
run;

*create student in five time point;
data student1_4;
			set student1;
			time1 = -1.5;
			time2 = -0.5;
			time3 = 0.5;
			time4 = 1.5;
run;

*Create student file in nine time point;
data student1_7;
			set student1;
			time1 = -1.5;
			time2 = -1;
			time3 = -0.5;
			time4 = 0;
			time5 = 0.5;
			time6 = 1;
			time7 = 1.5;
run;

*transpose data;
data student4;
	set student1_4;
	array timevar [4] time1 - time4;
	do i = 1 to 4;
			time=timevar[i];
			output;
	end;
	drop i time1-time4;
run;

data student7;
	set student1_7;
```

```
array timevar [7] time1 - time7;
do i = 1 to 7;
        time=timevar[i];
        output;
end;
drop i time1-time7;
run;

*restructures the e values to a column vector;
data evalues4;
        set overallerror4;
        array e[4] e1-e4;
        do i = 1 to 4;
                eti = e[i];
                output;
        end;
        keep eti;
run;

data evalues7;
        set overallerror7;
        array e[7] e1-e7;
        do i = 1 to 7;
                eti = e[i];
                output;
        end;
        keep eti;
run;

*generates the dependent variable;
*This is the complete dataset;
data complete4;
        replication = &rep;
        merge student4 evalues4;
        time2 = time*time;
y = &b00 +&b01*Wi + &b10*time + &b11*Wi*time
 +&b20*time2+&b21*Wi*time2+ u0i +u1i*time +u2i*time2+eti;
run;

data complete7;
        replication = &rep;
        merge student7 evalues7;
        time2 = time*time;
y = &b00 +&b01*Wi + &b10*time + &b11*Wi*time
 +&b20*time2+&b21*Wi*time2+ u0i +u1i*time +u2i*time2+eti;
run;
```

```
/******* generate the other datasets with missing values ******/
data indicator4;
    set student1_4(drop = Wi--u2i);
    x0 = 0;
    x1 = ranbin(&seed1, 1, &attrate);
    x2 = ranbin(&seed1+1, 1, 2*&attrate);
    x3 = ranbin(&seed1+2, 1, 3*&attrate);
run;

    *transpose data;
data student1_4Long;
        set indicator4;
        array timevar [4] time1 - time4;
        array xs[4] x0 - x3;
        do i = 1 to 4;
            time=timevar[i];
            missing_indicator = xs[i];
            output;
        end;
        drop i time1-time4 x0-x3;
run;

data indicator7;
    set student1_7;
    x0 = 0;
    x1 = ranbin(&seed1, 1, &attrate);
    x2 = ranbin(&seed1+1, 1, 2*&attrate);
    x3 = ranbin(&seed1+2, 1, 3*&attrate);
    x4 = ranbin(&seed1+3, 1, 4*&attrate);
    x5 = ranbin(&seed1+4, 1, 5*&attrate);
    x6 = ranbin(&seed1+5, 1, 6*&attrate);
run;
*transpose data;
data student1_7Long;
        set indicator7;
        array timevar [7] time1 - time7;
        array xs[7] x0 - x6;

        do i = 1 to 7;
            time=timevar[i];
            missing_indicator = xs[i];
            output;
        end;
        drop i time1-time7 x0-x6;
run;
```

```
data missing4;
merge complete4 student1_4Long;
by stu_ID time;
if missing_indicator = 1 then y = .;
completed_data = 0;
run;

data missing7;
merge complete7 student1_7Long;
by stu_ID time;
if missing_indicator = 1 then y = .;
completed_data = 0;
run;

%HLManalysis_4(inputdata = complete4, datatype = 1, sample &rep,complex_r = &R_effectsize,
outdata = complex_R_simple_G_4);

%HLManalysis_4(inputdata = missing4, datatype = 0, sample = &rep,
complex_r =&R_effectsize, outdata = complex_R_simple_G_missing_4);

%HLManalysis_7(inputdata = complete7, datatype = 1, sample = &rep,
        complex_r =&R_effectsize, outdata = complex_R_simple_G_7);

%HLManalysis_7(inputdata = missing7, datatype = 0, sample = &rep,
complex_r =&R_effectsize, outdata = complex_R_simple_G_missing_7);

                %end;
            %end;
          %end;
    %end;
    %mend complex_R_simple_G;


    *MACRO OF RUNNING THE ANALYSIS;
    %macro HLManalysis_4(inputdata = , datatype = , sample = ,
              complex_r =, outdata=);
    *Calculate the correct total variance first;
    proc corr data = Overallerror4 cov;
    var e1-e4;
    ods output cov = e_cov4;
    run;

    proc corr data = Randomstudent cov;
    var u0i u1i u2i;
    ods output cov = u_cov4;
    run;
```

```
proc iml;
reset print;
        use e_cov4;
        read all into within_cov_matrix [colname=varname];

        use u_cov4;
        read all into Tau;

        ZGZ = &Z_matrix_4*Tau*&Z_matrix_4`;
        Total_variance1 = ZGZ + within_cov_matrix;

    Total_variance = shape(total_variance1, 1, 16);

    create Total_covariance_correct4 from Total_variance;
        append from Total_variance;

        variance_of_stu1=shape(Tau,1,9);

        create random_effect_generate from variance_of_stu1;
        append from variance_of_stu1;
quit;

data random_effect_generate;
fit_covariance = 1;
set random_effect_generate;
drop col2 col3 col6;
rename col1 = random_UN_1_1_
        col4 = random_UN_2_1_
        col5 = random_UN_2_2_
        col7 = random_UN_3_1_
        col8 = random_UN_3_2_
        col9 = random_UN_3_3_;
run;

data total_covariance_correct4;
fit_covariance = 1;
set total_covariance_correct4;
drop col2-col4 col7-col8 col12;
rename col1 = Total_variance_UN_1_1_
        col5 = Total_variance_UN_2_1_
        col6 = Total_variance_UN_2_2_
        col9 = Total_variance_UN_3_1_
        col10 = Total_variance_UN_3_2_
        col11 = Total_variance_UN_3_3_
        col13 = Total_variance_UN_4_1_
        col14 = Total_variance_UN_4_2_
```

```
            col15 = Total_variance_UN_4_3_
            col16 = Total_variance_UN_4_4_;
    run;

    data coefficient_generated;
    fit_covariance = 1;
    beta_intercept = &b00;
    beta_time = &b10;
    beta_time2 = &b20;
    beta_Wi = &b01;
    beta_time_Wi = &b11;
    beta_time2_Wi = &b21;
    run;

     /*Model with simple R = ID and complex G*/

proc mixed data = &inputdata noclprint covtest method = reml;
         class stu_id;
model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
     random intercept time time2/subject = stu_id type = un v;
   ods output v = v_correct_ID CovParms = Covariance_correct_ID
           solutionF = Coefficient_correct_ID
           ConvergenceStatus=Convergen_correct_ID
           fitstatistics= AIC_correct_ID;
    run;

    %if &complex_r = 1 %then %do;

    /*Fit with time2, but time2 is fixed effect only, no random effect: correct model*/
proc mixed data = &inputdata noclprint covtest method = reml;
         class stu_id;
model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
   random intercept time/subject = stu_id type = un v;
   repeated /subject = stu_id type = CS;
   ods output v = v_t2fixed_CS CovParms = Covariance_t2fixed_CS
           solutionF = Coefficient_t2fixed_CS
           ConvergenceStatus=Convergen_t2fixed_CS
           fitstatistics= AIC_t2fixed_CS;
    run;

    %end;
    %if &complex_r = 2 %then %do;


    /*Fit with time2, but time2 is fixed effect only, no random effect, correct model*/
proc mixed data = &inputdata noclprint covtest method = reml;
   class stu_id;
```

```
model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
        random intercept time/subject = stu_id type = un v;
        repeated /subject = stu_id type = AR(1);
        ods output v = v_t2fixed_AR CovParms = Covariance_t2fixed_AR
                 solutionF = Coefficient_t2fixed_AR
                 ConvergenceStatus=Convergen_t2fixed_AR
                 fitstatistics= AIC_t2fixed_AR;
          run;

          %end;
          %if &complex_r = 3 %then %do;

          /*Fit with time2, but time2 is fixed effect only, no random effect, correct model*/
proc mixed data = &inputdata noclprint covtest method = reml;
        class stu_id;
model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
        random intercept time/subject = stu_id type = un v;
        repeated /subject = stu_id type = TOEP(2);
ods output v = v_t2fixed_TOEP CovParms = Covariance_t2fixed_TOEP
                solutionF = Coefficient_t2fixed_TOEP
                ConvergenceStatus=Convergen_t2fixed_TOEP
                fitstatistics= AIC_t2fixed_TOEP;
          run;

          %end;

          %mend HLManalysis_4;


          %macro HLManalysis_7(inputdata = , datatype = , sample = ,
                       complex_r =, outdata=);
          proc corr data = Overallerror7 cov;
          var e1-e7;
          ods output cov = e_cov7;
          run;

          proc corr data = Randomstudent cov;
          var u0i u1i u2i;
          ods output cov = u_cov7;
          run;

          proc iml;
          reset print;
                use e_cov7;
                read all into within_cov_matrix [colname=varname];
                use u_cov7;
                read all into Tau;
```

```
ZGZ = &Z_matrix_7*Tau*&Z_matrix_7`;
Total_variance1 = ZGZ + within_cov_matrix;

 Total_variance = shape(total_variance1, 1, 49);

create Total_covariance_correct7 from Total_variance;
      append from Total_variance;

quit;

data total_covariance_correct7;
fit_covariance = 1;
set total_covariance_correct7;
drop col2-col7 col10-col14 col18-col21 col26-col28 col34 col35 col42;
rename col1 = Total_variance_UN_1_1_
       col8 = Total_variance_UN_2_1_
       col9 = Total_variance_UN_2_2_
       col15 = Total_variance_UN_3_1_
       col16 = Total_variance_UN_3_2_
       col17 = Total_variance_UN_3_3_
              col22 = Total_variance_UN_4_1_
              col23 = Total_variance_UN_4_2_
              col24 = Total_variance_UN_4_3_
              col25 = Total_variance_UN_4_4_
              col29 = Total_variance_UN_5_1_
              col30 = Total_variance_UN_5_2_
              col31 = Total_variance_UN_5_3_
              col32 = Total_variance_UN_5_4_
              col33 = Total_variance_UN_5_5_
              col36 = Total_variance_UN_6_1_
              col37 = Total_variance_UN_6_2_
              col38 = Total_variance_UN_6_3_
              col39 = Total_variance_UN_6_4_
              col40 = Total_variance_UN_6_5_
              col41 = Total_variance_UN_6_6_
              col43 = Total_variance_UN_7_1_
              col44 = Total_variance_UN_7_2_
              col45 = Total_variance_UN_7_3_
              col46 = Total_variance_UN_7_4_
              col47 = Total_variance_UN_7_5_
              col48 = Total_variance_UN_7_6_
              col49 = Total_variance_UN_7_7_;
run;
     /*This is the complex G model with simple R*/
proc mixed data = &inputdata noclprint covtest method = reml;
```

```
        class stu_id;
model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
        random intercept time time2/subject = stu_id type = un v;
        ods output v = v_correct_ID CovParms = Covariance_correct_ID
                solutionF = Coefficient_correct_ID
                ConvergenceStatus=Convergen_correct_ID
                fitstatistics= AIC_correct_ID;
         run;

         %if &complex_r = 1 %then %do;

         /*Fit with time2, but time2 is fixed effect only, no random effect, correct model*/

proc mixed data = &inputdata noclprint covtest method = reml;
        class stu_id;
        model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
        random intercept time/subject = stu_id type = un v;
        repeated /subject = stu_id type = CS;
        ods output v = v_t2fixed_CS CovParms = Covariance_t2fixed_CS
                solutionF = Coefficient_t2fixed_CS
                ConvergenceStatus=Convergen_t2fixed_CS
                fitstatistics= AIC_t2fixed_CS;
         run;

         %end;
         %if &complex_r = 2 %then %do;

         /*Fit with time2, but time2 is fixed effect only, no random effect, correct model*/
proc mixed data = &inputdata noclprint covtest method = reml;
        class stu_id;
        model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
        random intercept time/subject = stu_id type = un v;
        repeated /subject = stu_id type = AR(1);
        ods output v = v_t2fixed_AR CovParms = Covariance_t2fixed_AR
                solutionF = Coefficient_t2fixed_AR
                ConvergenceStatus=Convergen_t2fixed_AR
                fitstatistics= AIC_t2fixed_AR;
         run;

         %end;
         %if &complex_r = 3 %then %do;

         /*Fit with time2, but time2 is fixed effect only, no random effect, correct model*/
proc mixed data = &inputdata noclprint covtest method = reml;
        class stu_id;
        model y = time time2 Wi Wi*time wi*time2/solution ddfm = satterth;
        random intercept time/subject = stu_id type = un v;
```

```
repeated /subject = stu_id type = TOEP(2);
ods output v = v_t2fixed_TOEP CovParms = Covariance_t2fixed_TOEP
        solutionF = Coefficient_t2fixed_TOEP
        ConvergenceStatus=Convergen_t2fixed_TOEP
        fitstatistics= AIC_t2fixed_TOEP;
  run;

  %end;

  %mend HLManalysis_7;
```

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