Error of Estimation and Sample Size in the Linear Mixed Model

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ABSTRACT

Daniel Serrano: Error of Estimation and Sample Size in the Linear Mixed Model
(Under the direction of Patrick Curran)

The linear mixed model is increasingly used in psychological applications. Whereas the model was once only applied rarely, because designs that would require the model were either avoided, or analyzed improperly, the model has found such favor in psychology that study designs are being contrived so as to allow use of the model. A potential complication of this trend is the intersection of the small sample sizes routine in psychological applications and the potential sensitivity of the model to small sample sizes. In truth, little is known about the small sample properties of the linear mixed model (Demidenko, 2004). Over the past three decades a handful of articles have attempted to understand the finite sample properties of linear mixed model estimators. Each of these studies has contributed to our understanding of the behavior of point estimation in the linear mixed model. A limitation of these preceding studies has been:

1. The simulation of balanced data, which rarely occurs in psychological applications

2. The use of simple models, which are also rarely used in psychological applications.

In this study both of these limitations are addressed. Outcomes of interest include model convergence rates, point estimate bias and point estimate root mean squared error (RMSE). Findings indicate that high rates of non-convergence are observed under unbalanced data when both few independent sampling units (ISUs) are sampled and few observations are sampled per ISU. Fixed effect point estimates are nearly unbiased in all sample sizes. Consistent with theory (Demidenko, 2004), for some (co)variance parameters, when few ISUs are sampled, no matter how many observations are sampled per ISU, problematic bias remains. Complex models exhibit greater bias than simpler models. (Co)variance parameter estimates exhibit more bias when population values are small than when they are large. When population (co)variance parameters generating values are small, RMSE is smaller than when population values are large. Consistent with theory and previous studies, full maximum likelihood (FML) estimates are more biased than restricted maximum likelihood (REML) estimates. I conclude with implications for the use of these models in applied research.

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In memory of the poor dog who attempted committing suicide under my front left wheel, and to my friend Patrick, who continues to distort the events of that day.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER 1

Introduction

The linear mixed model (Harville, 1977; Laird & Ware, 1982; Raudenbush & Bryk, 2002; Demidenko, 2004) is a flexible and powerful tool for modelling dependent data. Whether independent sampling units (ISUs) are clusters in a sampling design or subjects in a repeated measures design, the model elegantly accommodates the complexities unique to dependent data in ways classical methods such as analysis of variance (ANOVA) and regression cannot. The great advantage of the linear mixed model (LMM) over classical methods is that the LMM estimates sample averaged parameters, known as fixed effects, as well as both ISU-specific and observation-specific disturbance terms, known as random effects. The inability of classical methods to estimate ISU specific disturbance terms when analyzing dependent data often results in negatively biased standard errors (SEs) and biased test statistics (Scott & Holt, 1982).

In contrast to classical methods, the linear mixed model (LMM) provides standard errors (SEs) corrected for the dependence in the data. The model easily accommodates a wide array of covariance structures (Keselman, Algina, Kowalchuck, & Wolfinger, 1998; Wolfinger, 1993, 1996), as compared to classical methods which are limited to either homogeneous or compound symmetric covariance structures (Muller & Stewart, 2006). Moreover, missing and unbalanced data, which in classical methods require either case deletion or complex methods of estimation (Henderson, 1953), provide little difficulty for LMM estimation (Muller & Stewart, 2006). However, the model is not without its limitations. Each of the above mentioned benefits comes at the cost of model assumed asymptotic sample size (Demidenko, 2004; Muller & Stewart, 2006). Consequences of violating the asymptotic sample size requirement include imprecision of SEs (Demidenko, 2004; Kackar & Harville, 1984), imprecision of the degrees of freedom estimator (Kackar & Harville, 1984; Kenward & Roger, 1997), and consequently, inexact small sample inference (Muller & Stewart, 2006). In addition, certain estimators of the LMM are not guaranteed to exist under certain sample size conditions (Demidenko, 2004). Yet this assumption is difficult to interpret in the LMM, for the definition of sample size is more ambiguous in the LMM than it is in classical methods. Nor is it clear exactly how violations of this assumption impact parameter estimation.

There are two components in dependent data which constitute sample size: ISUs and observations sampled within ISUs. It is therefore not easy to intuit to what exactly an asymptotic sample size requirement applies: ISUs, observations, or both. Nor is it clear whether a general sample size requirement makes sense: Might ISUs be more important than observations or vice versa? In fact, Demidenko (2004) proves that ISUs play a larger role than number of observations in achieving asymptotic properties of variance component estimators. Preliminary empirical work is consistent with the work of Demidenko (2004), indicating that estimation error of variance components is minimized when the number of ISUs is maximized (Bassiri, 1988; Mok, 1995). This is logical, given that common estimators of variance components depend on the number of ISUs N.

Sample size also plays a role in inference in the LMM, particularly for fixed effects. While fixed effects tend to be quite robust, mis-specification or estimation error in the covariance matrix of random effects can result in bias of fixed effect standard errors (Kenward & Roger, 1997). This is because SEs of the fixed effects are computed as a function of the estimated covariance matrix of random effects. In small samples, the precision of the covariance matrix of random effects is compromised, which results in misspecified SEs of the fixed effects (Kenward & Roger, 1997). Thus sample size is a vexing problem that permeates both estimation and inference of the linear mixed model.

Given the seeming importance of this issue it is surprising that so little is known and so little has been done to elucidate the small sample properties of the LMM. While some attention has been paid to small sample inferential properties of the LMM (Harville & Jeske, 1992; Kackar & Harville, 1984; Kenward & Roger, 1997; Prasad & Rao, 1990), little is known about small-sample estimation (Demidenko, 2004).

In this thesis I seek to elucidate the finite sample behavior of linear mixed model estimators. Particular attention is paid to the bias and efficiency of point estimates across a range of ISU and observation sizes. Importantly, the issue is addressed in a sequence of models that vary in complexity of their fixed and random effects structures. Examining a sequence of models permits the generalization of findings to a broader class of modelling conditions. Selecting model types and sample sizes commonly encountered in social science research provides particular guidance for applied researchers in this field.

I begin with a formal explication of the model and theory underlying estimation. A review of applied articles in which empirical data sets with few data points were analyzed with the LMM demonstrates the increasing use of the LMM by psychologists in cases where model assumptions about sample size may be violated. In an attempt to understand the trend, attention is paid to recommendations by methodologists which have encouraged this practice. I next review prior simulation work investigating the role of sample size in parameter estimation. I then provide an overview of the limitations of prior simulation work in order to motivate the design of my study.

1.1 Theoretical Background

The linear mixed model equations are usually written for observation i in ISU_j (for example, the reduced form equation of Raudenbush & Bryk, 2002). However, expressing the model through the matrix equations for ISU_j clarifies the model implied distribution of $\mathbf{y}_j$. As most readers are familiar with the model for obs_{ij}, I begin by presenting the reduced form equation for a two predictor model, and discuss how this model generalizes directly to the vector model for ISU_j. The linear mixed model for obs_{ij} is written in scalar form as

$$y_{ij} = \gamma_{00} + \gamma_{10}x_{1ij} + \gamma_{20}x_{2ij} + u_{0j} + u_{1j}z_{1ij} + u_{2j}z_{2ij} + e_{ij} \tag{1.1}$$

where the γ are fixed effect parameters, the u parameters are unobservable random effects, and e_{ij} is an observation specific disturbance term. There are three quantities assumed fixed and known, the outcome y_{ij}, the fixed effect predictors x_{ij}, and the random effect predictors z_{ij}. A distinction is maintained between fixed and random effect predictors in order to allow for random effects without fixed effects and vice versa in the model for ISU_j. Extending this model to the model for ISU_j results in expanding all parametric components to vectors and observed quantities, except the outcome, to matrices. Consequently, the γ parameters become elements in the $k \times 1$ vector of fixed effects $\mathbf{\Gamma}$, the x_{ij} become elements in the $n_j \times k$ matrix of fixed effects predictors $\mathbf{X}_j$, the u parameters become elements in the $k \times 1$ vector of unobservable random effects $\mathbf{U}_j$, the z_{ij} become elements in the $n_j \times k$ matrix of random effects predictors $\mathbf{Z}_j$, the y_{ij} become elements in the $n_j \times 1$ outcome vector $\mathbf{y}_j$, and the observation specific disturbance terms e_{ij} become elements in the $n_j \times 1$ vector of observation specific disturbance terms contained in ISU_j, $\mathbf{e}_j$. Under this specification, the total sample size (N_t) can be expressed as $N \times n_j$ in balanced data (where N is the number of ISUs) and as $\sum_{j=1}^{j} n_j$ in unbalanced data.

Thus, the linear mixed model for ISU_j composed of n_j observations can be written as

$$\mathbf{y}_j = \mathbf{X}_j\mathbf{\Gamma} + \mathbf{Z}_j\mathbf{U}_j + \mathbf{e}_j. \tag{1.2}$$

For this model, $\mathbf{X}_j$ and $\mathbf{\Gamma}$ constitute the first moment structure of the outcome $\mathbf{y}_j$,

$$E(\mathbf{y}_j) = \mathbf{X}_j\mathbf{\Gamma}. \tag{1.3}$$

The ISU specific disturbance terms, or random effect parameters, $\mathbf{U}_j$, are assumed Gaussian, $\mathbf{U}_j \sim N(\mathbf{0}, \mathbf{T})$, while the observation specific disturbance terms, $\mathbf{e}_j$, are assumed independent Gaussian, $\mathbf{e}_j \sim N(\mathbf{0}, \mathbf{I}_j\sigma^2)$. As the densities for both $\mathbf{U}_j$ and $\mathbf{e}_j$ have zero mean, and both components are mutually statistically independent, by properties of Gaussian densities they contribute only to the second moment structure of $\mathbf{y}_j$,

$$\mathbf{V}_j = E(\mathbf{y}_j - \mathbf{X}_j\mathbf{\Gamma})^2 = \mathbf{Z}_j\mathbf{T}\mathbf{Z}_j' + \mathbf{I}_j\sigma^2. \tag{1.4}$$

From these equations it is apparent that the linear mixed model is a member of the general linear model family with mean structure $\mathbf{X}_j\mathbf{\Gamma}$ and covariance structure $\mathbf{Z}_j\mathbf{T}\mathbf{Z}_j' + \mathbf{I}_j\sigma^2$. We can therefore write the model implied distribution for the outcome as

$$\mathbf{y}_j \sim \boldsymbol{N}(\mathbf{X}_j\mathbf{\Gamma}, \mathbf{Z}_j\mathbf{T}\mathbf{Z}_j' + \mathbf{I}_j\sigma^2). \tag{1.5}$$

As each ISU has this model implied distribution, and by definition the ISUs are independent of one another, the full covariance matrix, $\mathbf{V}$ can be written:

$$\mathbf{V} = \mathbf{I} \otimes \mathbf{Z}_j\mathbf{T}\mathbf{Z}_j' + \mathbf{I}_j\sigma^2. \tag{1.6}$$

Where $\otimes$ is the left Kronecker product which results in a block diagonal matrix whose diagonal blocks are the ISU specific values of $\mathbf{Z}_j\mathbf{T}\mathbf{Z}_j' + \mathbf{I}_j\sigma^2$. For the case of two ISUs, $\mathbf{V}$ can be expressed as

$$\mathbf{V} = \begin{pmatrix} \mathbf{Z}_1\mathbf{T}\mathbf{Z}_1' + \mathbf{I}_1\sigma^2 & \mathbf{0} \\ \mathbf{0} & \mathbf{Z}_2\mathbf{T}\mathbf{Z}_2' + \mathbf{I}_2\sigma^2 \end{pmatrix}. \tag{1.7}$$

A major consequence of this structure is that the fixed and random effects are orthogonal (Demidenko, 2004).

A common summary statistic computed as a function of the variance components is the intra-class correlation coefficient, or heritability. The statistic is computed as a ratio of variance components, indicating the proportion of variance attributable to between ISU variance:

$$ICC = \frac{\sigma_b^2}{\sigma_b^2 + \sigma_w^2}, \tag{1.8}$$

where σ_b^2 is the between ISU variance and σ_w^2 is the within ISU variance.

Likelihood estimation is the favored method for obtaining parameter estimates. There are two likelihoods commonly employed: full maximum likelihood (Hartley & Rao, 1967) and restricted maximum likelihood (Harville, 1974; Patterson & Thompson, 1971). Full maximum likelihood (FML) jointly maximizes both the fixed and random effects, estimating the covariance matrix as if the fixed effects were known. Thus, as with all full maximum likelihood estimators, in balanced data the FML estimate of $\mathbf{T}$ is biased by a factor of $\frac{N}{N-k}$ where N is the number of ISUs and k is the number of elements in $\mathbf{\Gamma}$ (i.e., the number of fixed effects).

Following the work of Hartley and Rao (1967) the log likelihood for the LMM with Gaussian errors may be written as

$$\boldsymbol{\ell}(\boldsymbol{\theta}) = N_t ln\sigma^2 + ln\sum|\mathbf{V}_j| + \sigma^{-2}\sum(\mathbf{y}_j - \mathbf{X}_j\mathbf{\Gamma})'\mathbf{V}_j^{-1}(\mathbf{y}_j - \mathbf{X}_j\mathbf{\Gamma}), \tag{1.9}$$

where $\boldsymbol{\theta}$ is the vector of estimable parameters contained in $\mathbf{\Gamma}$, $\mathbf{T}$, and σ^2. However, the variance-profile log-likelihood is often much easier to work with because it requires likelihood estimation of one fewer parameter than the full likelihood. The variance-profile log-likelihood is obtained by replacing σ^2 with $\hat{\sigma}^2$, and re-expressing $\mathbf{V}_j$ as $(\mathbf{Z}_j\mathbf{T}\mathbf{Z}_j' + \mathbf{I}_j)$. The resulting log-likelihood can be written as

$$\boldsymbol{\ell}(\mathbf{\Gamma}, \mathbf{T}) = N_t + ln\sum|\mathbf{V}_j| + \sum(\mathbf{y}_j - \mathbf{X}_j\mathbf{\Gamma})'\mathbf{V}_j^{-1}(\mathbf{y}_j - \mathbf{X}_j\mathbf{\Gamma}). \tag{1.10}$$

The profiled residual variance estimator is given for both FML and REML as

$$\hat{\sigma}^2 = \frac{1}{\mathbf{N}_t}\sum_{i=1}^{N}(\mathbf{y}_i - \mathbf{X}_i\mathbf{\Gamma})'(\mathbf{I} + \mathbf{Z}_i\mathbf{T}\mathbf{Z}_i')^{-1}(\mathbf{y}_i - \mathbf{X}_i\mathbf{\Gamma}). \tag{1.11}$$

The fixed effects estimator can be obtained by solving the following derivative for $\mathbf{\Gamma}$

$$\frac{\partial \boldsymbol{l}(\mathbf{\Gamma}, \mathbf{T})}{\partial \mathbf{\Gamma}} = \sum \mathbf{X}_j'\hat{\mathbf{V}}_j^{-1}(\mathbf{y}_j - \mathbf{X}_j\mathbf{\Gamma}) \tag{1.12}$$

which gives

$$\hat{\mathbf{\Gamma}} = (\sum \mathbf{X}_j'\hat{\mathbf{V}}_j^{-1}\mathbf{X}_j)^{-1}\sum \mathbf{X}_j'\hat{\mathbf{V}}_j^{-1}\mathbf{y}_j, \tag{1.13}$$

This can be seen to be a generalized least squares (GLS) estimator. The fixed effects estimate, $\hat{\mathbf{\Gamma}}$, can be shown to be an unbiased estimate of $\mathbf{\Gamma}$. However, the MLE of $\mathbf{V}_j$ is known to be biased. This bias propagates through to inference on the MLE for $\mathbf{\Gamma}$. For, while $\hat{\mathbf{\Gamma}}$ is unbiased with $E(\hat{\mathbf{\Gamma}}) = \mathbf{\Gamma}$ by

$$E[(\mathbf{X}_j'\mathbf{V}_j^{-1}\mathbf{X}_j)^{-1}\mathbf{X}_j'\mathbf{V}_j^{-1}\mathbf{y}_j] = (\mathbf{X}_j'\mathbf{V}_j^{-1}\mathbf{X}_j)^{-1}\mathbf{X}_j'\mathbf{V}_j^{-1}\mathbf{X}_j\mathbf{\Gamma}, \tag{1.14}$$

mis-specification in the covariance matrix for the asymptotic limiting distribution of $\hat{\mathbf{\Gamma}}$, $(\sum \mathbf{X}_j'\mathbf{V}_j^{-1}\mathbf{X}_j)^{-1}$, by the bias of $\mathbf{V}_j$, results in biased estimates of the standard errors and tests for $\hat{\mathbf{\Gamma}}$ (Kackar & Harville, 1984; Kenward & Roger, 1997; Prasad & Rao, 1990). However, the robustness of the unbiasedness property of the fixed effects renders estimation error nearly trivial even in very small samples (Kenward & Roger, 1997)

Restricted maximum likelihood (REML) is a solution to the inherent bias of the FML estimator. The REML for the linear mixed model with Gaussian errors can be written as

$$\begin{aligned}\boldsymbol{\ell}(\sigma^2, \mathbf{T}) = (N_t - k)ln\sigma^2 + ln\sum|\mathbf{X}_j'\mathbf{V}_j\mathbf{X}_j| + ln\sum|\mathbf{V}_j| \\ +\sigma^{-2}\sum(\mathbf{y}_j - \mathbf{X}_j\hat{\mathbf{\Gamma}})'\mathbf{V}_j^{-1}(\mathbf{y}_j - \mathbf{X}_j\hat{\mathbf{\Gamma}}),\end{aligned} \tag{1.15}$$

As before, the variance-profile log-likelihood is easier to work with. In the case of REML, the variance-profile log-likelihood is easier to work with, and can be written as

$$\begin{aligned}\boldsymbol{\ell}(\mathbf{T}) = (N_t - k) + ln\sum|\mathbf{X}_j'\mathbf{V}_j\mathbf{X}_j| + ln\sum|\mathbf{V}_j| \\ +\sum(\mathbf{y}_j - \mathbf{X}_j\hat{\mathbf{\Gamma}})'\mathbf{V}_j^{-1}(\mathbf{y}_j - \mathbf{X}_j\hat{\mathbf{\Gamma}}).\end{aligned} \tag{1.16}$$

$$\hat{\mathbf{\Gamma}} = (\sum \mathbf{X}_j'\hat{\mathbf{V}}_j^{-1}\mathbf{X}_j)^{-1}\sum \mathbf{X}_j'\hat{\mathbf{V}}_j^{-1}\mathbf{y}_j. \tag{1.17}$$

Restricted maximum likelihood estimates (RMLEs) are obtained by capitalizing on the orthogonality property of the fixed and random effects. Specifically, given an initial value of $\mathbf{V}_j$, GLS estimates for $\mathbf{\Gamma}$ are obtained from equation 1.17, conditional upon this GLS estimate, the first likelihood estimate for $\mathbf{V}_j$ is obtained by solving equation 15. This initial likelihood estimate of $\mathbf{V}_j$ is then used to update the GLS estimate of the fixed effects, which is in turn used to update the likelihood estimate of $\mathbf{V}_j$. This process is repeated until some convergence criterion is achieved. As with FML, $\hat{\mathbf{\Gamma}}_{GLS}$ is unbiased (Kackar & Harville, 1984). Of equal, or greater importance, the covariance matrix for the asymptotic limiting distribution of $\hat{\mathbf{\Gamma}}_{GLS}$, $(\sum \mathbf{X}_j' \mathbf{V}_j^{-1} \mathbf{X}_j)^{-1}$, is unbiased in balanced data.

The SAS system implements a sweep operator in the construction of the log likelihood and derivatives which permits estimation of $\mathbf{T}$ independent of $\hat{\mathbf{\Gamma}}$ (Wolfinger, Tobias, & Sall, 1994). The Algorithm used by SAS capitalizes on an equivalent expression for the residuals:

$$\mathbf{e}_j = \mathbf{y}_j - \mathbf{X}_j \hat{\mathbf{\Gamma}} = \mathbf{y}_j - \mathbf{X}_j ((\mathbf{X}_j' \hat{\mathbf{V}}_j^{-1} \mathbf{X}_j) \mathbf{X}_j' \hat{\mathbf{V}}_j^{-1} \mathbf{y}_j) \tag{1.18}$$

which does not require explicit estimation of $\hat{\mathbf{\Gamma}}$. This results in a likelihood that only involves observed variables ($\mathbf{X}$ & $\mathbf{Z}$) and variance parameters ($\mathbf{V}_j$).

Though REML and FML differ in their approach to estimating the covariance matrix of random effects, REML and FML have identical estimators for the residual variance:

$$\hat{\sigma}^2 = \frac{1}{\mathbf{N}_t} \sum_{i=1}^{N} (\mathbf{y}_i - \mathbf{X}_i \mathbf{\Gamma})' (\mathbf{I} + \mathbf{Z}_i \mathbf{T} \mathbf{Z}_i')^{-1} (\mathbf{y}_i - \mathbf{X}_i \mathbf{\Gamma}). \tag{1.19}$$

Whereas the beneficial properties of the estimators of the covariance matrix of random effects are attained as $\mathbf{N} \to \infty$, it can be seen from equations (1.17) and (1.19) both $\hat{\mathbf{\Gamma}}$ and $\hat{\sigma}^2$ attain optimal properties as $\mathbf{N}_t \to \infty$.

As FML is approximately biased by a factor of $\frac{N}{N-k}$, in the case of balanced data the REML estimator can be obtained by premultipying

$$\hat{\mathbf{T}}_{FML} = \frac{1}{N \hat{\sigma}_{FML}^2} (\mathbf{Z}'\mathbf{Z})^{-1} \mathbf{Z}' \hat{\mathbf{E}} \hat{\mathbf{E}}' \mathbf{Z} (\mathbf{Z}'\mathbf{Z})^{-1} - (\mathbf{Z}'\mathbf{Z})^{-1} \tag{1.20}$$

by $\frac{N}{N-k}$ to obtain

$$\hat{\mathbf{T}}_{REML} = \frac{1}{N - k \hat{\sigma}_{FML}^2} (\mathbf{Z}'\mathbf{Z})^{-1} \mathbf{Z}' \hat{\mathbf{E}} \hat{\mathbf{E}}' \mathbf{Z} (\mathbf{Z}'\mathbf{Z})^{-1} - (\mathbf{Z}'\mathbf{Z})^{-1} \tag{1.21}$$

where $\hat{\mathbf{E}}\hat{\mathbf{E}}'$ can be defined as

$$(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\Gamma}})(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\Gamma}})' \tag{1.22}$$

Pre-multiplication by the factor $\frac{N}{N-k}$ adjusts the degrees of freedom for the k estimated fixed effects. This difference – adjusting for the estimation of the k fixed effects or treating the estimates as a priori known constants – is the key difference between REML and FML (Corbeil & Searle, 1976). It is important to note the emphasis on balanced data here, for in the case of unbalanced data neither estimator is unbiased, though REML is less biased than FML (Demidenko, 2004; Muller & Stewart, 2006). However, as the number of ISUs tends toward infinity, FML and REML converge.

In addition to the bias of the FML estimator of $\mathbf{V}_j$ and its effect on fixed effects inference, there is a second source of estimation error in the LMM. Both FML and RML estimates of $\mathbf{V}_j$ are compromised as sample size decreases. Pioneering theoretical work on this topic was done by Kackar and Harville (1984), and supported empirically by Corbeil and Searle (1976) and Swallow and Monahan (1984). Small sample sizes are believed to impact the LMM in two ways. First, estimates of $\mathbf{V}_j$ show inflated estimation error (Demidenko, 2004). Second, inference about the fixed effects is likely to deteriorate as estimation error increases in $\mathbf{V}_j$. This results from the role played by $\mathbf{V}_j$ in the SEs of $\hat{\boldsymbol{\Gamma}}$. The problem of imprecise inference regarding the fixed effects extends to both FML and REML, though such problems are likely compounded in FML as a function of the inherent bias in the weight matrix, $\mathbf{V}_j$, outlined above (Demidenko, 2004). Another factor likely to affect estimation in the LMM that is related to small sample sizes is the degree to which data are unbalanced. While estimation is known to be more complex in the presence of unbalanced data (Henderson, 1953; Searle, Casella, & McCulloch, 1992), little work has brought empirical evidence to bear on the question.

While the REML adjustment is appealing given the inherent bias of the FML estimator, there are conditions related to model selection, inference, and estimation properties that imbue FML with desirable properties. Using either REML or FML, one can test the relative fit of any LMM against another when the model of comparison is obtained by imposing linear constraints on the parameters of the first model and taking the difference of the likelihoods of the two models (Longford, 1995; Morrell, 1998). In FML estimation, both the fixed and random effects are contained in the likelihood, and thus one can impose linear constraints on either fixed or random parameters to obtain the likelihood for a model nested within the original model. However, because the fixed effects are not contained in the restricted likelihood presented in equation 1.15, constraints imposed on the fixed effects result in a model that is not nested within the original model (Longford, 1995), though Wald tests do exist for linear contrasts of fixed effects within a model. Consequently, in the case of model selection, FML has some advantages over REML. Other advantages of FML over REML include the fact that the FML estimator attains the supremum of the likelihood surface while REML does not, thus FML is a true Maximum Likelihood Estimator (MLE), while REML is not. As a result of this fact FML possesses the desirable properties of MLEs while REML does not.

Specifically, there are three main asymptotic properties of MLEs that make them desirable estimators. Under suitable regularity conditions (Hoel, Port, & Stone, 1971) the estimators are asymptotically Gaussian, consistent, and efficient. While both FML and REML are asymptotically Gaussian, only FML is asymptotically consistent (Rao, 1977). In addition, FML is empirically more efficient than REML (Corbeil & Searle, 1976; Swallow & Monahan, 1984). Related to these advantages is the fact that the REML function is not a minimally sufficient function of the parameters by virtue of its omission of the fixed effects – thus, while FML is a full information estimator, REML is not (Rao, 1977). Taken together, each of these issues provides applied researchers with distinct and compelling reasons for using *both* REML and FML. However, none of the information provided thus far provides guidance on the use of the model in small sample sizes. While asymptotic properties are invoked in estimation and inference, theoretical information guiding application of the model in finite conditions is limited if not absent. This fact, coupled with the increasing use of the model in small samples, serves as the impetus for my thesis. In this context, research detailing finite sample sizes under which optimal estimation properties are obtained would be of great assistance to applied researchers.

1.2 Applications of the LMM to Small Samples

Researchers have increasingly applied the linear mixed model to ever smaller sample sizes. While not yet a common practice, the existing examples provide a substantive motivation for this project.

In a cluster sampling application, Kellam, Ling, Merisca, Brown, and Ialongo (1998) used the LMM to assess the degree of variability in aggressive behavior of children nested within 41 classrooms in 19 schools. No information was provided by Kellam et al. (1998) on the number of observations per school. As part of a larger modeling scheme the authors estimated a model with fixed effects for gender and random slopes for school, though they provide no parameter estimates.

Use of the linear mixed model in the case of few ISUs is not restricted to applied researchers. In their seminal book on the LMM, Raudenbush and Bryk (2002) use the Huttonlocher, Haight, Bryk, and Sletzer (1991) data set for illustrative purposes. This data set was composed of repeated measures on 22 infants with 6 to 8 observations per infant. In some analyses presented in Raudenbush and Bryk (2002), data on only 11 infants were analyzed. The data provided information on infant vocabulary growth as a function of maternal speech, and were modeled using a second order polynomial growth curve. Fixed and random effects were estimated for all polynomial terms, thus an unrestricted 3-dimensional covariance matrix was estimated in the presence of only 11 ISUs.

A common theme in these examples was the use of few ISUs and many observations per ISU. While the number of ISUs sampled in the reviewed applications seem small relative to what is implied by asymptotic requirements, the sample sizes encountered in the social sciences and particularly in psychological applications are, by nature, limited in the number of subjects that can be practically and economically assessed. Compound the problem of small sample size with attrition and item non-response, and the expectation that applied researchers restrict use of the LMM to data sets of approximate asymptotic ISU size seems impractical and insensitive. Thus the provision of information guiding applied researchers through the finite sample behavior and properties of LMM estimators is imperative. For while applied researchers can not be expected to sample approximately asymptotic numbers of ISUs, the empirical behavior of the estimators may reveal realistically attainable finite sample sizes under which estimation error is sufficiently minimized.

A small body of simulation research has provided preliminary information regarding minimally sufficient sample sizes applied researchers can use and still estimate parameters with minimal error. Unfortunately, the majority of the studies have examined limited covariance structures and almost exclusively balanced data conditions. While this literature provides insight for applied researchers, the limitations of these studies leave many questions unanswered. Specifically, the effects of unbalanced data, complex covariance structures, and systematic variations in the number of fixed and random effects on parameter estimation in small samples remain unclear. These are the focus of my thesis.

1.3 Literature Review

In the first empirical study looking into the role of sample size and estimation error Corbeil and Searle (1976) examined the behavior of both REML and FML estimators across multiple models, both balanced and unbalanced data, and a range of sample size conditions. Though some of their sample size conditions were quite low, this was not unreasonable given that most models had closed form solutions. Nonetheless, they acknowledged that their sample sizes were smaller than ideal. ISU sizes examined were $10, 20, 60$, and 100, and observation sample sizes examined were $6, 10, 15$, and 25. Thus, the largest total sample size contained 2500 data points.

Corbeil and Searle (1976) showed that the FML estimator for each model under balanced data was more efficient than the REML estimator. The authors suggest that the role played by bias in the computation of the MSE, coupled with the noted negative bias of FML estimators might imbue FML with an inherent efficiency advantage over REML. Given this finding, Corbeil and Searle (1976) derive a modified MSE measure designed to minimize this possibility. Evaluation of these modified MSEs produced boundaries below which REML was more efficient than FML. Using this modified efficiency criterion, and restricting examination to variance values falling below the boundary for each model, REML was found to be more efficient. However, in unbalanced data, no closed form solution to the MSE could be obtained. Consequently, an adjusted MSE could not be computed, and, as expected, using the empirical MSE, in unbalanced data FML was found to be more efficient than REML in all cases. These findings were replicated by Swallow and Monahan (1984) who also demonstrated the relationship between the bias of FML and its superior MSE properties.

In a subsequent analysis of the simulation work presented in Swallow and Searle (1978), Swallow and Monahan (1984) examined bias and MSE properties of several estimators, including REML and FML, for the variance component model. The simulation design employed manipulations of sample size, intra-class correlation coefficient (ICC), and balancedness of the data. The primary focus of the paper was the estimation of variance components obtained via the one-way random ANOVA under varying degrees of unbalancedness. The two primary sampling patterns consisted of sequences of ISUs with fixed observation size. For example, the smallest sample size cells in the two patterns consisted of three ISUs having $3, 5$, and 7, and $1, 5$, and 9 observations, respectively. These two conditions had the same number of ISUs, different numbers of observations per ISU, and the same total sample size ($N_t = 15$). Increases in total sample size resulted from increasing the number of ISUs with fixed observations. Specifically, with six ISUs the number of ISUs with each of the above mentioned observation sizes was doubled, and with nine ISUs the number was tripled. Within each cell, $10,000$ replications were generated.

In examining point estimation of τ_{00}, Swallow and Monahan (1984) found that when ICC $< .5$ the FML estimator was the minimum variance estimator, as measured by the MSE. Moreover, FML had minimum bias of all estimators considered. When ICC $\geq .5$ FML had a downward bias which attenuated the MSE. The authors concluded that the shrinking of the MSE translated into an illusory advantage of FML over REML. In fact, bias correction of the FML estimator eliminated the relative advantage of FML over REML as measured by MSE. However, as proved by Corbeil and Searle (1976), the theoretical MSE of the FML estimator is smaller than that of the REML estimator in balanced data for a wide range of models. Whether this is related to theoretical bias or not, it is nonetheless an advantage of FML. While recent work has focussed on models with more complex fixed effects structures, only one has generalized the restricted covariance structures considered by Corbeil and Searle (1976) and Swallow and Monahan (1984). This is an unfortunate shortcoming, because under balanced data closed form solutions exist for such models.

In a brief note published in the *Multilevel Modelling Newsletter*, Mok (1995) presented the results of a small simulation investigating the impact of sample size under a known and constant ICC (.1459) on the efficiency and bias of Restricted Iterative Generalized Least Squares (RIGLS) estimates in the linear mixed model. RIGLS is the generalized least squares analog of REML, and the two estimators are identical when $\{U_j, e_j\} \sim N(0, \mathbf{\Sigma}_j)$, with the form of $\mathbf{\Sigma}_j$ varying as a function of the parameter, U_j or e_j, considered (Goldstein, 1986). Because Mok (1995) focused exclusively on the case of Gaussian balanced data, her work on RIGLS generalizes directly to REML. The model of interest to Mok (1995) was a mixed model with a fixed intercept and slope, each having random components and possessing a two-dimensional unstructured covariance matrix. Mok (1995) employed a fully balanced symmetric sample size design. Eleven ISU and observation sizes were considered: 5, 10, 20, 30, 40, 50, 60, 70, 80, 100, and 150. Every ISU size was crossed with every observation size resulting in 121 sample size conditions.

Within each sample size condition 100 replications were generated and analyzed. For each cell the empirical MSE and bias of the RIGLS estimates for the model parameters were computed.

Mok (1995) found that when the number of ISUs was equal to the number of observations or when the number of ISUs exceeded the number of observations fixed effects estimates were estimated with near identical precision. However, estimates in both conditions exhibited substantially smaller MSE and bias than did those obtained when the number of observations exceeded the number of ISUs. Random effect estimates, though consistent across all conditions, were more biased when the number of observations exceeded the number of ISUs than when the converse was true. There was no difference across conditions in the bias of residual variance estimates. Mok (1995) concluded that it was better to maximize ISU size in order to minimize estimation error.

Consistent with the conclusions of Mok (1995), Bassiri (1988) demonstrated the importance of ISUs in estimating LMM parameters. Bassiri (1988) examined changes in REML estimates as a function of ICC (.1 vs. .25), number of ISUs $(10, 30, 60, 150)$ and number of observation per ISU $(5, 25, 60, 150)$. The model was composed of three main fixed effects, one fixed interaction, and two random effects. The covariance matrix of the random effects was a two-dimensional heterogeneous variance component structure. Bassiri found that the number of ISUs was a better predictor of problems in REML estimation than the number of observations per ISU, with smaller numbers of ISUs resulting in the highest degrees of bias in both the fixed and random effects. Varying the number of observations within a fixed ISU size affected neither the estimation of fixed nor random effects. It is interesting to note that at a fixed sample size, estimates obtained under a large ICC (.25) exhibited less estimation error than when the ICC was small (.1). Bassiri (1988) suggested that because the ICC is a measure of the degree to which total variance is the result of between ISU variance, as ICC increases, so does the degree of variance associated with differences in ISUs. Such increases in variance parameters are tantamount to increases in the power to estimate parameters, for as parameters depart from zero they are likely to be more reliably estimated.

Hox and Maas (2002) also contributed to our understanding of the role of sample size in the linear mixed model. The model of interest to Hox and Maas (2002) was a multilevel model with four fixed effects (intercept, two slopes, and an interaction term) with two random effects (one intercept and one slope) modelled using a two dimensional homogeneous variance component covariance matrix. Hox and Maas (2002) examined 27 conditions in their design, consisting of three ISU conditions (30, 50, and 100 ISU), three observation size conditions (5, 30, and 50 observations per ISU), and three ICC conditions (ICC values of .1, .2, and .3). For each cell of the design 1000 replications were generated. Like Mok (1995), Hox and Maas (2002) examined bias only in REML estimates. Hox and Maas (2002) did not encounter any convergence or improper solution problems. They found negligible bias (average bias was .05%) in REML estimates of the fixed effects across sample size variations; however, in the smallest sample size condition $(\text{ISU} = 30, \text{observations} = 5)$ bias in the fixed effects was .3%. Peculiarly, Hox and Maas (2002) found the exact same pattern of bias in the random effects, with the average bias across sample size variations being .05%, and the highest bias of .3% being observed in the smallest sample size condition.

1.3.1 Summary

There are five general trends in the preceding empirical work: Increasing ISUs decreases bias more than increasing observations per ISU, the effect of model complexity has been ignored, the effect of unbalanced data has been ignored, and the effect of covariance magnitude has been ignored, though REML may be less biased than FML, it may have greater sampling variability.

First, consistent with theory, and as demonstrated in all empirical studies, REML is unconditionally less biased than FML. However, REML does not necessarily have the lowest sampling variance. In fact, for some models and sample sizes, REML may exhibit greater RMSE than FML.

Second, consistent with theory, Mok (1995) and Bassiri (1988) found that decreasing the number of ISUs had a substantial effect on (co)variance parameter estimation. In addition, fixed effects estimates became more precise as the total number of observations increased (Mok, 1995; Bassiri, 1988).

Third, the effect of model complexity has not been adequately examined. All but one of the reviewed studies examined the case of a variance component model. While this is a useful model, and has a rich history in many fields, the complexity of modern designs allow for estimating models of greater complexity. As a result, models with more than one random effect are now common in the applied literature. Thus, examining estimation error in more complex models is necessary.

Fourth, most studies have looked at data types that are both uncommon in applications and limit estimation error. All of the reviewed studies save Corbeil and Searle (1976) and Swallow and Monahan (1984) focused exclusively on the case of balanced data. Yet, we know from Corbeil and Searle (1976) and Searle et al. (1992) that closed form estimating equations exist for such models in the case of balanced data. Thus, contrary to Bassiri (1988), simulation studies of variance component models under balanced data result in a substantial loss of generality. The focus on balanced data has the potential to result in a loss of generality because it is in the case of unbalanced data that estimation error is most pervasive and problematic (Corbeil & Searle, 1976; Swallow & Monahan, 1984). The problem of unbalanced data is compounded by the fact that theory, which in balanced data nearly fully describes the nature of estimation error, provides little guidance in the case of unbalanced data (Corbeil & Searle, 1976; Swallow & Monahan, 1984). Thus, the need for empirical guidance is greatest in the case of unbalanced data.

Fifth, no study has manipulated the effect of covariance magnitude, assuming instead, that all covariance components are equally estimable. In contrast, one could conceive of larger and smaller covariance components being differentially estimable. As components tend toward boundary values, point estimation could become less precise and model convergence rates could decrease (Demidenko, 2004).

These five issues are the focus of my thesis.

1.4 Hypotheses

Based on analytic theory and prior research I tested five hypotheses.

1.4.1 Hypothesis 1: Estimator Effects

Previous research, both empirical and theoretical, has demonstrated the optimal bias properties of REML relative to FML. Across all conditions I predict that REML estimates of fixed effects and covariance components will be less biased than FML estimates. FML estimates of covariance components should be substantially negatively biased, while REML estimates should be only slightly negatively biased. In addition, based on the work of Corbeil and Searle (1976), Swallow and Monahan (1984), and Rao (1977), FML is predicted to have lower RMSE than REML.

1.4.2 Hypothesis 2: Effect of Varying Independent Sampling Units on T and Total Sample Size on σ^2 and $\mathbf{\Gamma}$

As the number of ISUs decrease, both FML and REML will exhibit increased bias in estimates of $\mathbf{T}$. However, FML bias is expected to exceed REML bias. At the same time, FML should exhibit greater efficiency than REML. While very small n_j may have an effect on estimation error in $\mathbf{T}$, this effect should be small relative to the impact of varying N. In contrast, fixed effect and residual variance estimates should be unaffected by decreasing ISU size. However, because $\hat{\sigma}^2$ and $\hat{\mathbf{\Gamma}}$ depend on the total sample size, as the total sample size decreases, the performance of their estimators should erode in terms of bias and efficiency.

1.4.3 Hypothesis 3: Effect of Varying the Number of Estimated Fixed Effects on Estimation of Covariance Parameters

REML estimation is motivated by the fact that the bias of $\mathbf{T}_{FML}$ increases as the number of fixed effects increases. A worst case scenario for the $\mathbf{T}_{FML}$ occurs when the number of ISUs is small and the number of fixed effects is large (Raudenbush & Bryk, 2002). Thus I predict that as model complexity increases, the REML estimator of the covariance parameters should exhibit lower bias and efficiency, than the FML estimator.

1.4.4 Hypothesis 4: The Effect of Unbalanced Data

Point estimation and inference are known to be more complex under unbalanced data (Henderson, 1953). For a subset of the cells, point estimates obtained under balanced data will be contrasted with point estimates obtained under unbalanced data. Theory would suggest that REML estimates would be unbiased under balanced data. Thus, I hypothesize that point estimates of all parameters will be more accurate under balanced data, exhibiting near zero bias, but only for REML; and FML estimates may exhibit some bias, but only trivial amounts.

1.4.5 Hypothesis 5: Magnitude of Covariance Matrix of Random Effects

Estimation of parameters of small magnitude poses difficulty in the mixed model (Bassiri, 1988). Consequently, I predict that bias and efficiency of covariance component estimates will increase and decrease respectively as magnitude of covariance components decrease.

CHAPTER 2

Method

The simulation employs a 2 (estimators) X 4 (ISU sizes) X 4 (observation sizes) X 3 (models) X 2 (covariance matrices) design. There are thus 192 cells in the design.

2.0.6 Estimators and ISUs

The two estimators considered in this design were REML and FML. Four ISU sizes were examined in order to study the behavior of estimators across a range of ISUs. These ISU sizes reflect the lower end of acceptable ISU sizes as well as one ISU size chosen to be representative of a very large number of ISUs. The ISU sizes considered were 15, 30, 60, and 120. Because the most complex model had 6 fixed effects, and in such a context Demidenko's Inequality 2.87 shows that the MLE exists with probability 1 when the number of ISUs exceed 13, 15 was employed as a minimum ISU size in order to protect against non-existence of the MLE.

2.1 Models Considered

A total of three model types were considered. They were: **Model 1**, which was a random intercept model, composed of an intercept term containing both fixed and random components; **Model 2**, which was a random regression model, composed of an intercept and two slope parameters, each having both fixed and random components; lastly, **Model 3** added a level 2 predictor, and two cross level interactions to **Model 2**. These models can be mathematically represented using reduced form equations as:

Model 1:

$$y_{ij} = \gamma_{00} + u_{0j} + e_{ij}, \tag{2.1}$$

Model 2:

$$y_{ij} = \gamma_{00} + \gamma_{10}x_{1ij} + \gamma_{20}x_{2ij} + u_{0j} + u_{1j}z_{1ij} + u_{2j}z_{2ij} + e_{ij}. \tag{2.2}$$

Model 3:

$$y_{ij} = \gamma_{00} + \gamma_{10}x_{1ij} + \gamma_{20}x_{2ij} + \gamma_{01}w_{1j} + \gamma_{11}w_{1j}x_{1ij} + \gamma_{21}w_{1j}x_{2ij} + u_{0j} + u_{1j}z_{1ij} + u_{2j}z_{2ij} + e_{ij}. \tag{2.3}$$

These three models were considered because of their prominence in many model building strategies. Specifically, in applications it is common to begin analyses by estimating a simple model, such as **Model 1**. This initial model is typically expanded by looking into the existence of additional random effects. This second stage of model building is represented by **Model 2**. Lastly, once an optimal number of random effects have have been specified, **Model 2** is expanded to include one or more predictors designed to explain the variability in the outcome across ISUs. The addition of such level-2 predictor(s) results in the addition of main effect(s) for the level-2 predictor(s) as well as interactions between the level-2 predictor(s) with every other level-1 predictor. This last stage of model building is captured by **Model 3**.

2.1.1 Parametric Specification

The fixed effect vector for **Model 1**, $\mathbf{\Gamma}_1$, had only a single element, γ_{00}. The fixed effect vector for **Model 2**, $\mathbf{\Gamma}_2$, was composed of three elements, $\gamma_{00}, \gamma_{10}, \gamma_{20}$. The specification of the fixed effect vector for **Model 3**, $\mathbf{\Gamma}_3$, was an extension of $\mathbf{\Gamma}_2$, where the first three elements were identical to those of $\mathbf{\Gamma}_2$. However, $\mathbf{\Gamma}_3$ was augmented by the inclusion of a level 2 predictor and all cross-level interactions. **Model 2** and **Model 3** each had a covariance matrix of random effects, $\mathbf{T}$ of dimension 3×3, while **Model 1** only had a single random effect variance component: τ_{00}.

A common manipulation employed in previous studies of sample size in the mixed model has been to vary the intra-class correlation (ICC). Since models with low ICCs generally have smaller intercept variances than do models with large ICCs, manipulating ICC has been used to determine differences in magnitude of estimation error as parameters diverged from zero. However, when the variance components are summarized by a covariance matrix rather than a scalar variance, the true meaning of manipulating the ICC is unclear. In such a context it is not clear whether the ICC, as traditionally computed, has any real meaning (Ahrens, 1976). Because the ultimate impact of such manipulations is to increase or decrease the magnitude of one element, in the case of a covariance matrix, a more meaningful manipulation would be to compare covariance matrices with elements of larger magnitude to covariance matrices with elements of smaller magnitude. Thus, two covariance matrices, $\mathbf{T}_1$ and $\mathbf{T}_2$, were generated in order to test Hypothesis 4.

The elements of $\mathbf{T}_1$ were of small magnitude, while the elements of $\mathbf{T}_2$ were of large magnitude. Therefore, **Model 2** and **Model 3** were estimated twice in the design, once under the covariance matrix of random effects corresponding to $\mathbf{T}_1$, and once under $\mathbf{T}_2$. In order to test hypothesis 5 on **Model 1**, the same procedure was employed, though instead of alternating covariance matrices, the value of τ_{00} was varied. Thus, **Model 1** was estimated with τ_{00} set equal to the 1,1 element of $\mathbf{T}_1$ and again with τ_{00} set equal to the 1,1 element of $\mathbf{T}_2$. For economy of writing, from hereon, the two fixed effects vectors and two covariance matrices of random effects will be generally referred to using an m subscript. When the reader encounters $\mathbf{\Gamma}_m$ and $\mathbf{T}_m$ this is meant to indicate a statement applying to either $\mathbf{\Gamma}_1$ and/or $\mathbf{\Gamma}_2$ etc.

2.1.2 Population Values

Because the fixed effects, residual variance, and random effects are orthogonal due to the block diagonal Hessian of the model (Demidenko, 2004), $\mathbf{\Gamma}_m$, $\mathbf{T}_m$ and σ^2 can be populated with values that are all mutually independent. Although, in principle, parameter estimates could take on infinitely many values, the integer values I chose for σ^2 and the elements of the matrices $\mathbf{\Gamma}_m$ and $\mathbf{T}_m$ were chosen to be representative of the values commonly encountered in applications or reported in literature. The fixed effects vectors I used for this thesis are given as:

$$\mathbf{\Gamma}_1 = \begin{pmatrix} 5 & .98 & 2.3 \end{pmatrix}', \tag{2.4}$$

$$\mathbf{\Gamma}_2 = \begin{pmatrix} 5 & .98 & 2.3 & 1.9 & 1.3 & .85 \end{pmatrix}'. \tag{2.5}$$

Proportion of Variance Explained by Fixed Effects

Effect sizes are are not uniquely defined for the linear mixed effect model. However, it is important to demonstrate how the population values for the fixed effects map onto commonly encountered or expected values in social science research. I used pseudo-effect size measures to demonstrate the correspondence between fixed effect value effect sizes associated with the generating values and Cohen's rules for effect size (Cohen, 1988). Because of varying model complexity, the means by which the pseudo-effect size measures were computed changed across models. All methods fell under the rubric of proportion of variance reduction methods advocated by Raudenbush and Bryk (2002). For model 2, all of the fixed effect estimates were associated with level 1 variables, and thus, according to Raudenbush and Bryk (2002) resulted in decreasing residual variance values. Thus proportion reduction in variance can be observed in residual variance estimates. In contrast, with model 3, level 1 predictors can be expected to remain associated with reductions in residual variance, but the level 2 predictor effect and the corresponding cross-level interactions can be expected to be associated with reductions in random effect variance.

For model 2, pseudo-effect size estimates were obtained by first fitting a null model with random and fixed intercepts, and then incrementally adding the level 1 fixed effects, at each stage computing the proportion reduction in variance between the fitted model and the baseline model according to the definition given by Raudenbush and Bryk (2002):

$$PR_{l1} = \frac{\sigma_c^2}{\sigma_u^2 + \sigma_c^2}. \tag{2.6}$$

For model 3, the process was more complex.

For models in which level 2 and cross level effects, Raudenbush and Bryk (2002) recommend calculating proportion reduction in variance measures on the random effect variances and not the residual variances. To the extent that the random effects are correlated, accuracy of proportion reduction in variance techniques will be attenuated. Nonetheless, the proportion reduction in variance equation used here for the $\mathbf{i}^{th}$ level 2 effects is given by Raudenbush and Bryk (2002) as:

$$PR_{l2} = \frac{\tau_{ii}^c}{\tau_{ii}^u + \tau_{ii}^c}, \tag{2.7}$$

where the c and u superscripts indicate conditional and unconditional values. Unconditional values are the estimates of τ_{ii} observed when the $\mathbf{i}^{th}$ level 2 effect is not included, and the conditional values are the estimates of τ_{ii}, when the $\mathbf{i}^{th}$ level 2 effect *is* included. Thus, τ_{11} is conditioned upon inclusion of the level 2 predictor ($W1$), τ_{22} is conditioned upon the inclusion of the first cross level interaction ($W1 * D1$), and τ_{33} is conditioned upon the inclusion of the second cross level interaction ($W1 * D2$). Results are given in Table 2.1. As can be seen, proportion reduction in variance values corresponded to small to moderate effect sizes as defined by Cohen (1988).

Table 2.1: Proportion Reduction in Variance Estimates for Models 2 and 3

	SR^2 for Fixed Effect Parameters				
	γ_{10}	γ_{20}	γ_{01}	γ_{11}	γ_{21}
Model 2 T1	0.09	0.14	-	-	-

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Table 2.1 – continued from previous page

	SR^2 for Fixed Effect Parameters				
	γ_{10}	γ_{20}	γ_{01}	γ_{11}	γ_{21}
Model 2 T2	0.07	0.14	-	-	-
Model 3 T1	0.05	0.12	0.13	0.15	0.17
Model 3 T2	0.12	0.20	0.26	0.29	0.37

Consistent with the examples provided in Raudenbush and Bryk (2002), the residual variance I considered in this thesis was large and constant. Thus the residual variance matrix was be parameterized as $\mathbf{I}\sigma^2$ for each model, with $\sigma^2 = 46.58$.

I generated $\mathbf{T}_1$ and $\mathbf{T}_2$ by first specifying one correlation matrix, $\mathbf{R}$. The correlations contained in $\mathbf{R}$ reflect medium to high correlations. Next, I generated two diagonal matrices, $\mathbf{D}_1$ and $\mathbf{D}_2$, corresponding to $\mathbf{T}_1$ and $\mathbf{T}_2$ respectively. The elements of $\mathbf{D}_1$ and $\mathbf{D}_2$ were the standard deviations of the desired covariance matrix ($\mathbf{T}_1$ or $\mathbf{T}_2$). The two diagonal matrices differed in magnitude, with $\mathbf{D}_1$ having small elements and $\mathbf{D}_2$ large elements. Pre and post-multiplication of the correlation matrix by the corresponding diagonal matrices resulted in two covariance matrices whose elements differ in magnitude.

Given $\mathbf{R}_1$:

$$\mathbf{R}_1 = \begin{pmatrix} 1 & 0.44 & 0.43 \\ 0.44 & 1 & 0.19 \\ 0.43 & 0.19 & 1 \end{pmatrix}, \tag{2.8}$$

and the diagonal matrix

$$\mathbf{D}_1 = \begin{pmatrix} 12 & 0 & 0 \\ 0 & 7 & 0 \\ 0 & 0 & 4 \end{pmatrix}, \tag{2.9}$$

the resulting covariance matrix composed of elements of large magnitude is given as:

$$\mathbf{T}_1 = \begin{pmatrix} 12 & 4 & 3 \\ 4 & 7 & 1 \\ 3 & 1 & 4 \end{pmatrix}. \tag{2.10}$$

Starting from the correlation matrix

$$\mathbf{R}_2 = \begin{pmatrix} 1 & 0.29 & 0.32 \\ 0.29 & 1 & 0.12 \\ 0.32 & 0.12 & 1 \end{pmatrix}, \tag{2.11}$$

and the diagonal matrix

$$\mathbf{D}_2 = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \tag{2.12}$$

the covariance matrix composed of elements of low magnitude is given as:

$$\mathbf{T}_1 = \begin{pmatrix} 4 & 1 & 0.9 \\ 1 & 3 & 0.3 \\ 0.9 & 0.3 & 2 \end{pmatrix}, \tag{2.13}$$

2.2 Data Generation

2.2.1 Unbalanced Data

All data examined in this project were unbalanced, except for the subset of cells in which balanced data were contrasted with unbalanced. There are several reasons why balanced data are not interesting to a study of iterative estimators. First, closed form estimators exist for many mixed models under balanced data (Corbeil & Searle, 1976; Searle et al., 1992). Second, it is rare for field-collected data to be balanced. Thus simulation findings based on balanced data are likely of limited use to applied researchers.

Unbalanced data were generated using the following mechanism. Unballanced observations were allocated to ISUs by first dividing the total number of ISUs within an

ISU condition (15, 30, 60, or 120) into thirds. The first third of the ISUs then sampled a number of observations within a given observation condition (15, 30, 60, or 120) equal to $\frac{1}{3}$ of the total number of observations in the condition. The second third of the ISUs then sampled a number of observations equal to $\frac{2}{3}$ of the total number of observations in a given observation condition. The final third of the ISUs sampled a number of observations equal to the total number of observations in a given observation condition. For example, with 15 ISUs in the 15 observations per ISU condition, the first 5 ISUs sampled 5 observations, the second 5 ISUs sampled 10 observations, and the last 5 ISUs sampled 15 observations. This process was repeated for each ISU and observation condition.

2.2.2 Generating Random Effects with Known Covariance Structure

In each replication a matrix of standard normal variables was sampled, transformed so that it was orthogonal to the fixed effect predictors and the errors. This matrix was then multiplied by the Cholesky factor of the population covariance matrix. The resulting matrix had column covariance corresponding to the population covariance matrix contaminated by the sampling error involved in generating the initial random normal matrix.

2.2.3 Generating Dependent Variable Under Model

1. After generating random effects with known covariance structure, the dependent variable was generated under the mixed model as an additive function of the fixed and random effects, with random error added to generate the level 1 error. Exogenous predictors were generated as realizations from the standard normal distribution.

2. Unbalanced observations were generated by deleting observations in each observation cell nested within the 4 ISU size conditions in a manner proportional to the number of observations under balanced data. Starting from balanced data, unbalanced observations were generated by deleting: $\frac{2}{3}$ of the observations in the first

third of the ISUs, $\frac{1}{3}$ of the observations in the second third of the ISUs, and zero observations in the final third of the ISUs. For example, under 15 ISUs and 15 observations per ISU, 10 observations were deleted from each of the first 5 ISUs, 5 observations were deleted from each of the next 5 ISUS, and zero observations were deleted from the last 5 ISUs. Under 15 ISUs and 30 observations per ISU, 20 observations were deleted from each of the first 5 ISUs, 10 observations were deleted from each of the next 5 ISUS, and zero observations were deleted from the last 5 ISUs. This process was repeated in each of the 16 sample size cells.

2.2.4 Manipulation Check of Data Generation Process

Because data generation does not vary by parameter values or model complexity, in order to determine whether the procedure generated valid data I restricted attention to a fixed and large sample size and generated data under model 2. The test simulation used 3000 ISUs and 2000 observations per ISU, resulting in a total sample size of 6 million data points. The Mixed procedure in SAS was used to determine whether parameters governing data generation could be adequately recovered in estimation

Table 2.2: Model 2 Manipulation Check of Data Generation

			T2	
Model	**Parameter**	**True**	**RML**	**FML**
$Model2$	γ_{00}	5	5	4.9
$Model2$	γ_{10}	.98	.98	.84
$Model2$	γ_{20}	2.3	2.29	2.16
$Model2$	σ^2	46.58	46.65	46.37
$Model2$	τ_{11}	4	4.03	4.02
$Model2$	τ_{21}	1	.94	1.03
$Model2$	τ_{22}	3	2.88	3.2

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Table 2.2 – continued from previous page

			T2	
Model	**Parameter**	**True**	**RML**	**FML**
$Model2$	τ_{31}	.9	.9	.77
$Model2$	τ_{32}	.3	.3	.4
$Model2$	τ_{33}	2	1.98	1.74

As can be seen, the parameter estimates were close to expectation at asymptotic sample sizes, thus empirical evidence suggests that the data generation procedure is valid.

2.3 Analyses

2.3.1 Improper and Non-converged Solutions

Non-converged solutions are defined as solutions in which, for some reason, a maximum is not obtained in 100 iterations. This is double the default number of iterations in Proc Mixed, and is employed to maximize the chance for models to converge in the smallest sample sizes. Improper solutions were defined as any solution in which the estimated covariance matrix of random effects was not positive definite at the last iteration.

To track the frequency of such problems as a function of sample size, indicator variables were generated tallying the number of non-converged or improper solutions relative to the total number of solutions in a given cell of the design.

2.3.2 Measuring Estimation Error

Estimation error was measured using percent relative bias (PRB), and root mean squared error (RMSE). These two statistics were computed using the following equations:

$$\mathrm{PRB} = 100 * \frac{\frac{1}{N}\sum_{i=1}^{N}(\hat{\theta}_i - \theta)}{\theta} \tag{2.14}$$

$$\text{RMSE} = [\frac{1}{N}\sum_{i=1}^{N}(\hat{\theta}_i - \theta)^2]^{\frac{1}{2}} \quad (2.15)$$

Values of the two measures of estimation error were computed by pooling across the 1000 replications in each cell of the design. Tabular estimation error results are presented in appendices. However, because it is often difficult to interpret tabular information in simulation studies, I employed two methods to further examine results: graphical summaries, and meta-modeling. Consistent with the guidelines presented by Kaplan (1988), bias values exceeding 10% were considered problematic.

2.3.3 Plots

In addition to examining the behavior of estimation error statistics arranged in tables, graphical summaries of estimation error were generated by plotting PRB and RMSE across ranges of sample size (ISUs for covariance parameters, and fixed effects). To permit simple contrasts across conditions, casement plots were generated for the sample size and estimator effects.

2.3.4 Testing Hypotheses 1 and 2: Meta-Model

Estimation error, as defined by $100 \times \frac{(\hat{\theta}_i - \theta)}{\theta}$, was calculated for the covariance parameters, and the residual variance estimates obtained from every model in every cell of the design. For each model (**Model 1**, **Model 2**, and **Model 3**) a general linear model (GLM) was fit to the outcome of statistics (PRB or RMSE) for each estimated parameter (each variance, covariance, and fixed effect). In order to determine the effect of varying the following facets of the design: the number of ISUs, the total sample size, and the type of estimator (REML or FML), reference cell coded main effects and interactions were estimated. Results were contrasted across covariance matrix condition to determine the effect of covariance element magnitude. All possible two way interactions were estimated. Least squares means for each cell of the design matrix corresponded to the PRB estimates for each cell of the simulation design.

Hypotheses regarding model complexity (hypothesis 3) and covariance matrix magnitude (hypothesis 5) were tested by contrasting meta-model effects (Multiple $\mathbf{R}^2$) as well as bias and RMSE cell means across the three models of interest and the two covariance matrix conditions.

CHAPTER 3

Results

3.1 Outline

I begin by describing a subset of results that I will not present in detail. First, cells with model convergence rates below 5% were excluded. Second, the fixed effects and balanced data results were excluded because they exhibited very low levels of bias and RMSE. Results obtained from the meta-models are presented next. I then present results for covariance parameter bias. Results are arranged in order of model complexity, starting with model 1 and finishing with model 3. Results initially focus on the estimator and covariance matrix effect. Subsequently, sample size and estimator effects are explored for each covariance matrix and model. A summary provides contrasts across all conditions examined. Following the parameter bias summary, results are provided in the same order for parameter RMSE.

3.2 Results Restricted to Cells With Less Than 5% NCV Solutions

Because the simulation was run in each cell until 1000 proper solutions were obtained, in the smallest sample size cells, where proper solutions were very rare, the probability that the 1000 obtained solutions were sampled from the extrema of the distribution of solutions was great. Solutions observed in such cells could provide idiosyncratic or inexplicable results, which could be expected to have very low external validity. In order to maximize the external validity of the study I excluded cells with initial attempt convergence rates less than 5%. In other words, I require that at least 50 of the first

1000 replications converge to a proper solution. Cells excluded from analysis because of rates of non-convergence exceeding the pre-specified threshold are indicated in Tables 3.1, 3.2, and 3.3 by red highlighting. Convergence rates are not presented for model 1 because all solutions converged in the first attempt. Thus, no cells were excluded for model 1.

As can be seen in Table 3.1, for model 2, FML and REML had nearly identical rates of excluded cells. The proportion of excluded cells varied over covariance matrix, with higher rates under T2 than under T1. Unfortunately, the result of these exclusions was the elimination of the smallest sample size cells from analyses, which were the cells of primary interest to this study. Though fewer cells were eliminated under T1, the eliminated cells were still among the absolute smallest sample size cells of the design. Cells of the design not displayed in Table 3.1 exhibited 100% convergence rates.

Table 3.1: Convergence Rates for Model 2

	% of Replications Converging in First Trial			
	T1 FML	T1 REML	T2 FML	T2 REML
15 ISU, 15 OBS	0.0%	0.0%	0.0%	0.0%
15 ISU, 30 OBS	0.20%	0.20%	0.20%	0.20%
15 ISU, 60 OBS	8.10%	8.30%	2.80%	3.10%
15 ISU, 120 OBS	25.30%	100.00%	2.60%	2.60%
30 ISU, 15 OBS	0.90%	4.90%	1.10%	1.30%
30 ISU, 30 OBS	12.80%	12.90%	5.00%	5.40%
30 ISU, 60 OBS	100.00%	100.00%	0.70%	0.70%
30 ISU, 120 OBS	100.00%	100.00%	100.00%	100.00%
60 ISU, 15 OBS	42.30%	85.10%	0.80%	7.70%

Table 3.2 demonstrates that under balanced data, rates of non-convergence and improper solutions were much lower than were observed under unbalanced data. As in Table 3.1, only the set of cells with convergence problems are presented, cells not presented in Table 3.2 exhibit 100% convergence rates. Under balanced data, only one cell, where 15 ISUs were sampled with 15 observations per ISU, was excluded based on the criterion set forth for admission to analysis. However, in order to provide a fair comparison between balanced and unbalanced data, in all analyses and plots the same cells excluded under model 2 unbalanced data were excluded under model 2 balanced data.

Table 3.2: Convergence Rates for Model 2, Balanced Data

	% of Replications Converging in First Trial			
	T1 FML	T1 REML	T2 FML	T2 REML
15 ISU, 15 OBS	2.4%	2.5%	0.1%	0.7%
15 ISU, 30 OBS	100.0%	100.0%	7.5%	23.3%
15 ISU, 60 OBS	100.0%	100.0%	100.0%	100.0%
15 ISU, 120 OBS	100.0%	100.0%	100.0%	100.0%
30 ISU, 15 OBS	100.0%	100.0%	15.0%	36.5%

As can be seen in Table 3.3, patterns of non-convergence and cell-exclusion under model 3 were nearly identical to the rates observed under model 2. Under model 2 for T2, REML and FML excluded cells coincided perfectly except for one cell; however, as observed in Table 3.3 under T2, for model 3 there were two cells for which exclusion was not coincident for REML and FML. A curious effect of interest was that, under model 3, when models failed to converge, the probability that all replications in a given cell would converge in the first attempt was virtually zero, whereas under model 2 there was a non-zero probability.

Table 3.3: Convergence Rates for Model 3

	% of Replications Converging in First Trial			
	T1 FML	T1 REML	T2 FML	T2 REML
15 ISU, 15 OBS	0.0%	0.0%	0.0%	0.0%
15 ISU, 30 OBS	0.40%	0.40%	0.0%	0.0%
15 ISU, 60 OBS	0.80%	4.10%	0.90%	0.90%
15 ISU, 120 OBS	14.70%	37.70%	3.50%	5.10%
30 ISU, 15 OBS	0.20%	0.30%	0.0%	0.0%
30 ISU, 30 OBS	12.50%	38.30%	0.0%	9.70%
30 ISU, 60 OBS	100.00%	100.00%	100.00%	100.00%
30 ISU, 120 OBS	100.00%	100.00%	100.00%	100.00%
60 ISU, 15 OBS	6.40%	6.40%	5.30%	6.00%

3.3 Exclusion of Fixed Effects

I restrict the detailed presentation of results to covariance parameters. There exist two compelling arguments for ignoring a detailed treatment of the fixed effect results. First, they are theoretically unbiased, with identical estimating equations for REML and FML. Second, results obtained in this study demonstrated that the asymptotic unbiasedness of the fixed effect estimator was robust to finite sample sizes. Because the MLEs of fixed effects do not differ between FML and REML, fixed effects estimates were nearly identical across estimators, with PRB values highly correlated, $\bar{\rho} = .99$, with no correlation in any condition below .98. In addition to the near zero bias observed in the fixed effects, both estimators exhibited identical and low levels of RMSE. These effects were consistent across all models, covariance matrices, and sample sizes. All plots depicting these effects are presented in appendix 1a, and full tabular results are presented in appendices 3 and 4.

3.4 Restriction of Attention to Unbalanced Results

This study focussed on estimation error under unbalanced data. However, the effect of unbalanced data is only meaningful to the extent that it is distinct from the effect for balanced data. Because a comprehensive treatment of the contrast between balanced and unbalanced data was beyond the scope of this project, but some treatment is important, in this section I provide a brief overview of the effect of balanced data on model 2. Full results for balanced data PRB are presented in Table 5.3, RMSE results are presented in 5.7, and graphical results are provided in appendix 1b. As expected, bias was greatly reduced when balanced data were analyzed. Across both estimators, covariance matrix conditions and sample sizes, balanced data estimates were much less biased and exhibited far lower RMSE than those observed for unbalanced data.

As observed in figure 5.19, under balanced data, bias exceeded $\pm 10\%$ for only τ_{11} & τ_{32}, and then only for FML, and only when 15 ISUs were sampled with 30 observations per ISU. However, as described in Table 3.2, under balanced data many more cells were accepted for analysis because of the higher rates of convergence and proper solutions observed. Figure 5.21 indicates that when analyzed cells were equated across data types, balanced data never exhibited bias exceeding $\pm 10\%$ under T1. As can be seen in figure 5.22, under T2, when analyzed cells were equated, balanced data exhibited very low bias, with only three estimates of τ_{11} exceeding $\pm 10\%$, and only for FML.

3.5 Meta-Model Results

For each estimated covariance parameter, general linear models were fit predicting variability in estimation error from the ISU effect, observations effect, and estimator effect, along with all possible two way interactions. Because the simulation design overpowers tests of point estimates of model effects, meta-model results are restricted to effect size estimates. Model $\mathbf{R}^2$ values are presented in Tables 3.4, 3.5, 3.6. Effects were generally small. Investigation of within-cell variance in estimation error indicated that cell variances ranged from approximately 8 to 20 times greater than cell means. Because Within-cell variance in estimation error exceeded between cell variance, multiple R^2 estimates were generally low.

Table 3.4: Meta-Model Results: Model 1

	Meta Model Multiple $\mathbf{R}^2$	
Parameter	**T1**	**T2**
σ^2	0.036	0.028
τ_{11}	0.097	0.087

Table 3.5: Meta-Model Results: Model 2

	Meta Model Multiple $\mathbf{R}^2$	
Parameter	T1	T2
σ^2	0.009	0.001
τ_{11}	0.013	0.009
τ_{21}	0.004	0.002
τ_{22}	0.007	0.004
τ_{31}	0.003	0.002
τ_{32}	0.001	0.001
τ_{33}	0.009	0.005

Table 3.6: Meta-Model Results: Model 3

	Meta Model Multiple R^2	
Parameter	T1	T2
σ^2	0.008	0.005
τ_{11}	0.035	0.028
τ_{21}	0.013	0.007
τ_{22}	0.02	0.014
τ_{31}	0.006	0.004
τ_{32}	0.002	0.003
τ_{33}	0.023	0.016

3.6 Covariance Parameter Bias

This section details the bias observed in parameter estimates of covariance components (variances and covariances). Five effects believed to impact severity of bias are considered: Number of ISUs sampled, number of observations sampled per ISU, estimator, covariance matrix magnitude, and model complexity. Recall that the ISU effect was parameterized with four levels, $15, 30, 60,\ \&\ 120$ ISUs. The observations effect was parameterized under an unbalanced model of thirds. Initially, $15, 30, 60,\ \&\ 120$ observations were allocated to each ISU. Which were then subjected to conditional elimination resulting in *average* observations per ISU of $10, 20, 40,\ \&\ 80$ respectively. Therefore, rather than referring to the observations allocated under balanced data, throughout the results section, when observations are referenced, they are referred to in terms of what the average observations per ISU is in a given condition. The estimator effect had two levels: FML and REML. The covariance matrix magnitude effect was tested by manipulating the generating matrix for the covariance matrix of random effects. The first generating matrix, T1, had elements of large magnitude, and the second, T2, had elements of small magnitude. Model complexity was manipulated with three models: a random effects ANOVA (model 1); a random effects regression model with an intercept and two predictors, each having a fixed and random component (model 2); and a random effects regression model with six predictors: an intercept and two predictors, each having fixed and random components, a level 2 predictor, and the two estimable cross level interactions (model 3).

The results are initially described within model by estimator and across covariance matrix, and then within model by estimator and sample size across covariance matrix.

3.6.1 The Covariance Matrix, Estimator, and Model Complexity Effect

Figures presented in this section detail the relationship between the estimator effects and differences as a function of the covariance matrix effect. FML and REML bias values are plotted against one another. REML bias is plotted along the vertical axis and FML bias is plotted along the horizontal axis. The horizontal line emanating from the REML axis indicates zero REML bias, while the vertical line emanating from the FML axis indicates zero FML bias. Bias values falling on the intersection of the two zero bias lines indicates zero bias for a specific covariance parameter in a given condition. A 45° line is overlaid and the points that fall on the line indicate where FML and REML bias estimates are identical. For PRB plots a green square demarcates the thresholds indicative of excess or problematic bias levels. Bias values outside of the green square along the vertical axis are estimates for which REML bias exceeds ±10%, while values outside the green square along the horizontal axis are estimates for which REML bias exceeds ±10%, and values outside the green square along both axes indicate excess bias in both estimators. Because some population values were less than 1, raw bias plots were examined to determine any effect of the relative bias metric on results. Though in a few cases the relative bias was different from raw bias, PRB never produced outliers, and observed discrepancies were consistent with expectations. Specifically, they were restricted to parameters with the smallest generating values. Given the general consistency between relative and raw bias, and the advantage of the interpretable metric associated with the relative bias metric, emphasis was placed on the relative bias findings.

Model 1

Under T1, REML PRB values ranged from -8 to 2.8, while FML PRB values ranged from -17.2 to 2.8; no REML estimates exceeded 10% bias, while 2 FML estimates exceeded 10% bias. Under T2, bias was more extreme, with REML PRB values ranging from -18.7 to 2.6, and FML PRB values ranging from -30.3 to 2.4; three REML estimates exceeded 10% bias and 7 FML estimates exceeded 10% bias. As observed in figure 3.1 and 3.2, REML and FML estimates of σ^2 were identical and exhibited trivial degrees of bias. There was no effect for covariance matrix on this parameter because the log likelihoods (both REML and FML) used in SAS' Mixed procedure profile out the residual variance, ensuring independence of the residual variance and covariance matrix of random effects. Profile estimation ensured that FML and REML estimates would be identical because the closed form estimator is identical across the two likelihoods. The random intercept parameter exhibited a different and slightly more complex pattern of bias. Though both FML and REML estimates of τ_{11} were uniformly negatively biased, the bias was more severe for FML under both T1 and T2. Compared to T1, T2 estimates of τ_{11} exhibited a much greater degree of bias. Examination of raw bias (see figures 3.3 and 3.4) revealed that the patterns observed in the relative bias metric were somewhat inconsistent with the raw bias metric. Whereas T2 raw bias levels were lower than T1 raw bias levels, T2 PRB levels were greater than T1 PRB levels. However, no extreme cases were produced in the PRB metric because the generating values for τ_{11} were both greater than 1. At the same time, because the T2 generating value was $\frac{1}{3}$ the magnitude of the T1 value, the PRB values under T2 were necessarily more extreme than the T1 values, all else being equal.

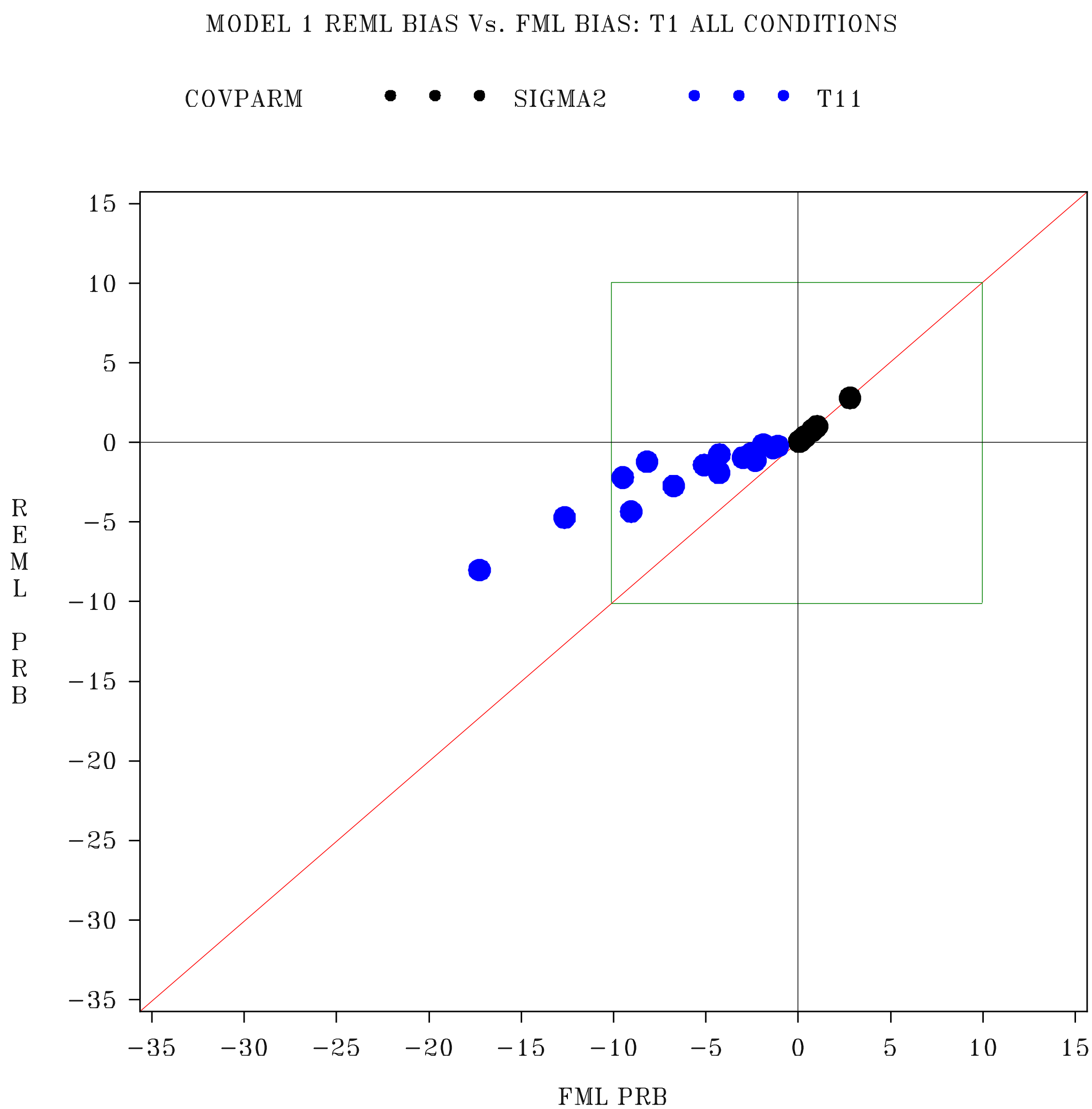

Figure 3.1: Random Effect PRB Model 1 T1 REML & FML

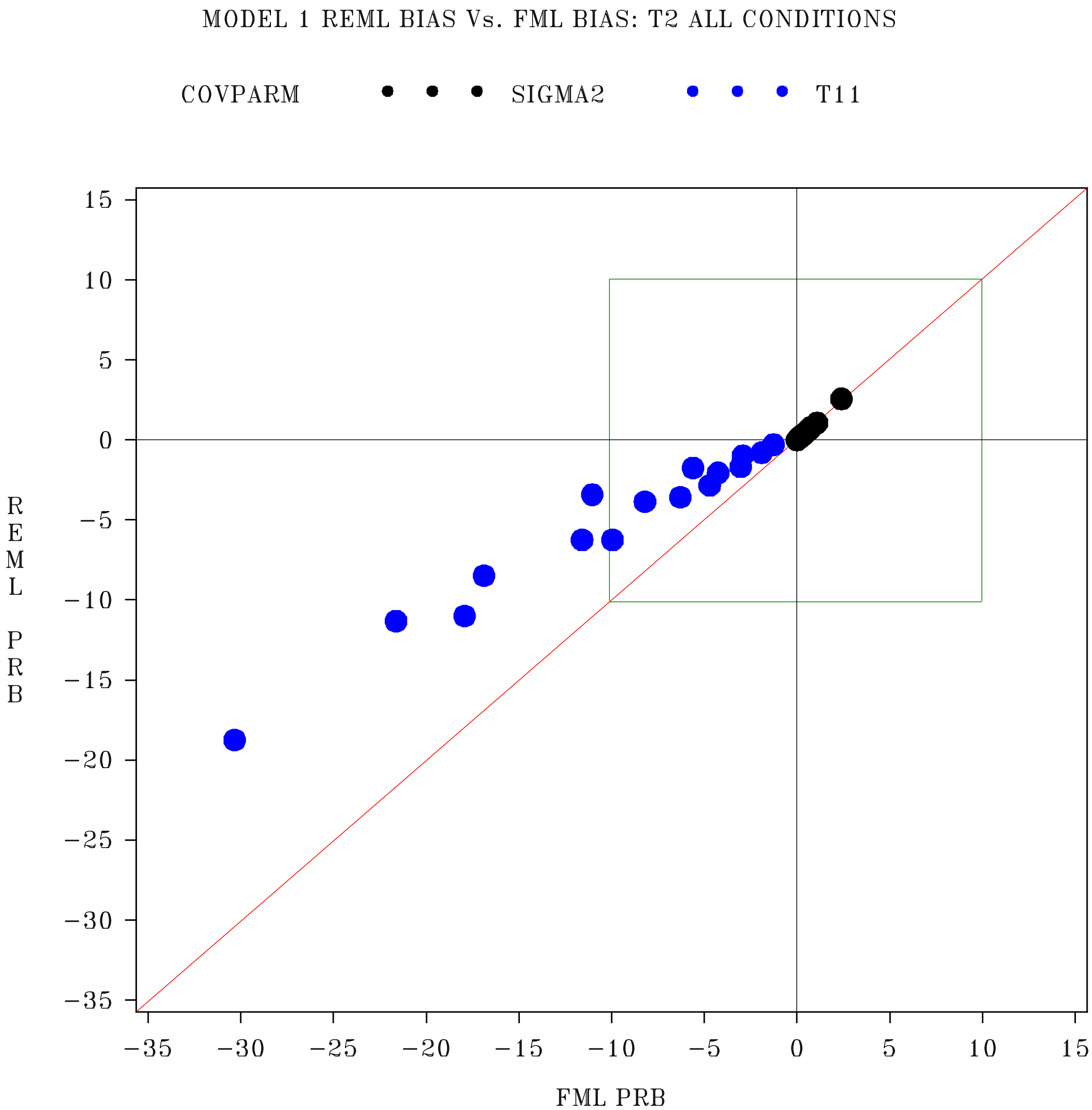

Figure 3.2: Random Effect PRB Model 1 T2 REML & FML

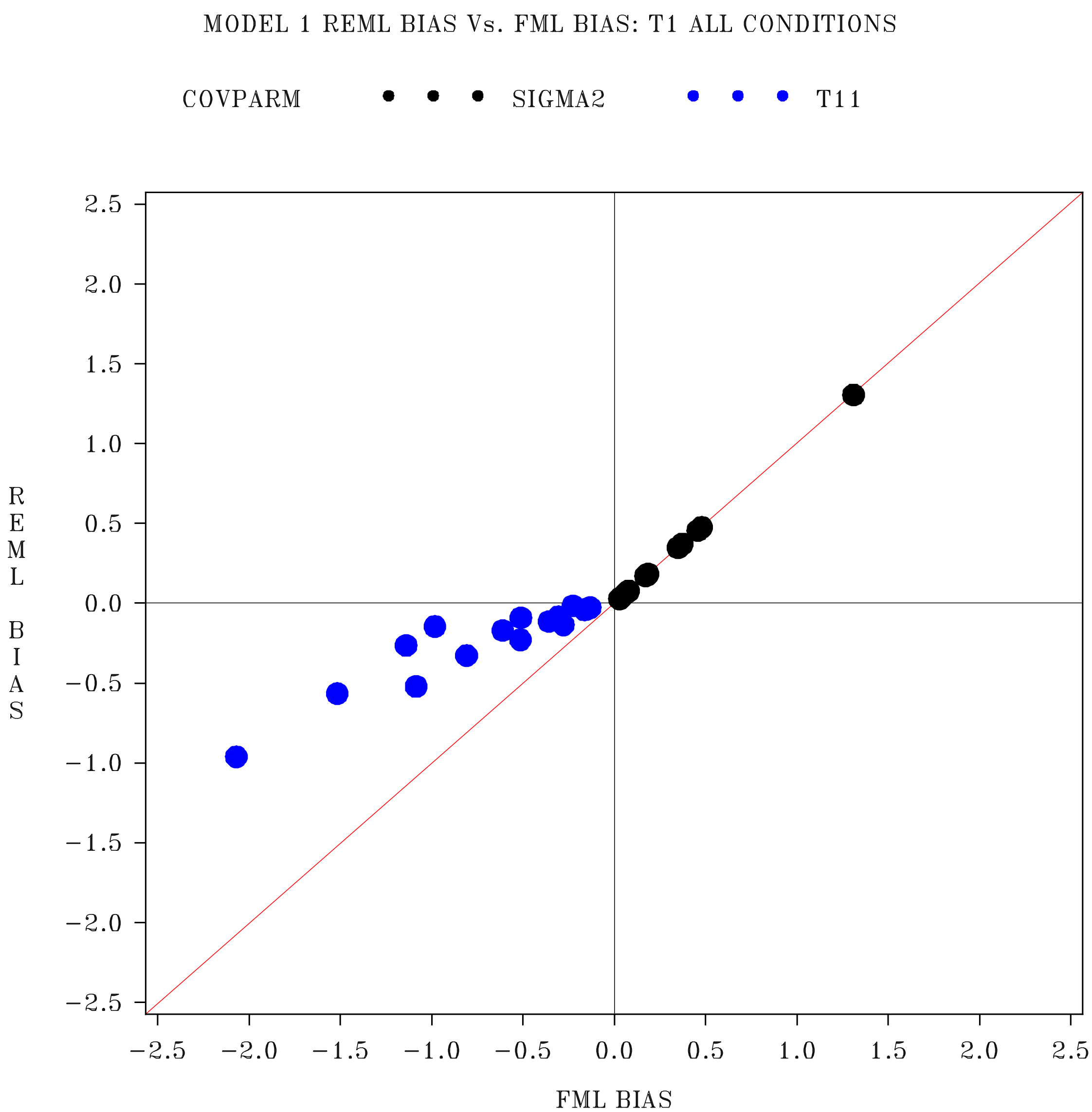

Figure 3.3: Random Effect Raw Bias Model 1 T1 REML & FML

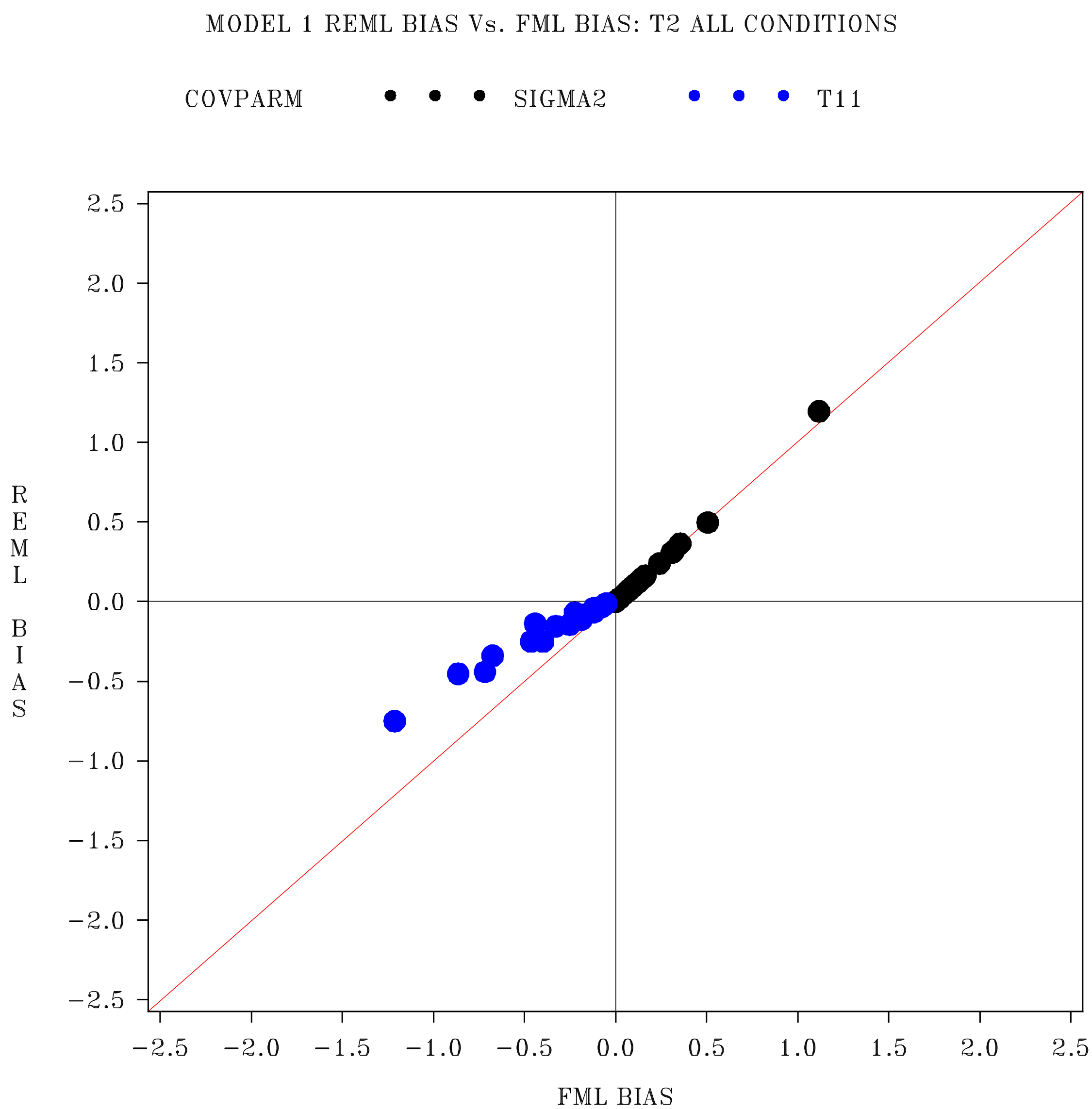

Figure 3.4: Random Effect Raw Bias Model 1 T2 REML & FML

Model 2

Under T1, REML PRB values ranged from -4.7 to 6.3, while FML PRB values ranged from -14.8 to 4.1; no REML estimates exceeded 10% bias, while four FML estimates exceeded 10% bias. Under T2, bias was more extreme, with REML PRB values ranging from -12.2 to 55.2, and FML PRB values ranging from -18.7 to 38.8; three REML estimates exceeded 10% bias and 5 FML estimates exceeded 10% bias. As can be seen in figure 3.5, under T1, FML was consistently negatively biased, with several values exceeding the threshold defining severe bias, while REML displayed a symmetric distribution of bias about zero, with no values exceeding the threshold defining severe bias. Though some substantial bias was observed in FML, there did not appear to be any extreme cases, indicating that the relative bias metric did not distort or exaggerate the magnitude of the observed bias. This was confirmed when figure 3.5 was contrasted with raw bias contained in figure 3.7. Both plots lead to the same conclusion regarding estimator performance within T1. Given that T1 was the generating matrix of large values, with no generating value less than 1, this finding was not surprising. Findings for T2, presented in figures 3.5 and 3.7 lead to different conclusions, both with regard to performance of the estimators and the influence of the relative bias metric on findings. As observed in both figures, FML exhibited the substantial negative bias observed under T1, however, for some parameters, so too did REML. However, REML bias was generally symmetrically distributed about zero. Unlike T1 PRB, contrasting figures 3.6 and 3.8 indicated that under T2, the relative bias metric appeared to exaggerate the bias effect. Specifically, the two most extreme PRB values corresponded to the two parameters, τ_{31} & τ_{32}, which had the smallest generating values, .9 & .3 respectively. If there were two parameters for which the relative bias metric could be expected to produce any extreme cases it would be these. Thus, the degree of bias observed for τ_{31} & τ_{32} was likely a combination of some bias and the exaggerating effect of PRB applied to parameters having small generating values.

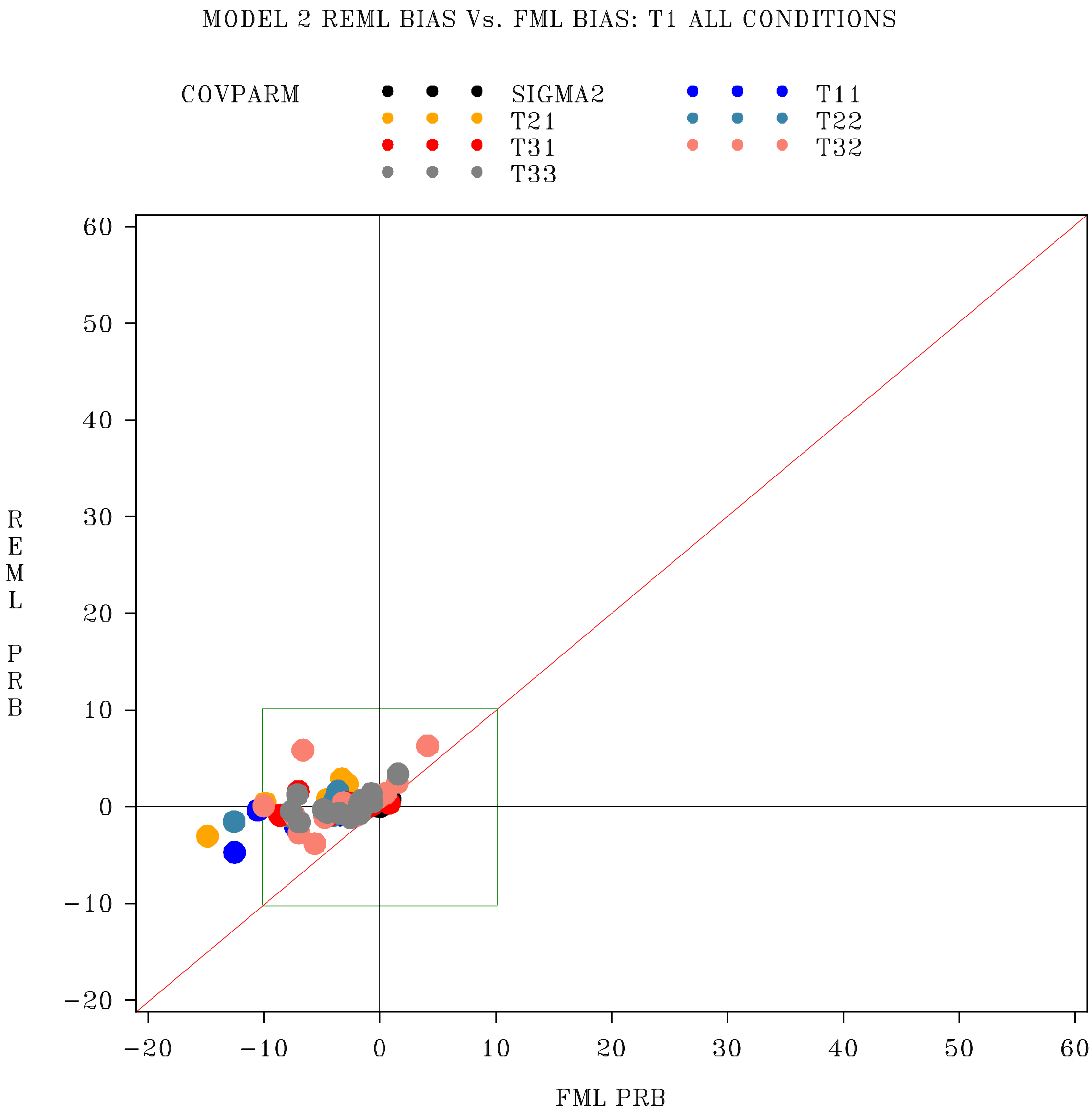

Figure 3.5: Random Effect PRB Model 2 T1 REML & FML

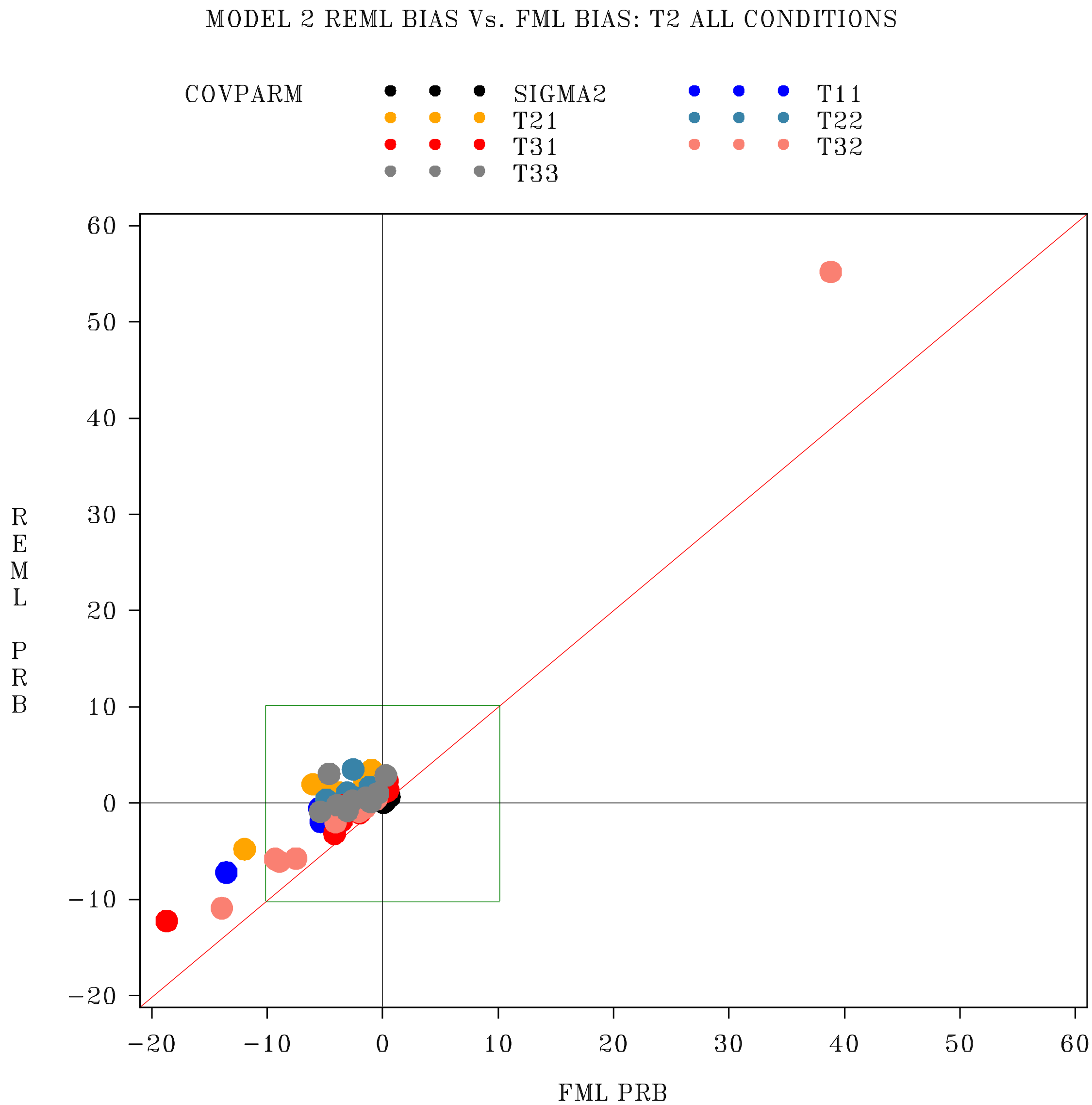

Figure 3.6: Random Effect PRB Model 2 T2 REML & FML

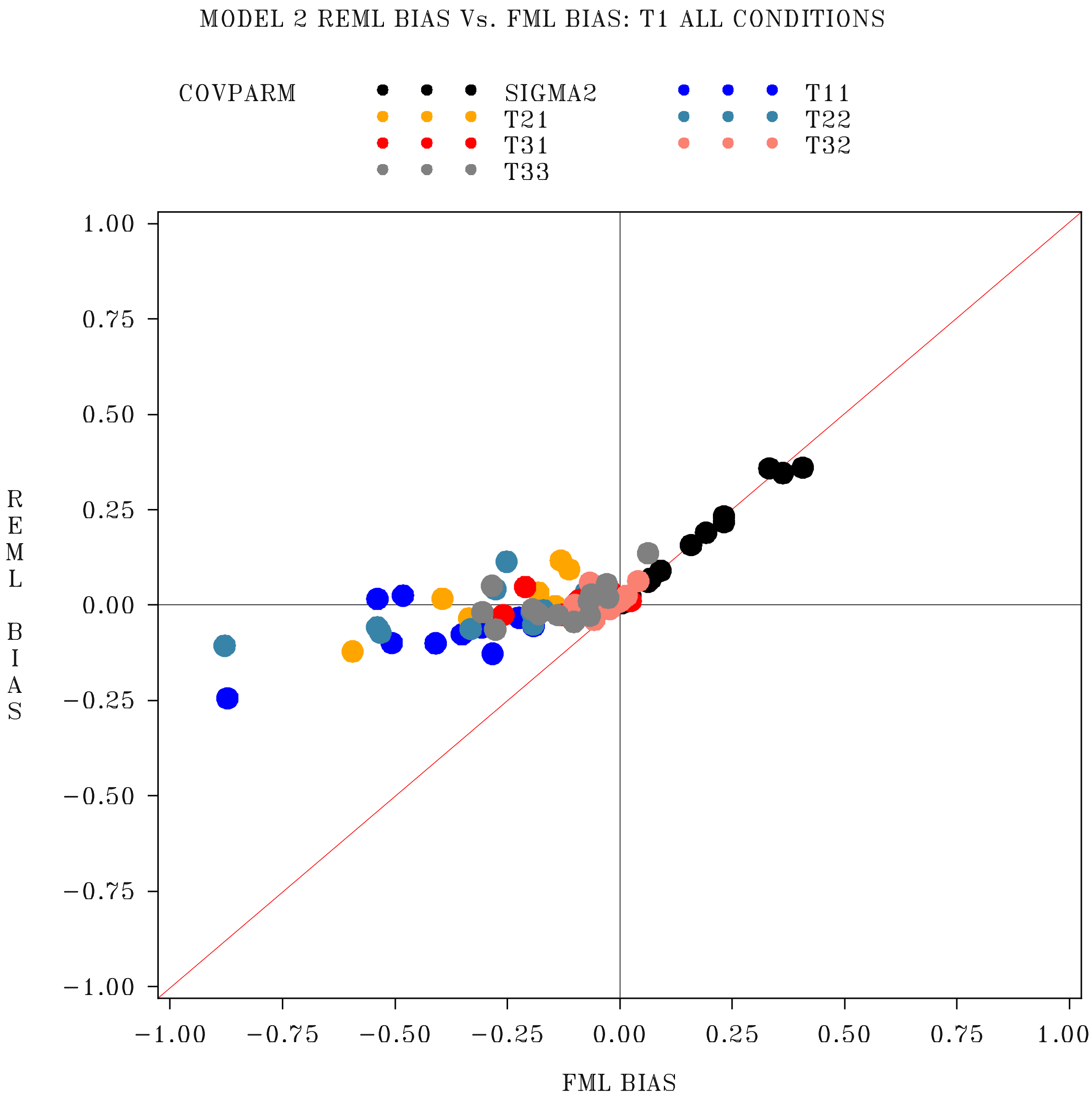

Figure 3.7: Random Effect Raw Bias Model 2 T1 REML & FML

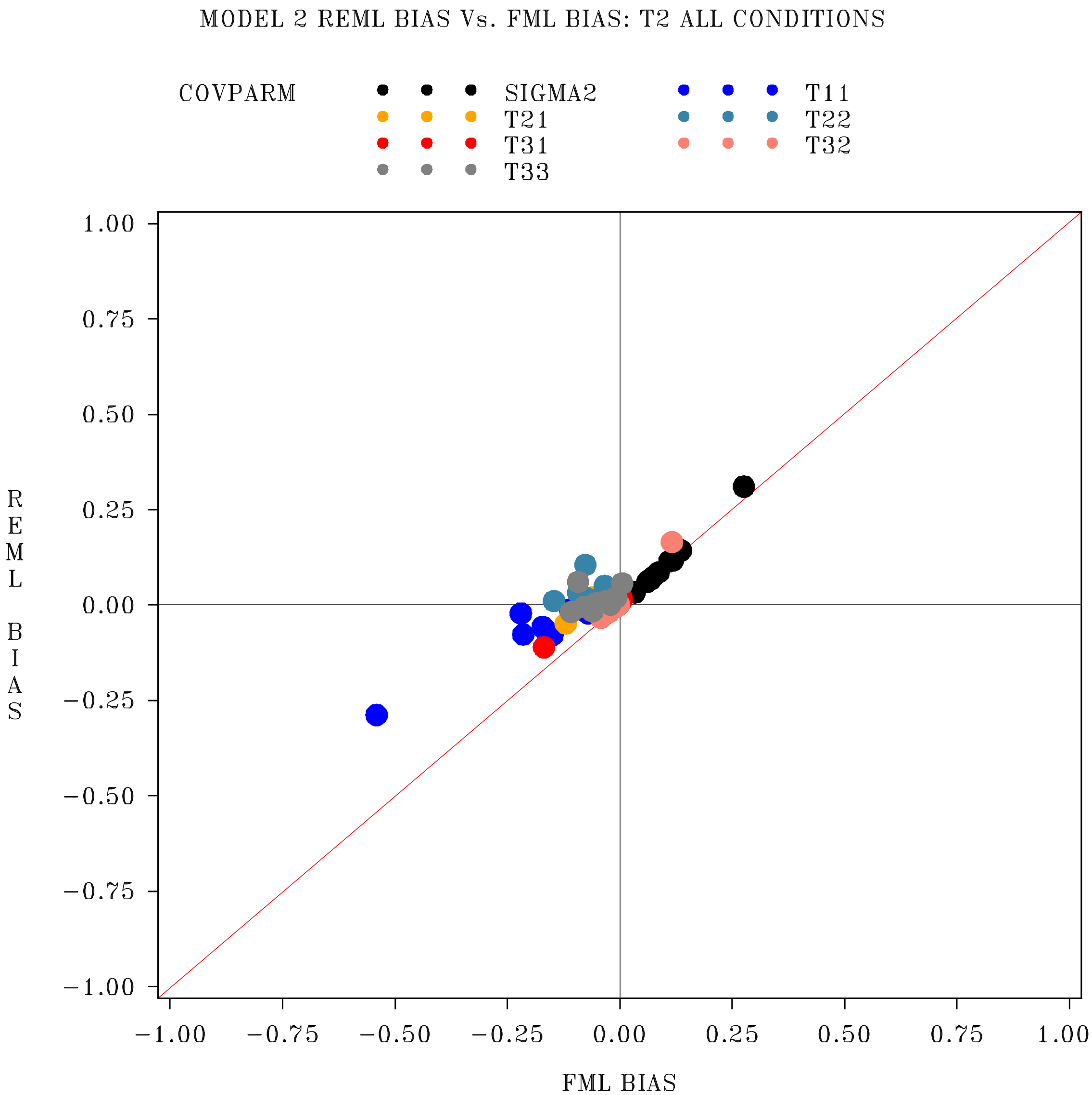

Figure 3.8: Random Effect Raw Bias Model 2 T2 REML & FML

Model 3

Under T1, REML PRB values ranged from -12.9 to 9, while FML PRB values ranged from -18.8 to .9. Under T2, bias was more extreme, with REML PRB values ranging from -73.5 to 14.2, and FML PRB values ranging from -81.1 to 6.3. Under model 3, extreme bias values tended to be negative, whereas under model 2 extreme values tended to be positive. As demonstrated in figure 3.9, under T1 only one REML estimate exceeded 10% bias, whereas 11 FML estimates exceeded 10% bias. Under T2, seven REML estimates exceeded 10% bias, while 16 FML estimates exceeded 10% bias. Figure 3.10 demonstrates that under T2, the extreme positive bias associated with τ_{32} observed in model 2 was replaced with extreme negative bias in model 3. The negative bias trend was not unique to τ_{32}. Under T2 the trend was observed in all covariance parameters. However, as with model 2, the covariances under T2 were associated with generating values less than 1, consequently, it is no surprise that extreme cases observed in the PRB plots were exclusively associated with covariance parameters. Examination of figures 3.11 and 3.12 revealed that the relative bias metric reversed the trend observed in the raw bias metric. T2 raw bias exhibited lower dispersion than T1 raw bias, but, as already discussed, T2 PRB exhibited greater dispersion than T1 PRB. This increased dispersion was a direct result of the relative bias metric, observed in covariances, whose generating values were less than 1, and thus an expected result of the relative bias metric.

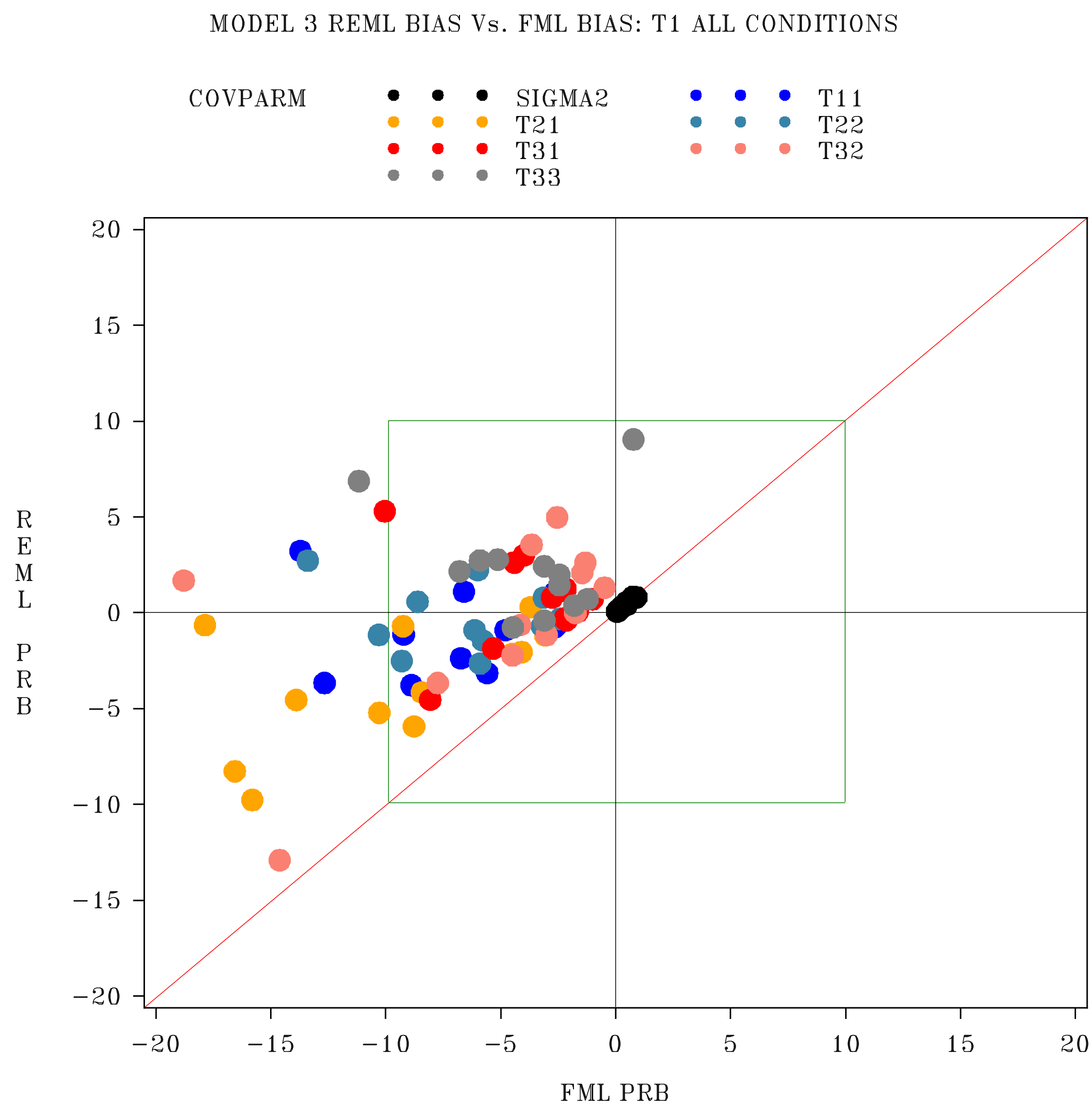

Figure 3.9: Random Effect PRB Model 3 T1 REML & FML

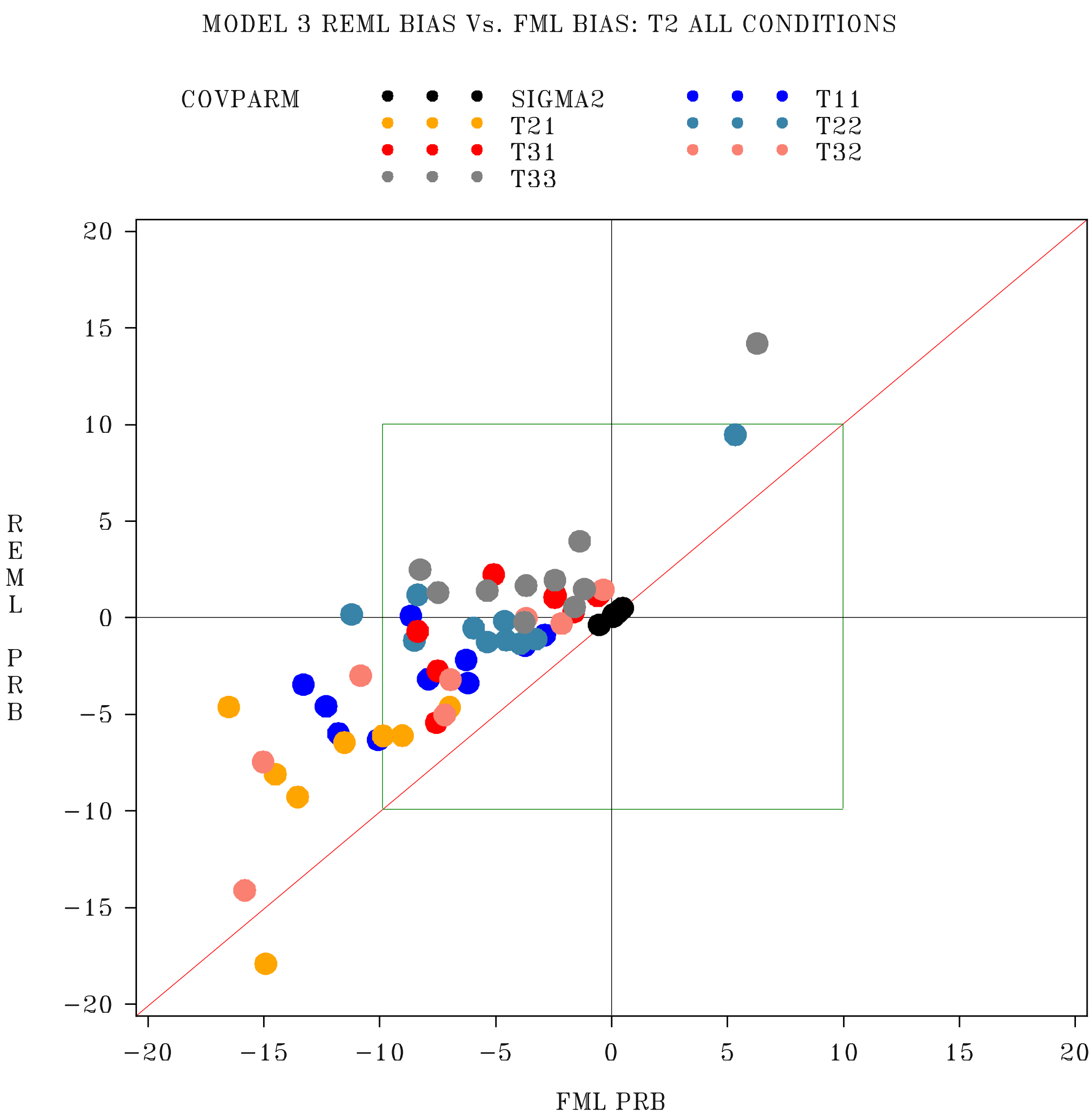

Figure 3.10: Random Effect PRB Model 3 T2 REML & FML

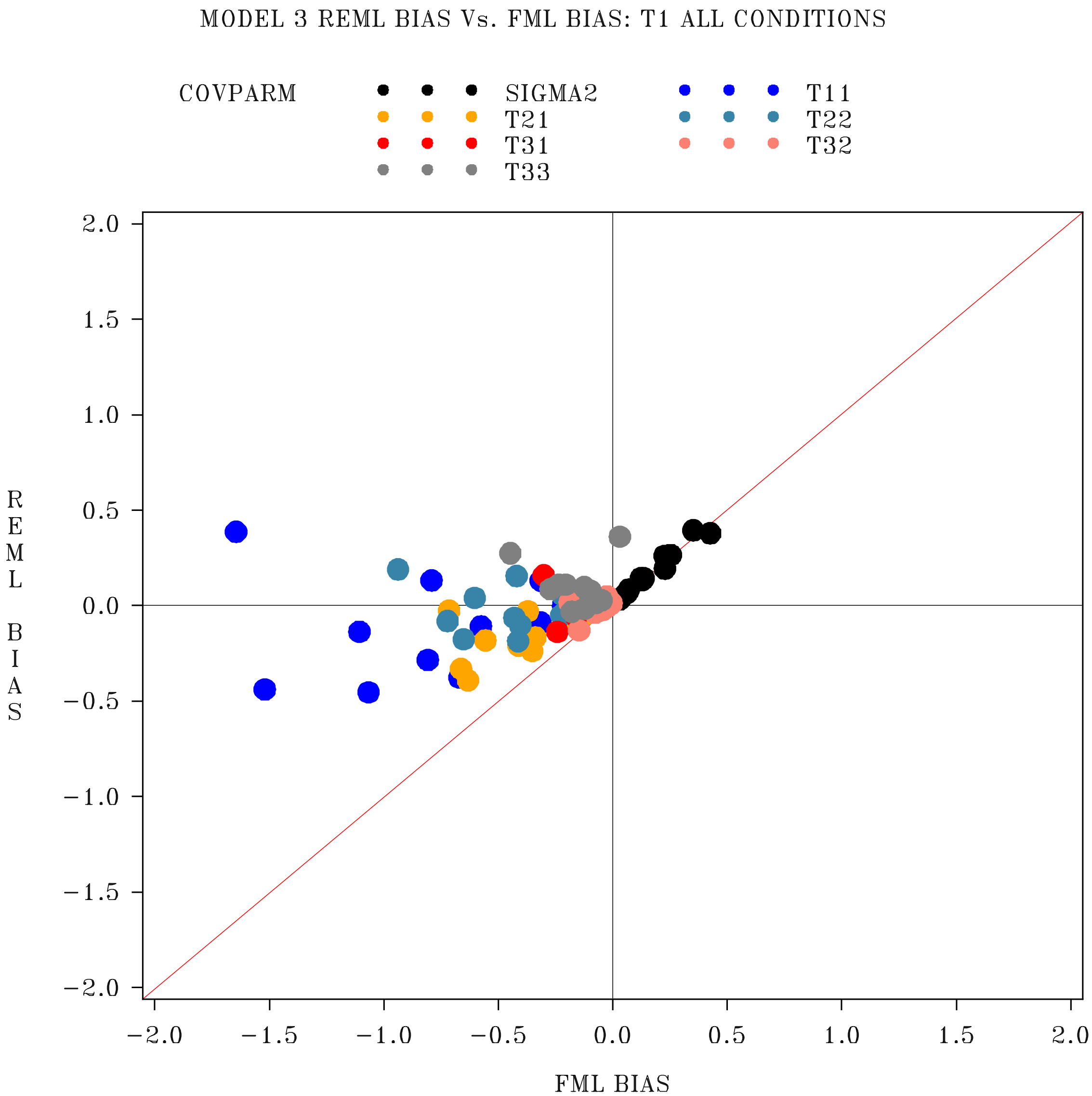

Figure 3.11: Random Effect Raw Bias Model 3 T1 REML & FML

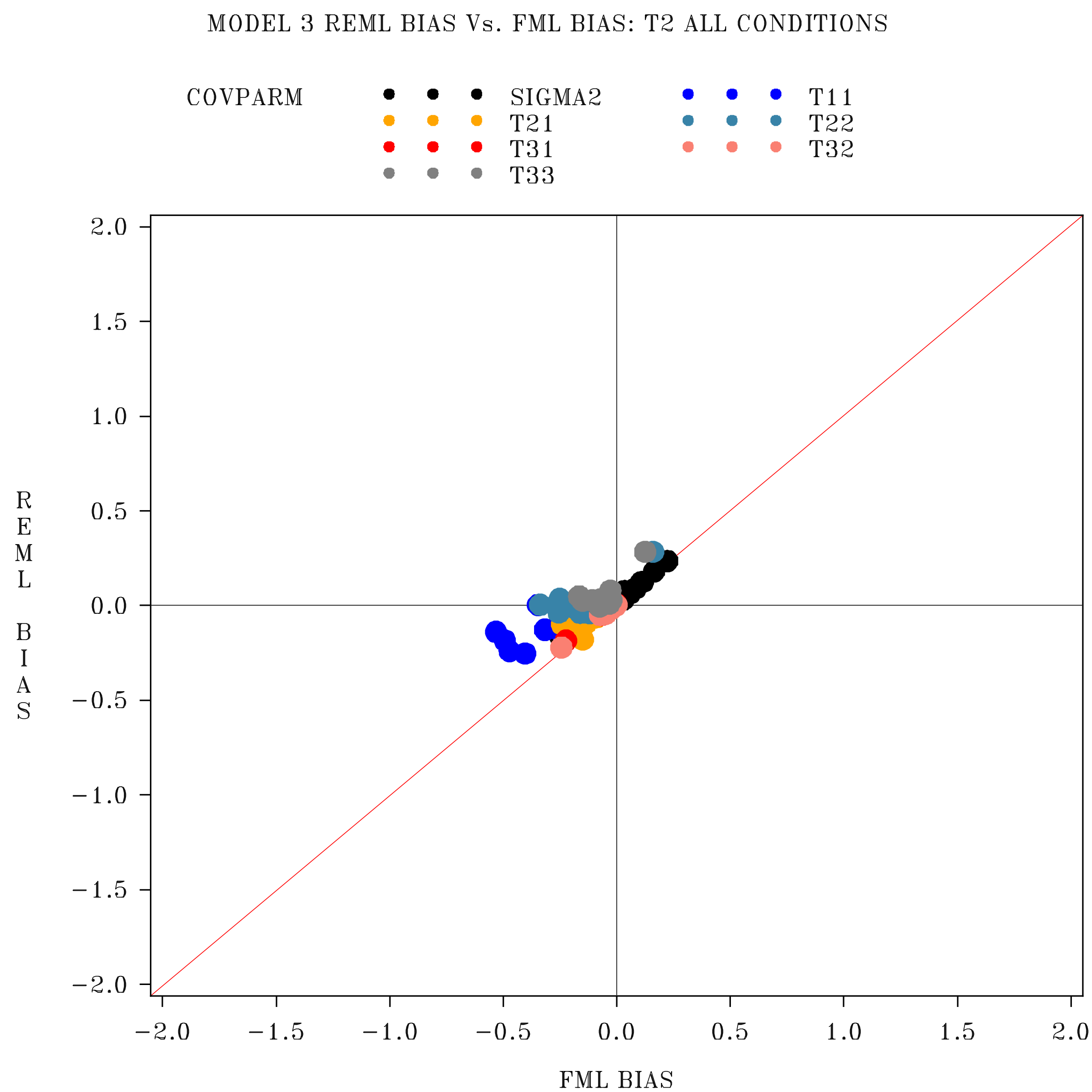

Figure 3.12: Random Effect Raw Bias Model 3 T2 REML & FML

3.6.2 Conditioning Upon ISUs and Observations: The Covariance Matrix, Estimator, and Model Complexity Effect

Figures presented in this section detail how the covariance matrix, estimator and model complexity effects vary over increasing ISUs and observations. Within a covariance matrix condition and model, casement plots graph the change in PRB (plotted along the ordinate) across increasing ISUs (plotted along the abscissa). Each sub-plot in the casement plot corresponds to a given average observations condition. Within each sub-plot, as many as three horizontal lines are overlain. In every graph a zero bias line is inserted; for graphs in which PRB only exceeds -10%, a line demarcating -10% is overlain; for those in which PRB only exceeds 10%, a line demarcating 10% is overlain; and for those in which PRB exceeds $\pm 10\%$, lines demarcating $\pm 10\%$ are overlain. PRB values exceeding the lines demarcating $\pm 10\%$ are considered problematic.

Model 1

As can be seen in figures 3.13 and 3.15, PRB for the residual variance parameter, σ^2, was the same across estimators, and uniformly low, never exceeding 4% bias in any sample size condition. Conversely, as demonstrated in figures 3.14 and 3.16, even for a relatively simple model like model 1, substantial bias was observed in estimates of τ_{11}. As seen previously, FML was more negatively biased than REML. Though the literature acknowledges REML bias under unbalanced data (Demidenko, 2004), for a simple model like model 1, REML only exhibited excess bias in finite sample sizes. When sample size was large (120 ISUs), REML appeared unbiased, with FML only slightly biased. Bias levels appeared greater across covariance matrices as well, with more extreme bias observed under T2 than under T1. Nonetheless, patterns of bias were consistent with expectation: bias decreased as sample size increased, and FML was uniformly more biased than REML. Full results for this model are contained in Table 3.1. Neither REML nor FML estimates of σ^2 ever exhibited bias levels exceeding 10% for any model, covariance matrix, or sample size, and are not discussed further.

Under T1, when 15 ISUs were sampled with an average of 10 or 20 observations per ISU, FML estimates of τ_{11} exhibited PRB levels exceeding 10%. Results described for τ_{11} can be seen in figure 3.17. Full details are given in Table 3.1. Only FML estimates exhibited problematic levels of PRB; all REML estimates were biased by less than 10%.

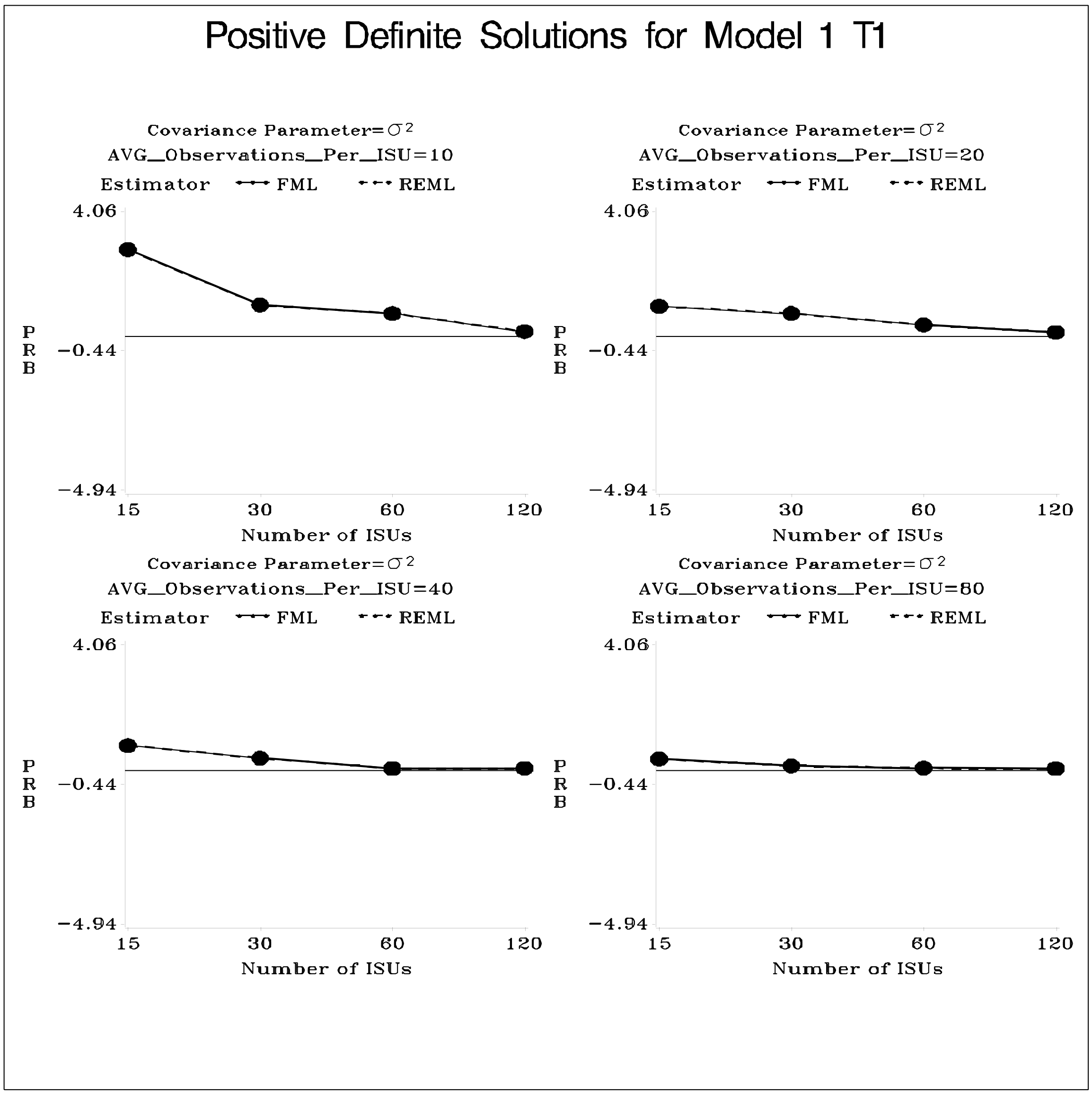

Figure 3.13: σ^2 PRB Model 1 T1 REML & FML

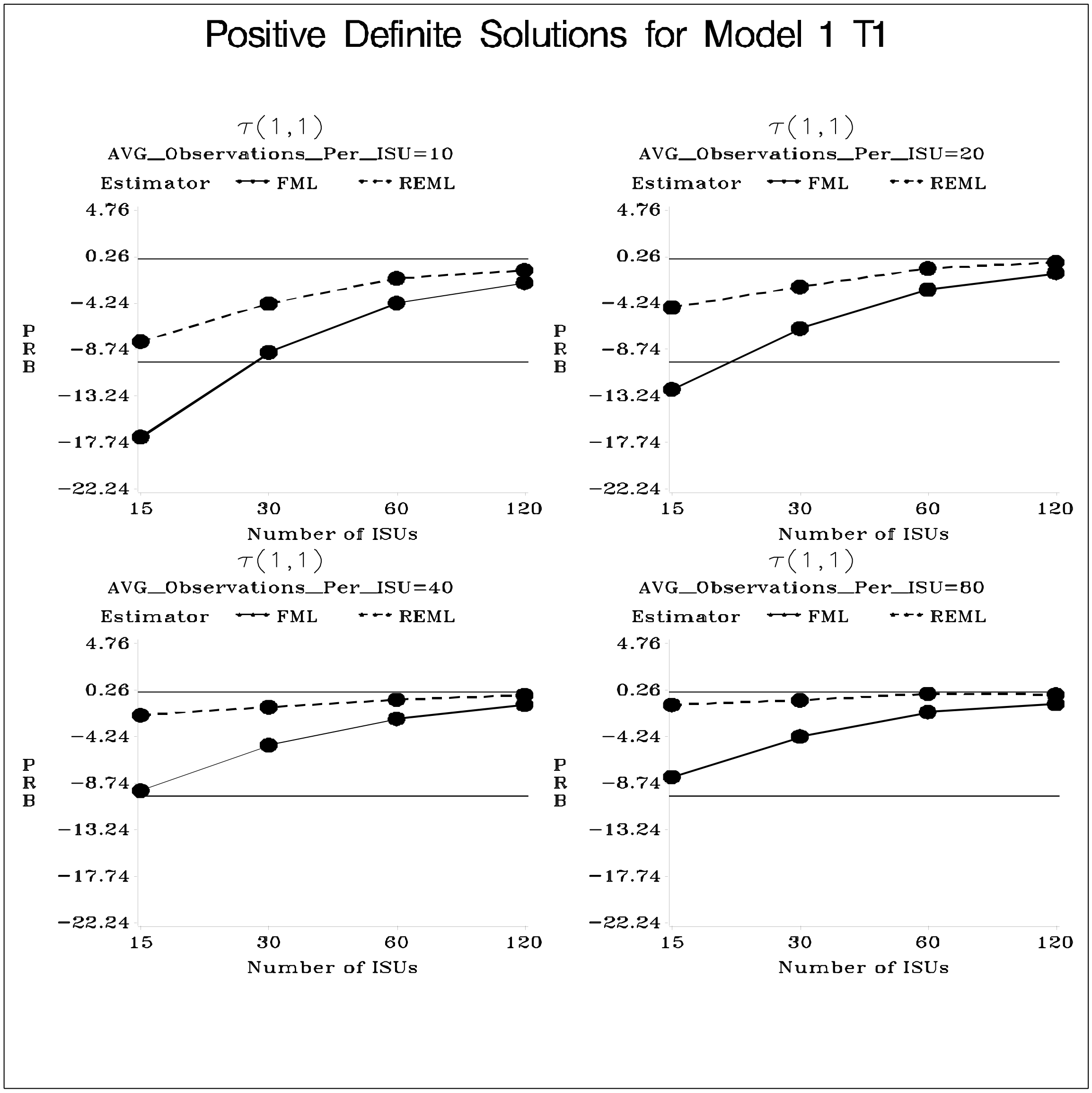

Figure 3.14: τ_{11} PRB Model 1 T1 REML & FML

Full Results for T2 are presented in figure 3.16 and Table 3.2; bias levels exceeding 10% are described in detail below. Both FML and REML estimates of τ_{11} exhibited problematic PRB levels. FML bias exceeded 10% whenever 15 ISUs were sampled, no matter how many observations (average observations of 10, 20, 40, or 80 per ISU) were sampled. When 30 ISUs were sampled with an average of 10 or 20 observations per ISU, FML bias exceeded 10%. When 60 ISUs were sampled with an average of 10 observations per ISU, FML bias exceeded 10%. When 15 ISUs were sampled with an average of 10 or 20 observations per ISU, REML bias exceeded 10%. When 30 ISUs were sampled with an average of 10 observations per ISU, REML bias exceeded 10%. FML was always more negatively biased than REML, but, consistent with theory, REML was not unbiased, simply less negatively biased than FML.

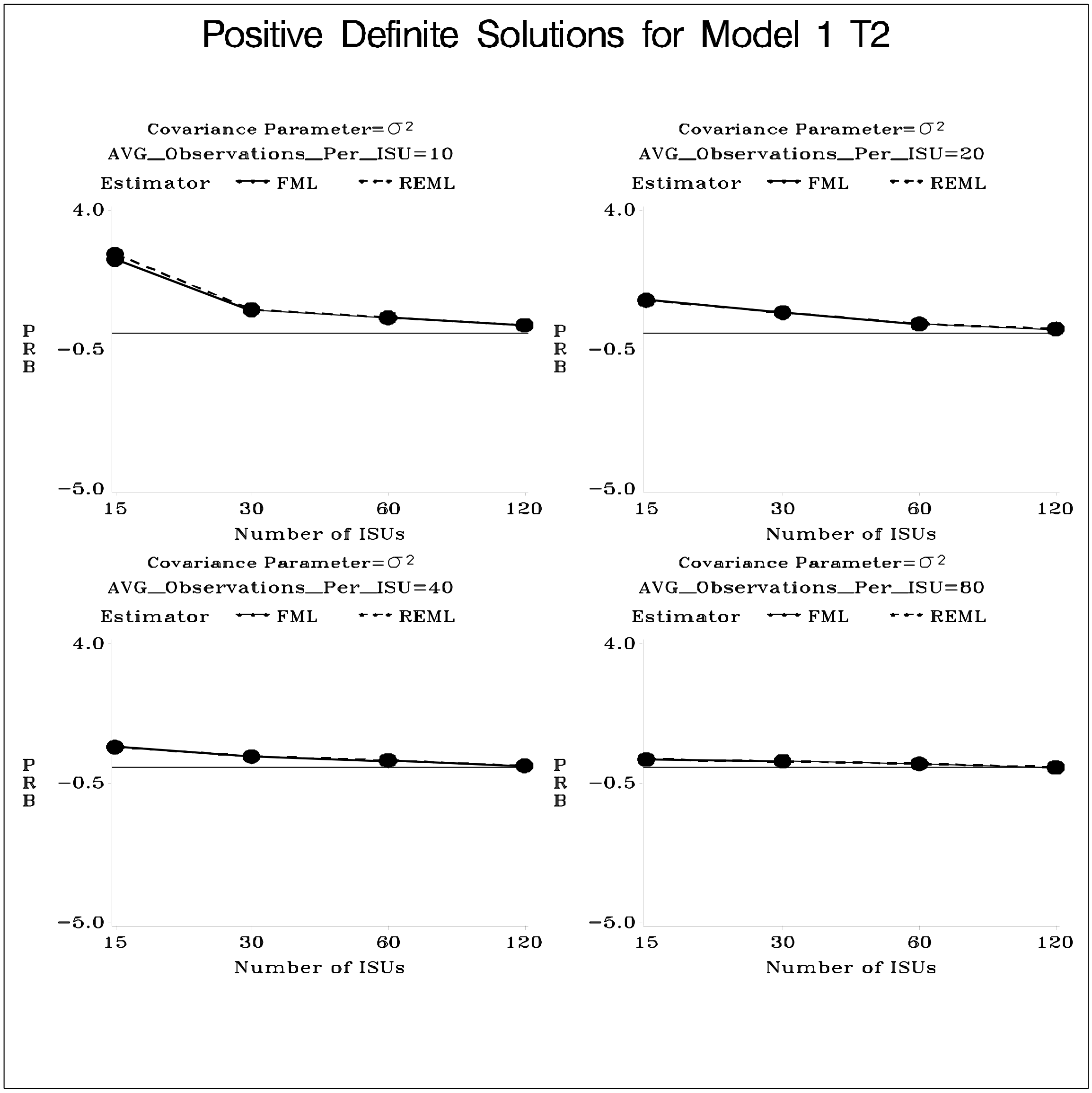

Figure 3.15: σ^2 PRB Model 1 T2 REML & FML

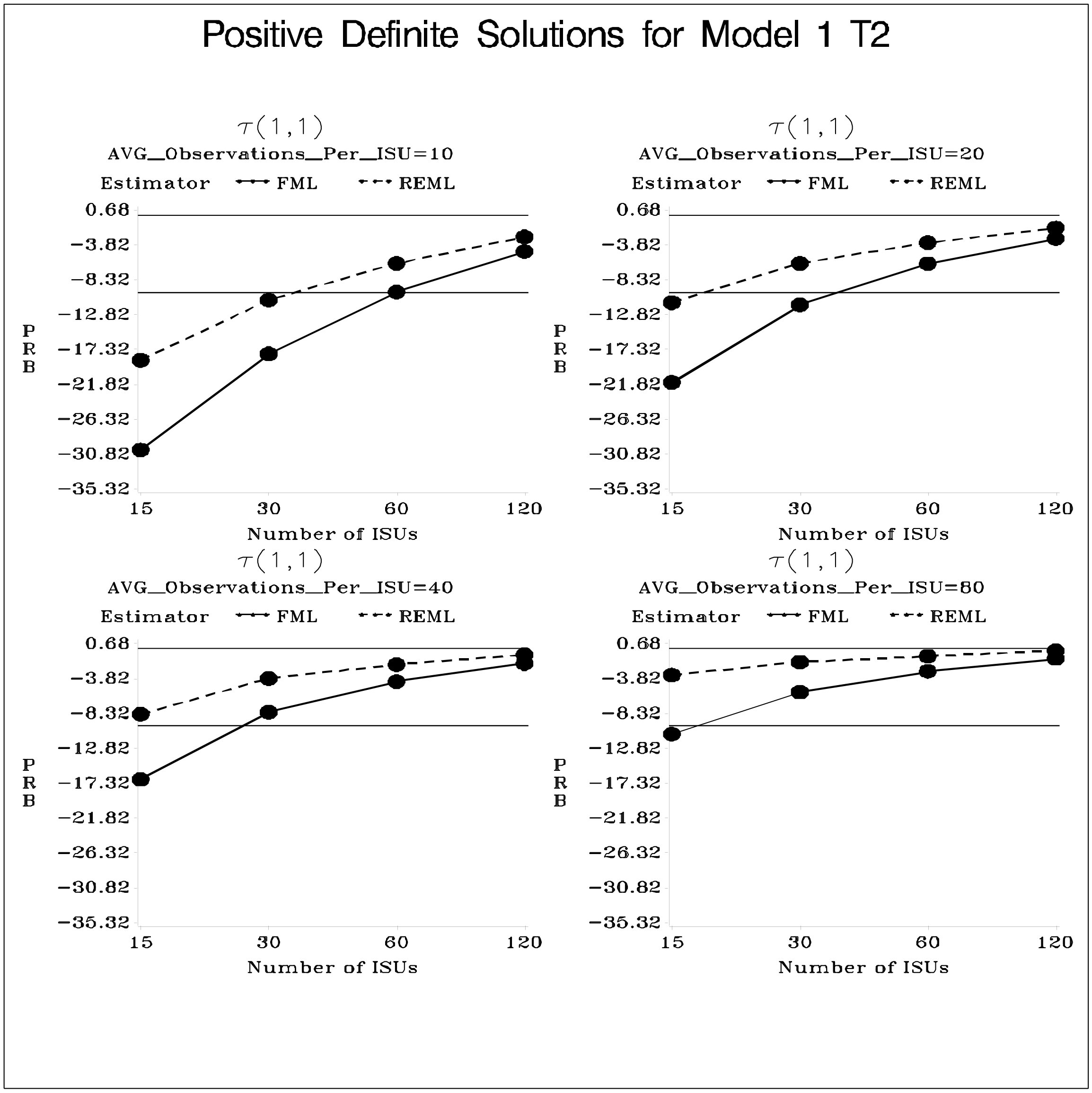

Figure 3.16: τ_{11} PRB Model 1 T2 REML & FML

Model 2

Results were more complicated to interpret under model 2. Except for a few covariances that exhibited severe positive bias (see figures 3.26 and 3.27), REML was uniformly less biased than FML. However, given the values observed in figures 3.26 and 3.27, it is more accurate to say that REML was more positively biased then FML, and when parameter estimates were negatively biased, as variance components tended to be, REML appeared to be the less biased estimator. But when the parameter estimates were positively biased, as covariances sometimes were, REML appeared to be the more biased estimator. Though some covariance components exhibited inconsistent trends in bias across increasing ISU sizes, overall, bias monotonically decreased for all variance and covariance components as the number of ISUs sampled increased. Of interest was the scarcity with which REML bias values exceeded 10%, especially given the frequency with which FML bias exceeded 10% in model 1. Recall however, that in model 1, all bias values exceeding 10% occurred whenever an average of 10 or 20 observations were sampled per ISU. In Model 2, as in model 3, those cells were excluded from analysis when few ISUs were sampled due to high rates of non-convergence, which reduced the chance of observing excessive bias levels because the excluded cells were the cells in which bias levels were expected to be greatest.

Under T1, FML estimates of $\tau_{11}, \tau_{21},$ & τ_{22} were biased by more than 10%, and are the focus of discussion here. Results described for τ_{11} can be seen in figure 3.17; for τ_{21}, in figure 3.18; for τ_{22}, in figure 3.19. Full details are given in Table 3.5. When 15 ISUs were sampled with an average of 40 or 80 observations per ISU, FML estimates of $\tau_{11}, \tau_{21},$ & τ_{22} exhibited negative bias exceeding 10%. Under T1, REML estimates never exhibited bias exceeding 10%; all covariance components were unbiased based on the criterion set forth for this study.

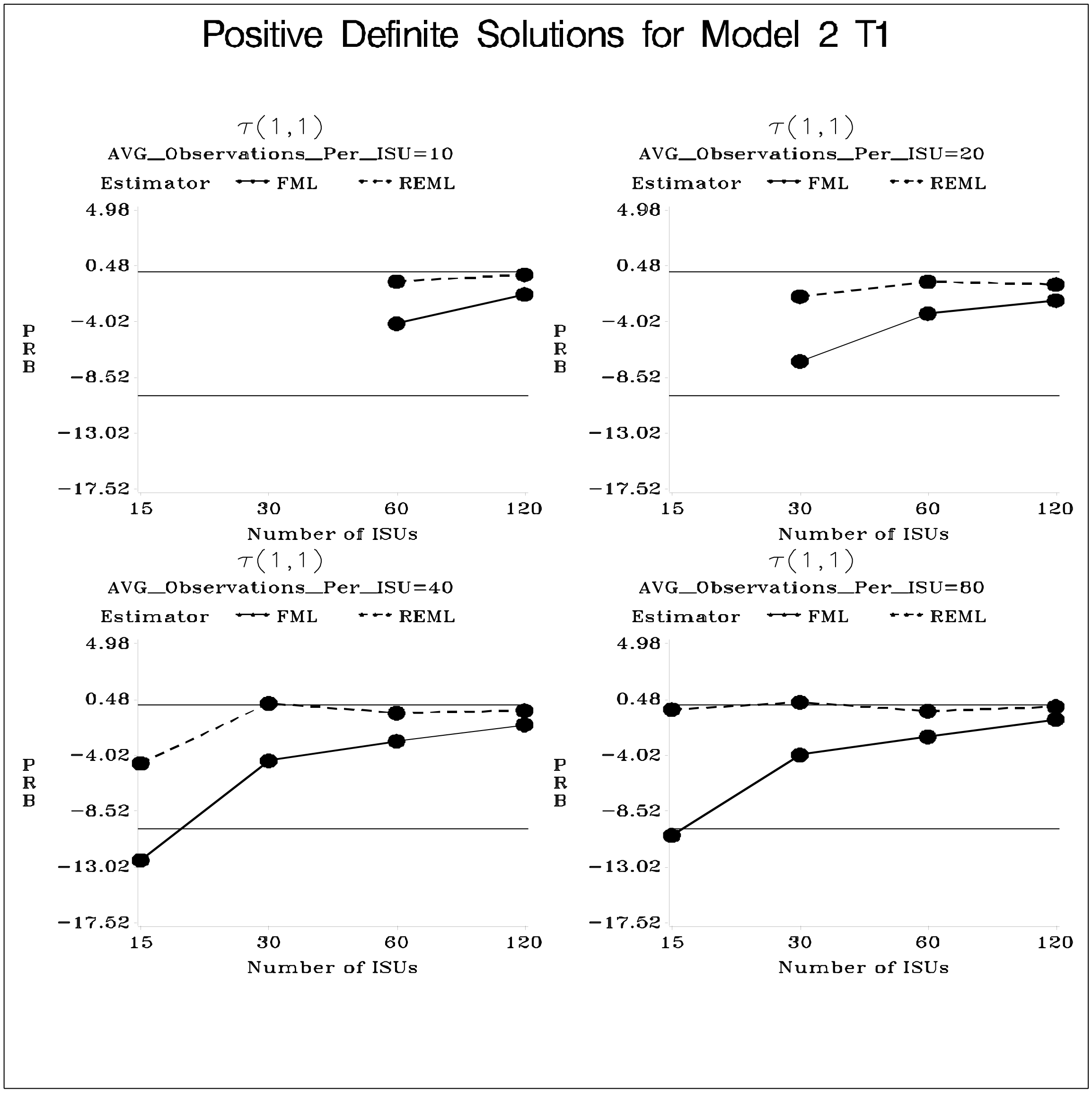

Figure 3.17: τ_{11} PRB Model 2 T1 REML & FML

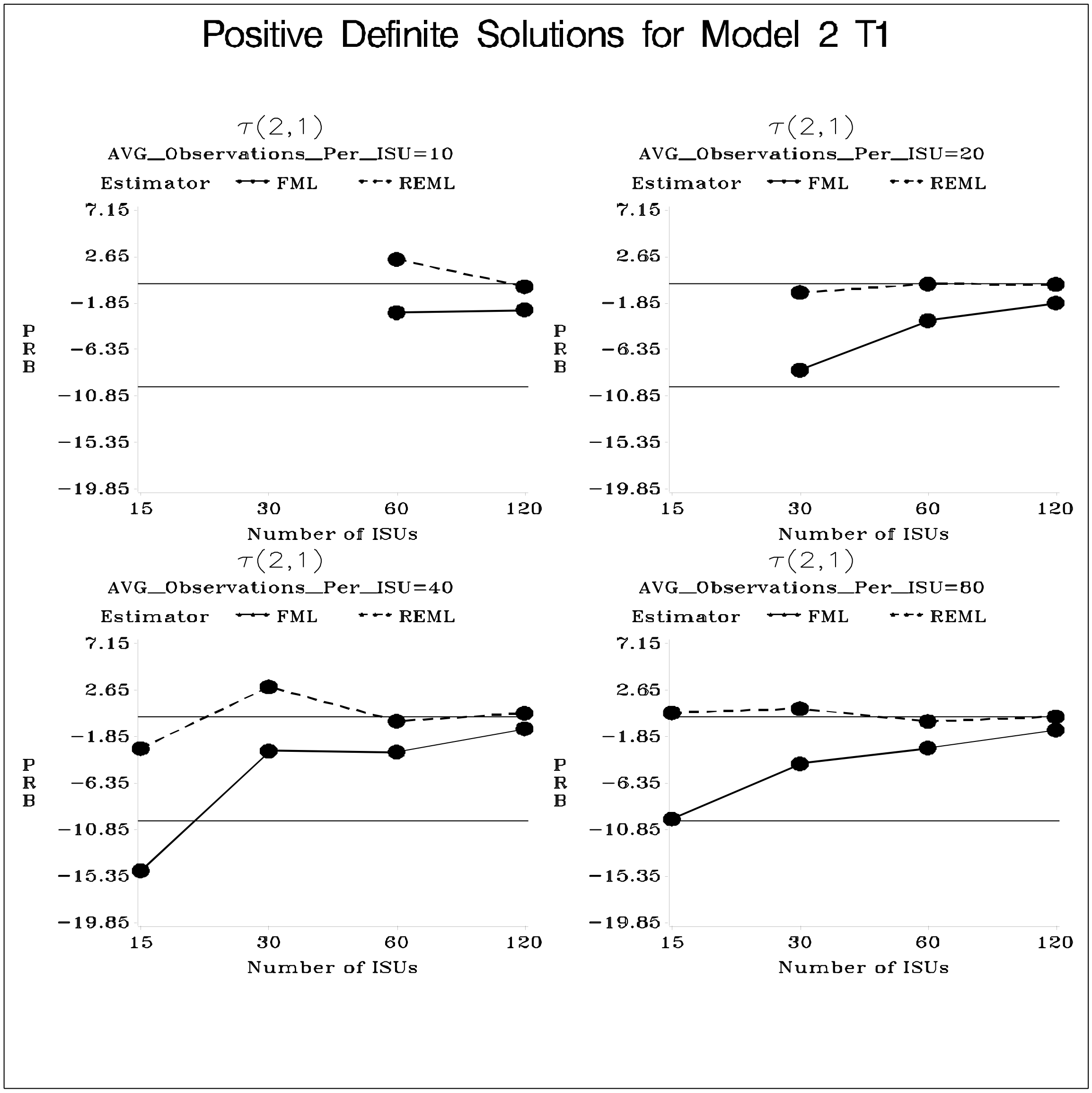

Figure 3.18: τ_{21} PRB Model 2 T1 REML & FML

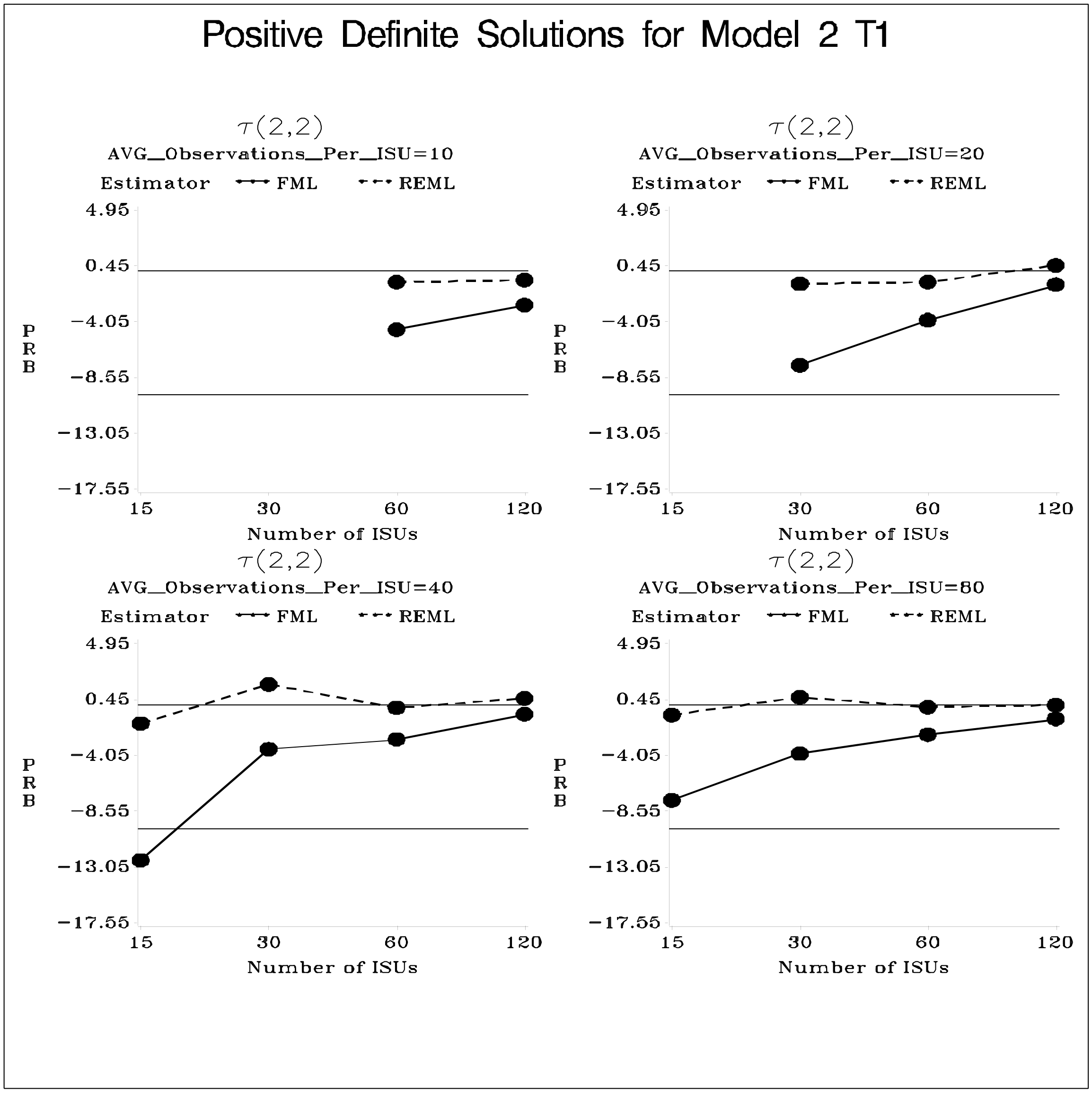

Figure 3.19: τ_{22} PRB Model 2 T1 REML & FML

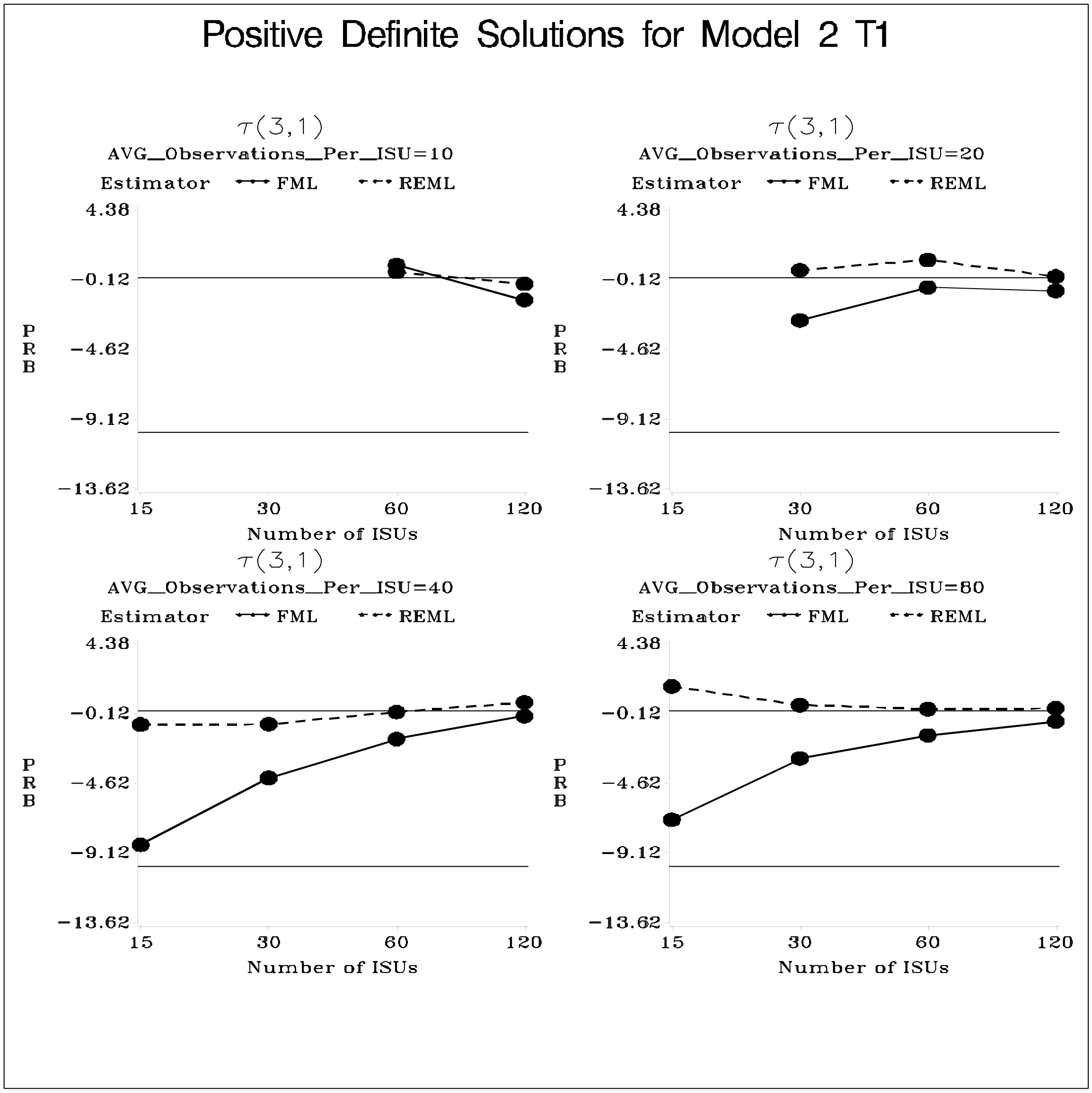

Figure 3.20: τ_{31} PRB Model 2 T1 REML & FML

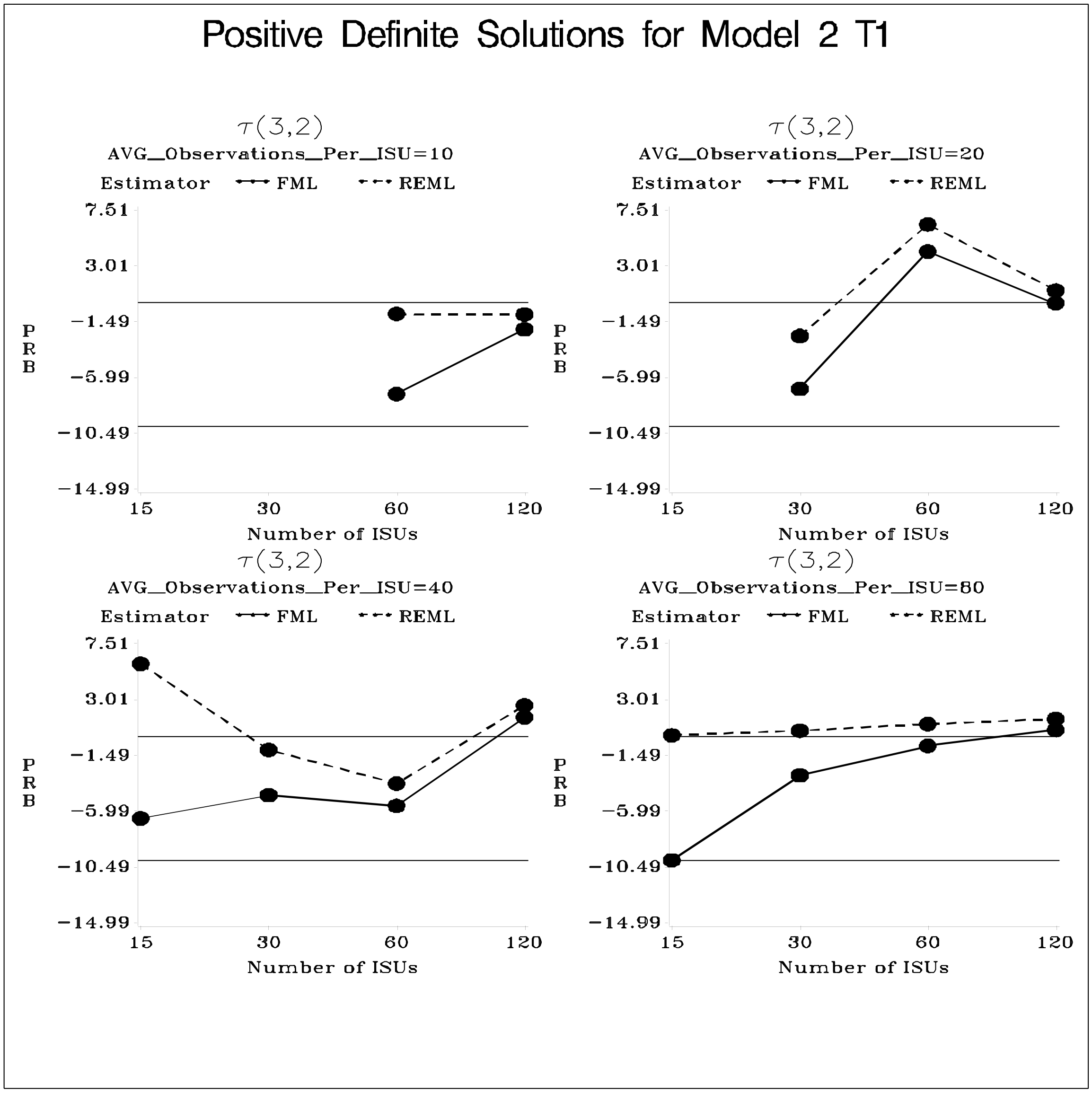

Figure 3.21: τ_{32} PRB Model 2 T1 REML & FML

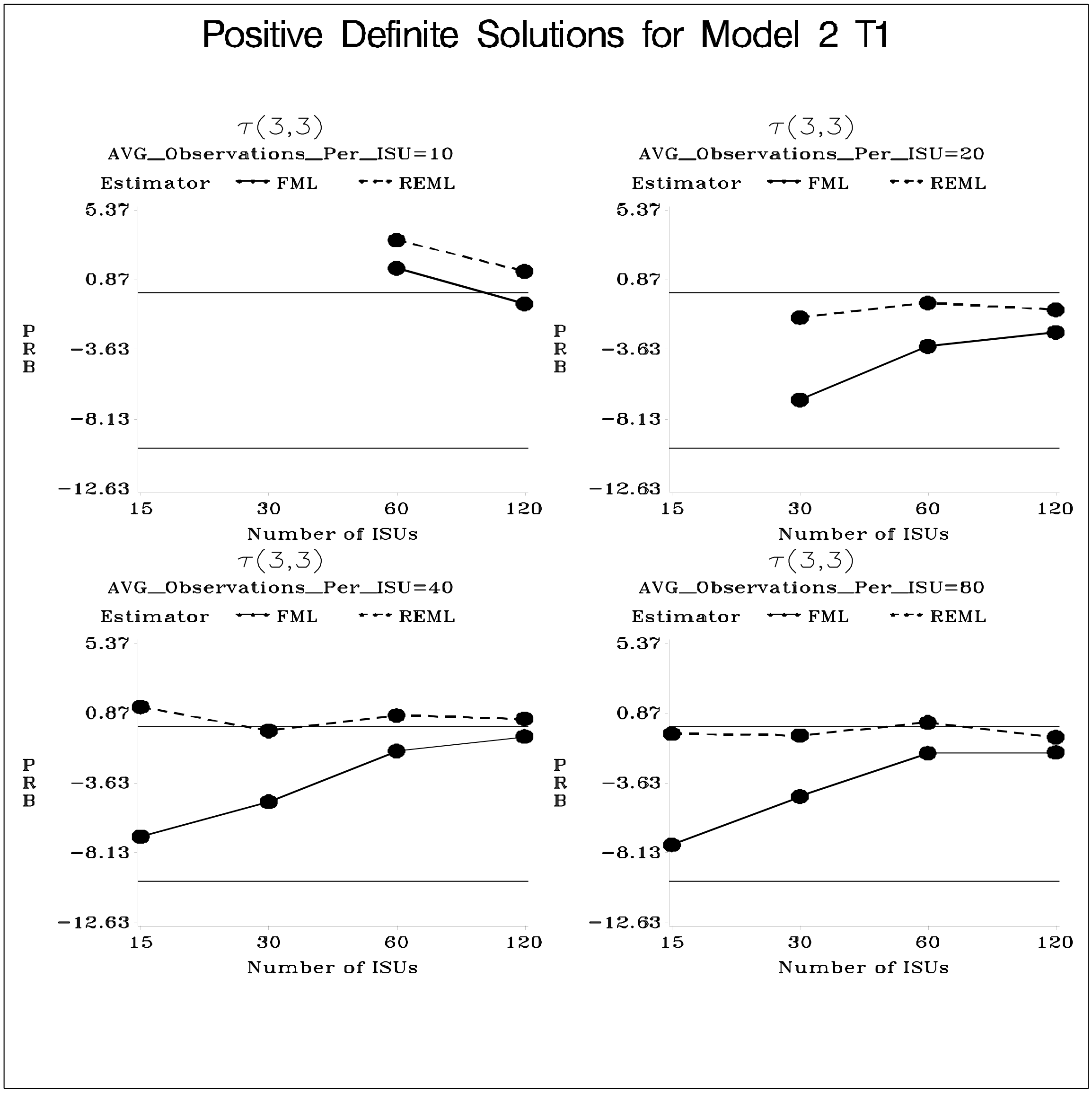

Figure 3.22: τ_{33} PRB Model 2 T1 REML & FML

Under T2, FML estimates of $\tau_{11}, \tau_{21}, \tau_{31}, \;\&\; \tau_{32}$ were biased by more than 10%, and are the focus of discussion here. Results described for τ_{11} can be seen in figure 3.23; for τ_{21}, in figure 3.24; for τ_{31}, in figure 3.26; and for τ_{32}, in figure 3.27. Full details are given in Table 3.6. When 30 ISUs were sampled with an average of 20 observations per ISU, FML estimates of $\tau_{11}, \tau_{21}, \;\&\; \tau_{31}$ were biased by -10% or more, while FML estimates of τ_{32} were biased by $+10\%$ or more. When 120 ISUs were sampled with an average of 10 observations per ISU, FML estimates of τ_{32} exhibited bias exceeding -10%. Under T2, when 30 ISUs were sampled with an average of 20 observations per ISU, REML estimates of τ_{31} were biased by -10% or more, while REML estimates of τ_{32} were biased by $+10\%$ or more. As with FML estimates, when 120 ISUs were sampled with an average of 10 observations per ISU, REML estimates of τ_{32} exhibited bias exceeding -10%, however, FML estimates were slightly more negatively biased than REML estimates.

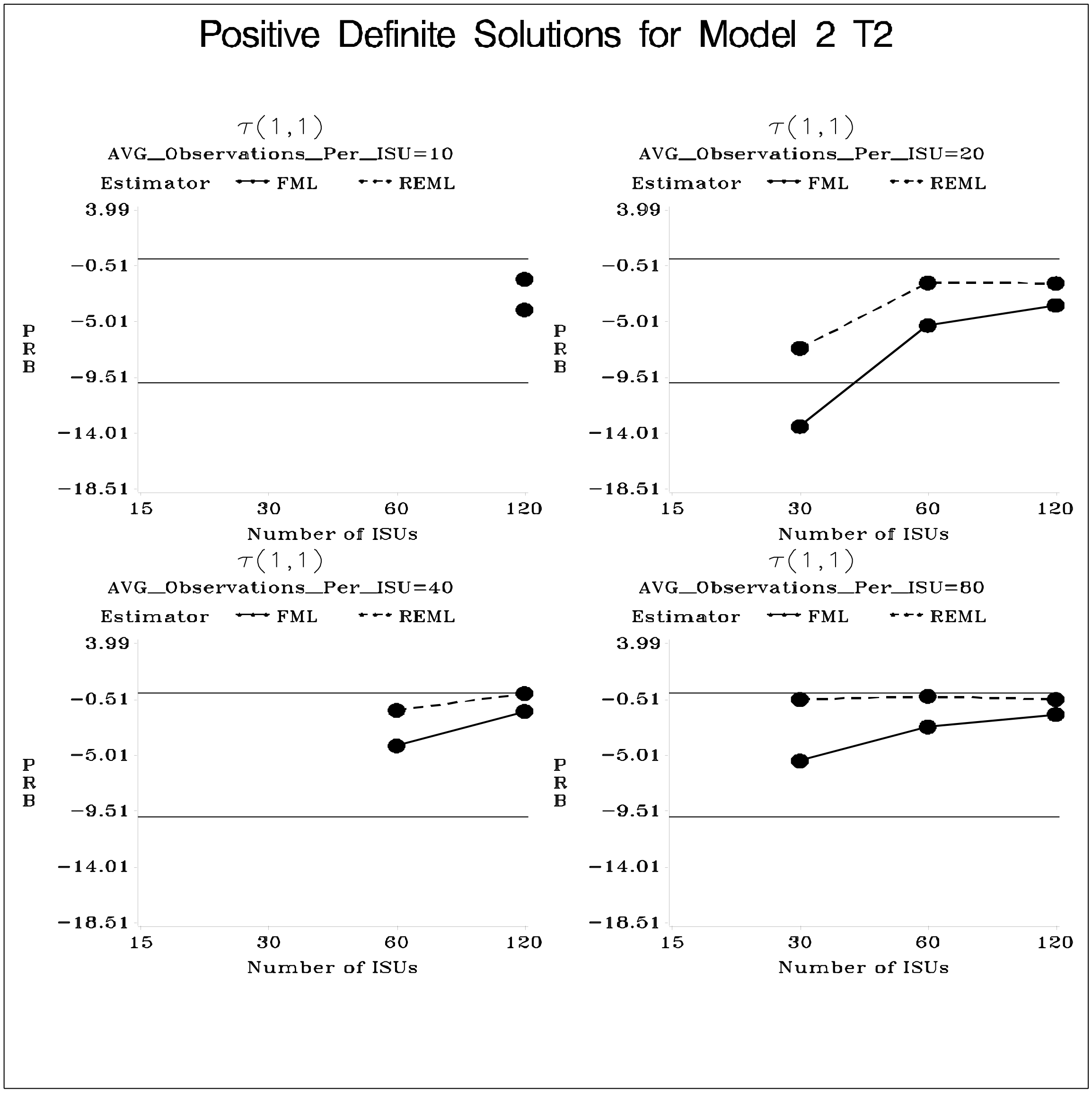

Figure 3.23: τ_{11} PRB Model 2 T2 REML & FML

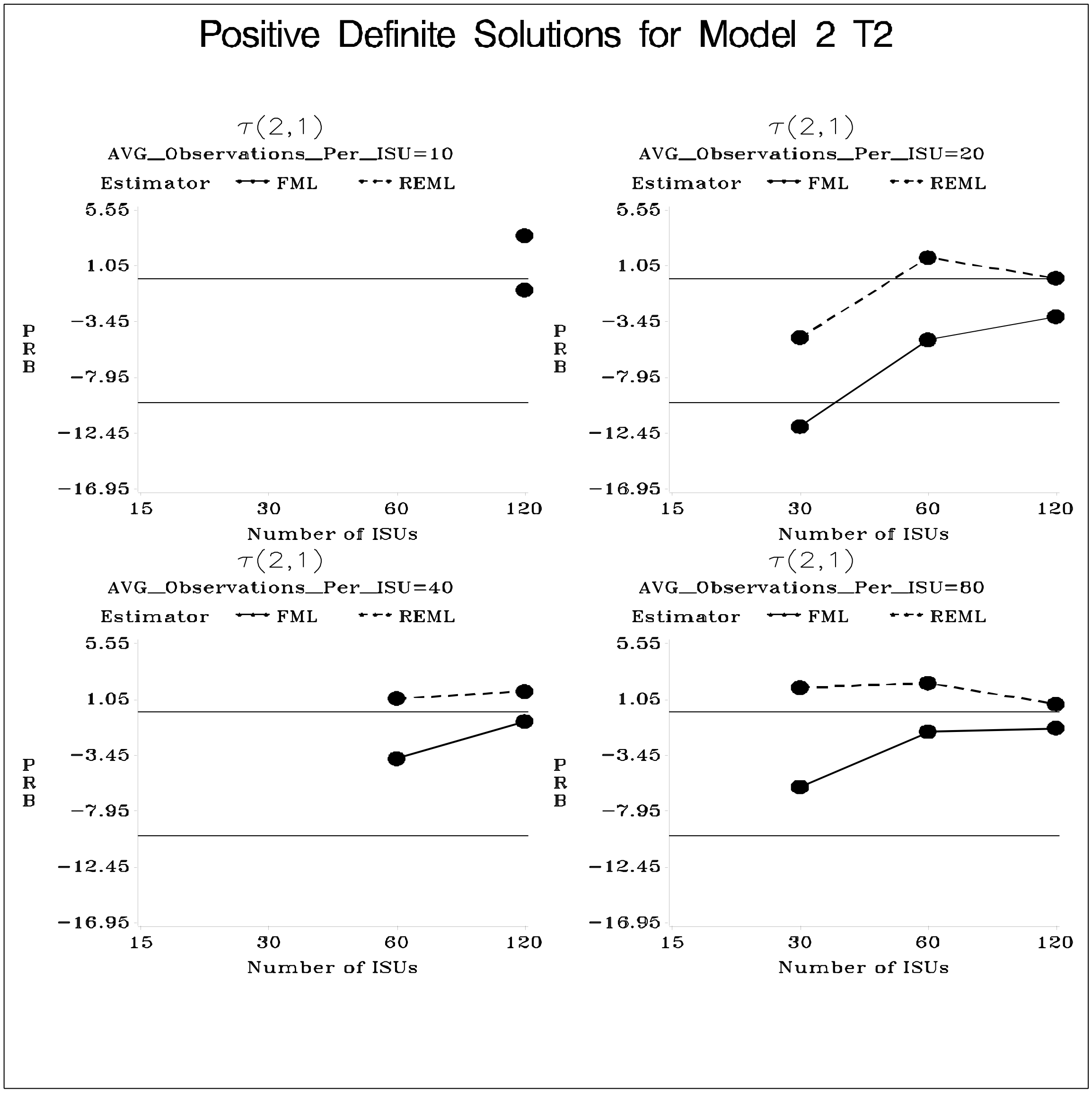

Figure 3.24: τ_{21} PRB Model 2 T2 REML & FML

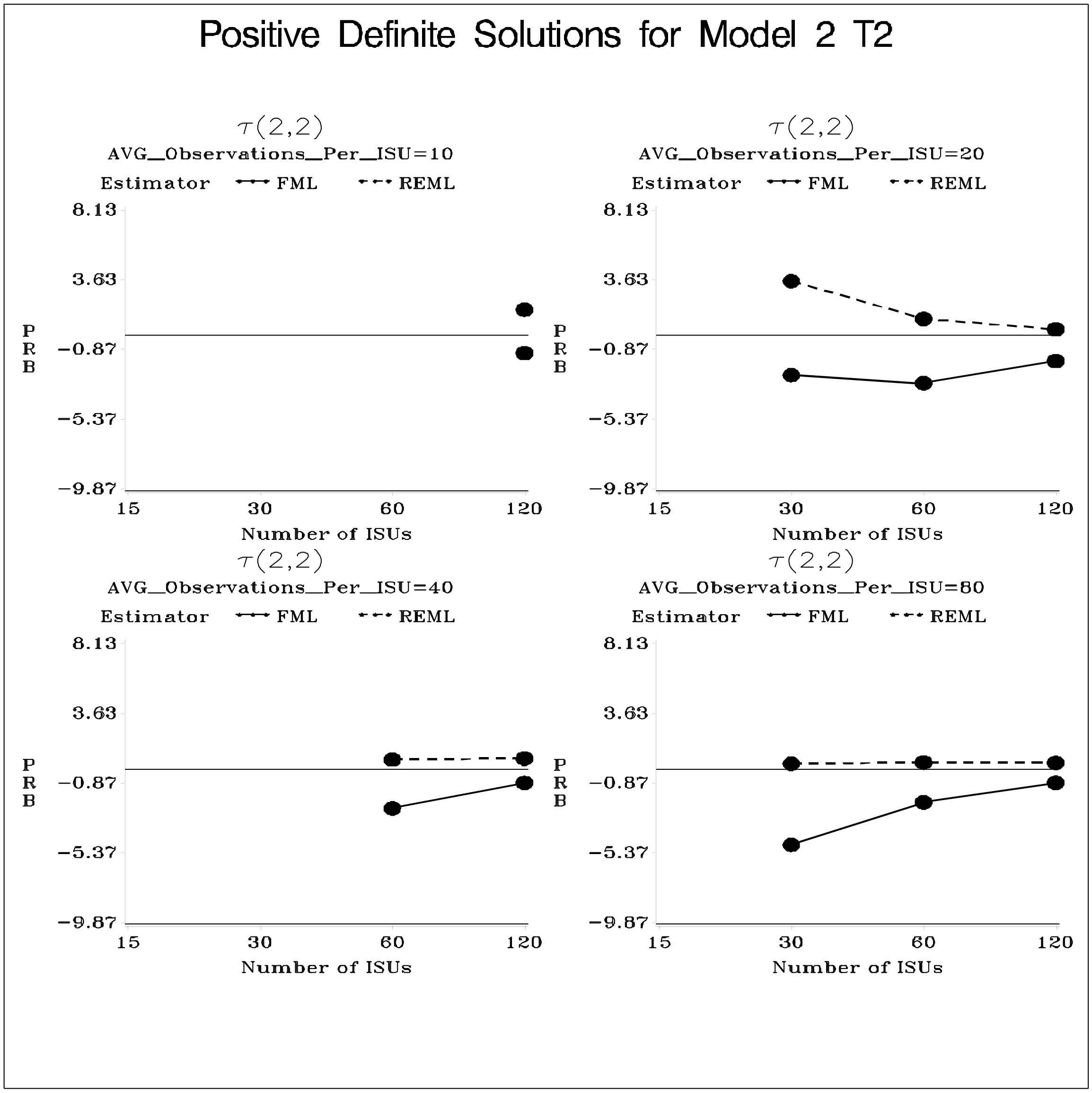

Figure 3.25: τ_{22} PRB Model 2 T2 REML & FML

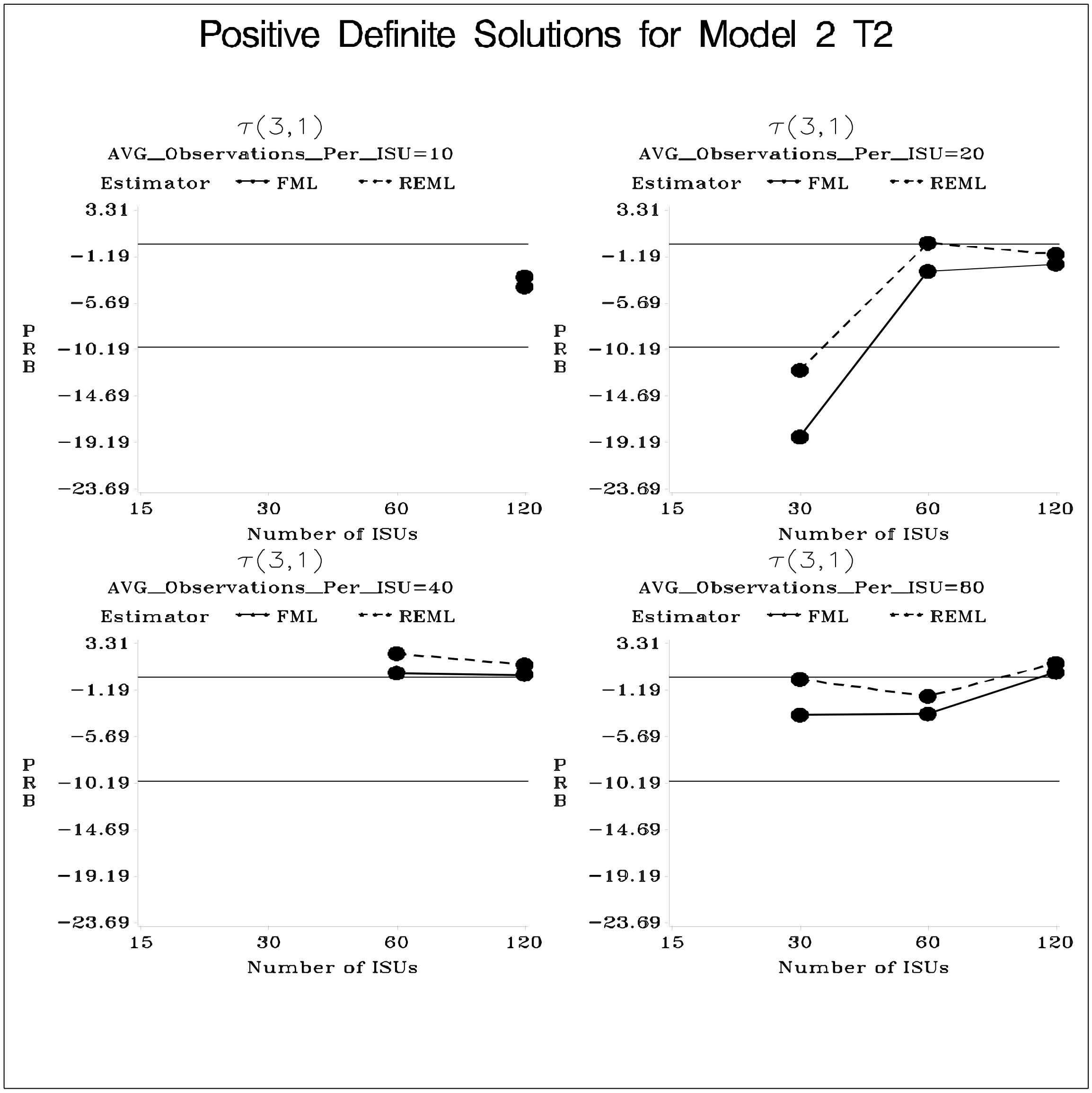

Figure 3.26: τ_{31} PRB Model 2 T2 REML & FML

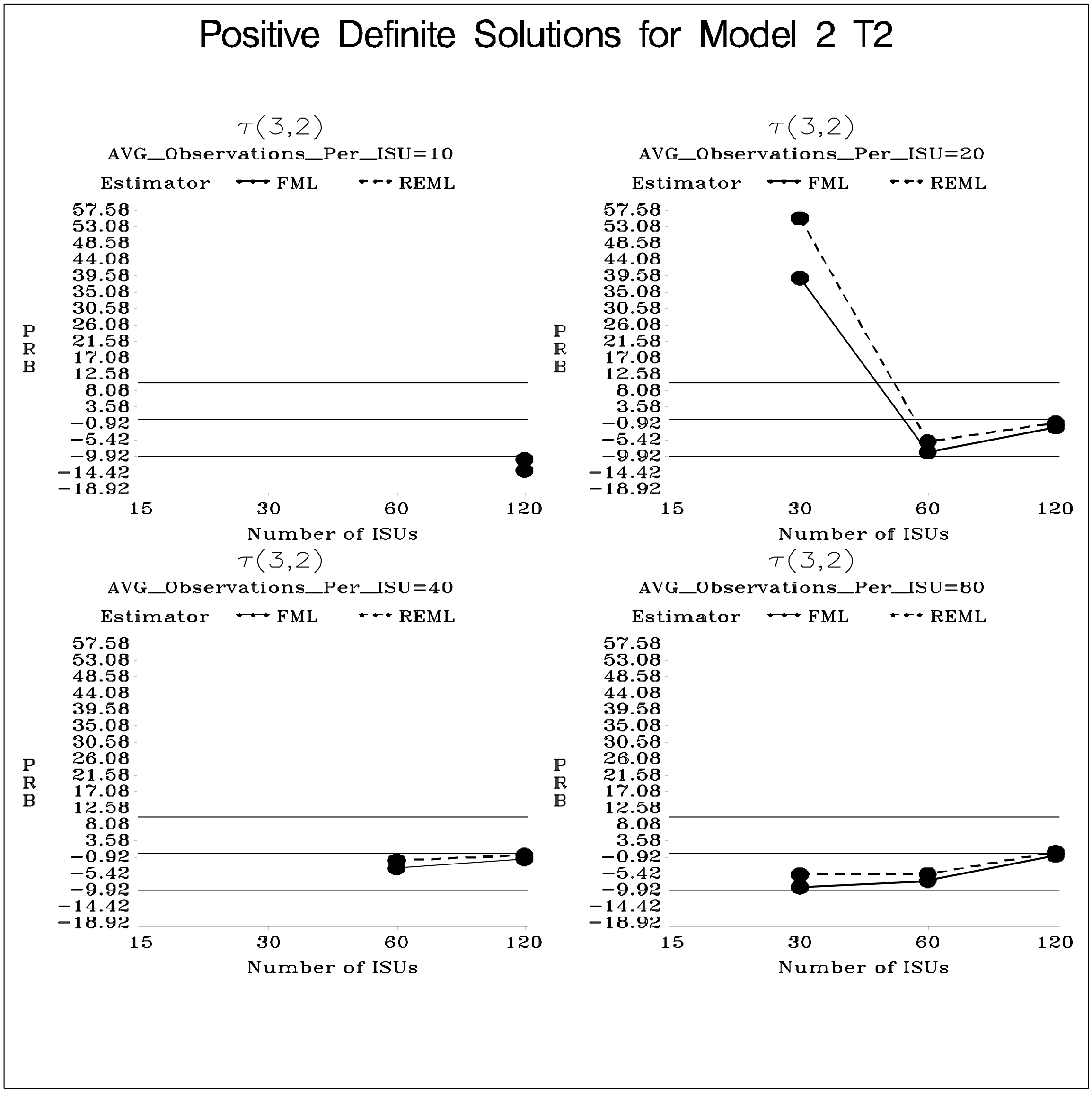

Figure 3.27: τ_{32} PRB Model 2 T2 REML & FML

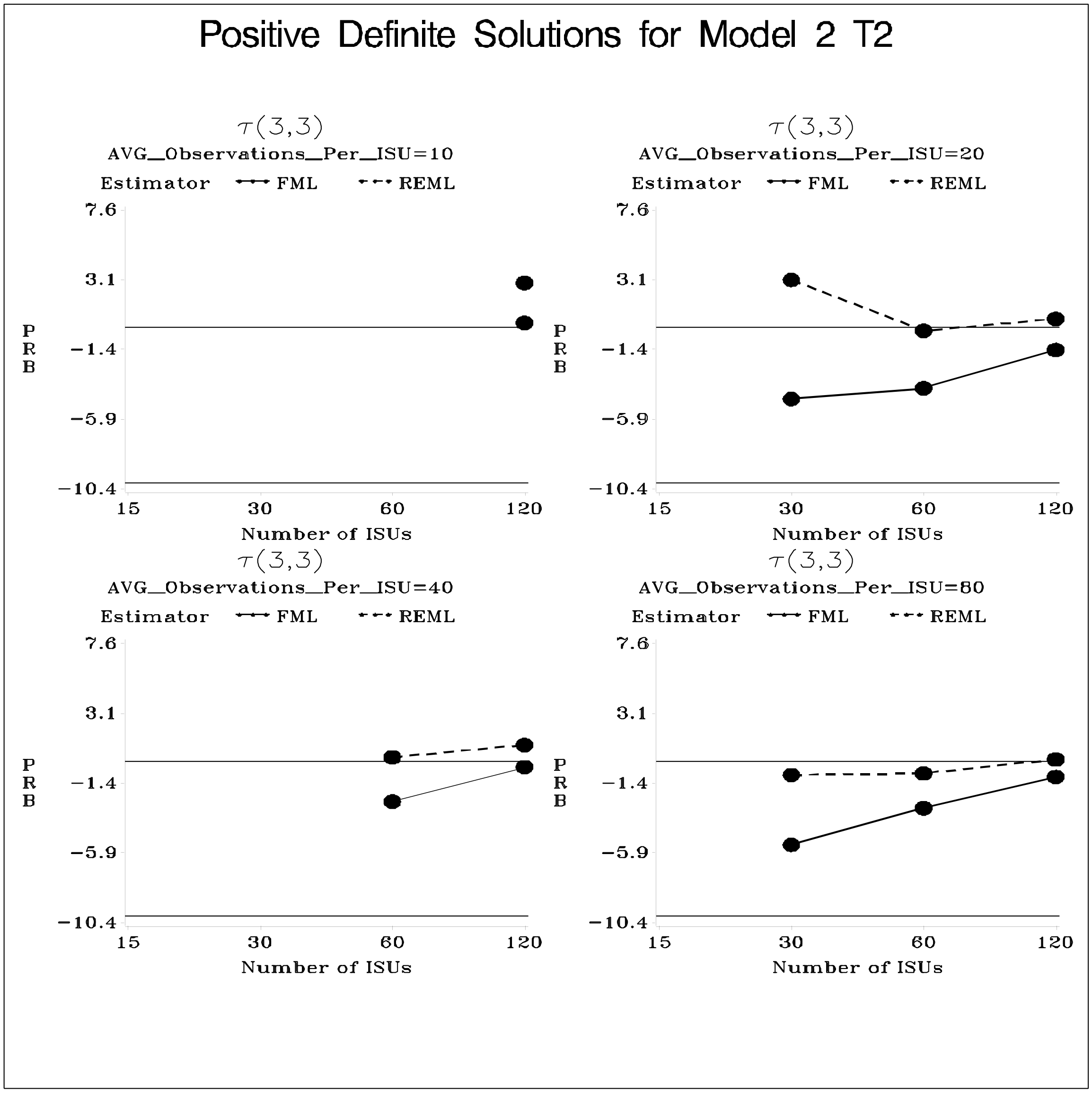

Figure 3.28: τ_{33} PRB Model 2 T2 REML & FML

Model 3

Under T1, when 15 ISUs were sampled, even with an average of 80 observations sampled per ISU, FML bias always exceeded -10% for every variance and covariance parameter. When 30 ISUs were sampled with an average of 20 observations per ISU, FML estimates of $\tau_{11}, \tau_{21}, \tau_{22}$, & τ_{32} were biased by -10% or more. When 30 ISUs were sampled with an average of 40 observations per ISU, FML estimates of τ_{21} were biased by -10% or more. Sampling 60 ISUs with an average of 10 or 20 observations per ISU resulted in FML bias exceeding -10% for τ_{21} Unlike FML, under T1, only REML estimates of τ_{32} exhibited bias of -10% or more, and only when 30 ISUs were sampled with an average of 20 observations per ISU.

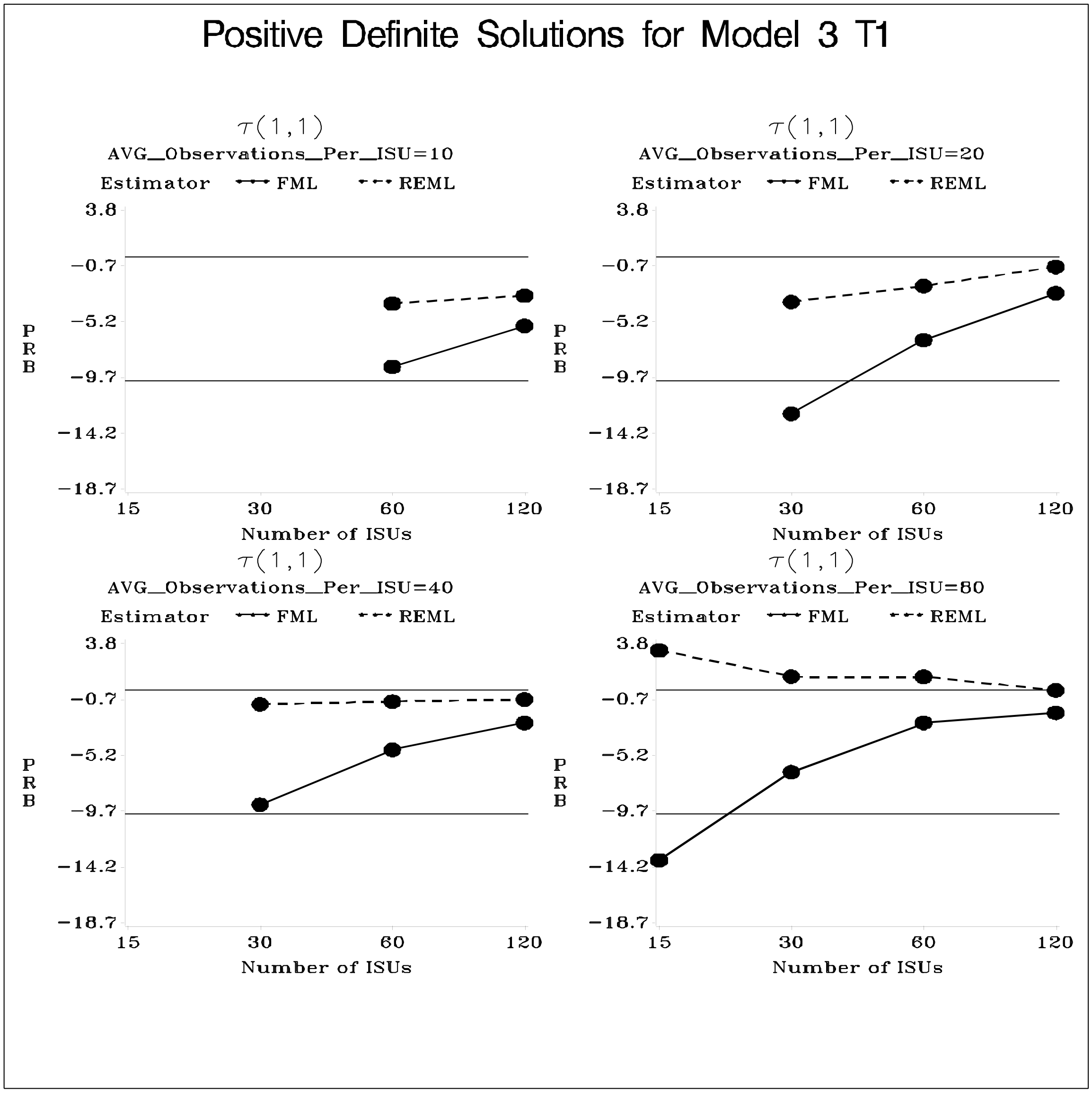

Figure 3.29: τ_{11} PRB Model 3 T1 REML & FML

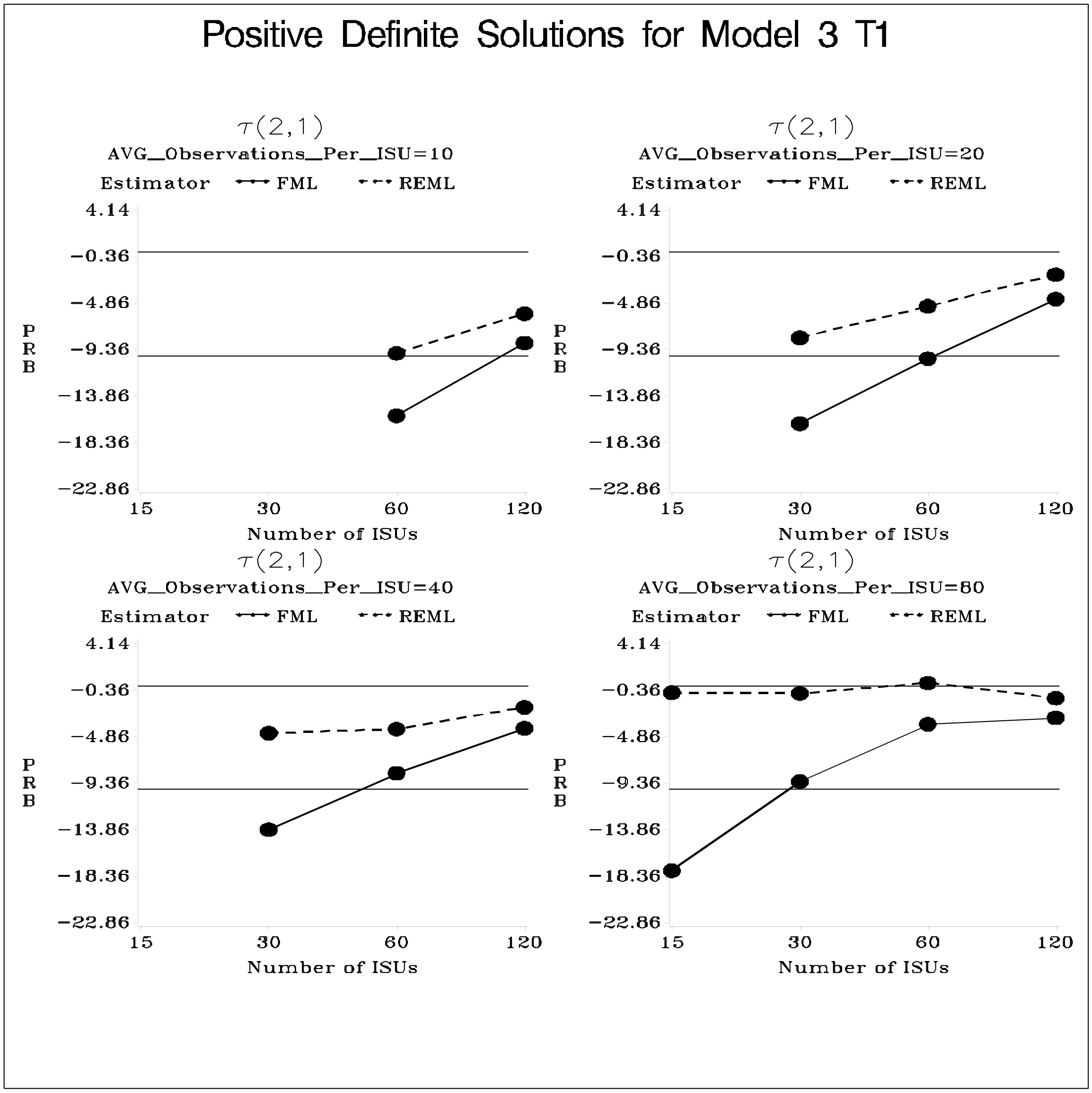

Figure 3.30: τ_{21} PRB Model 3 T1 REML & FML

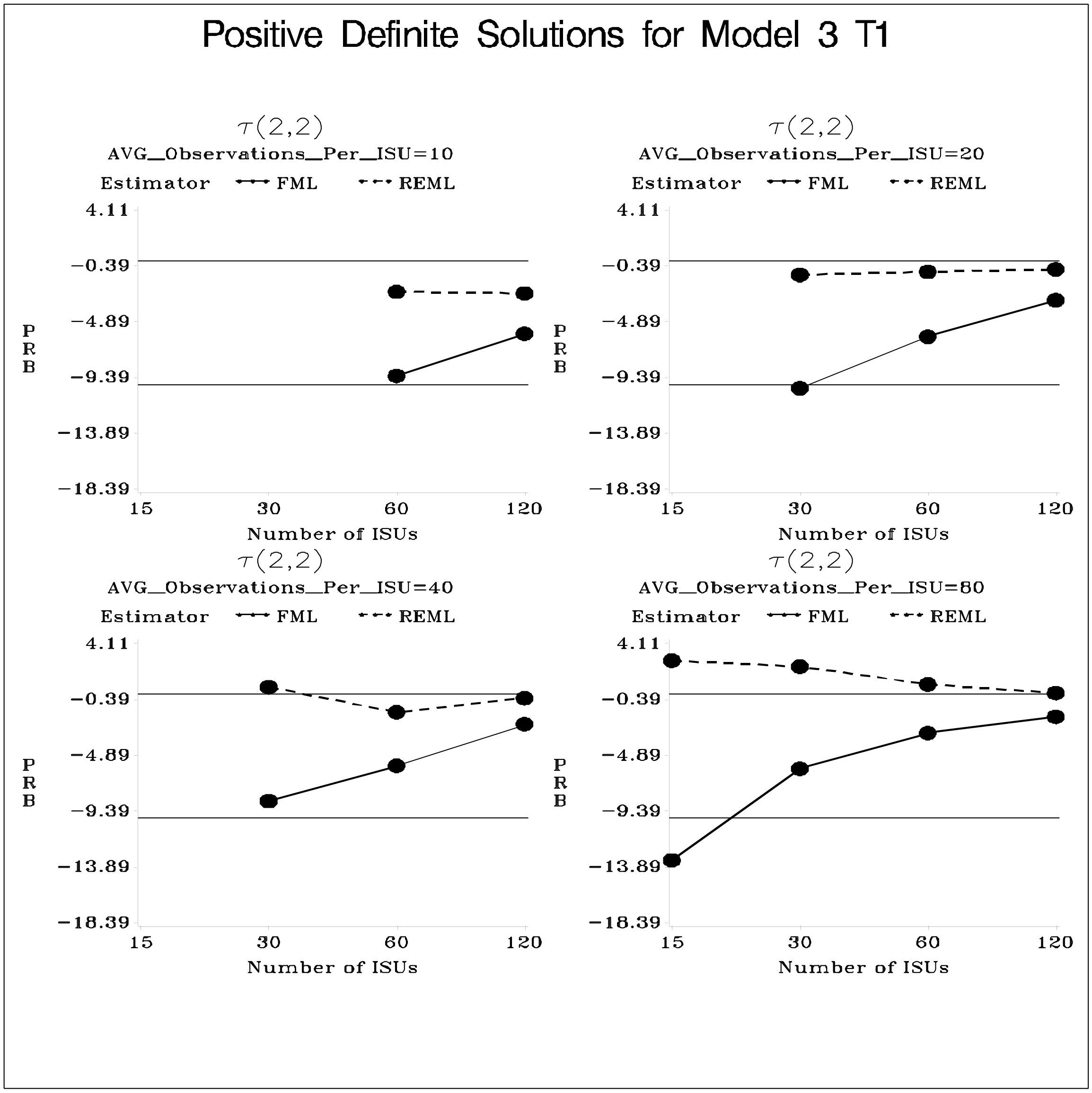

Figure 3.31: τ_{22} PRB Model 3 T1 REML & FML

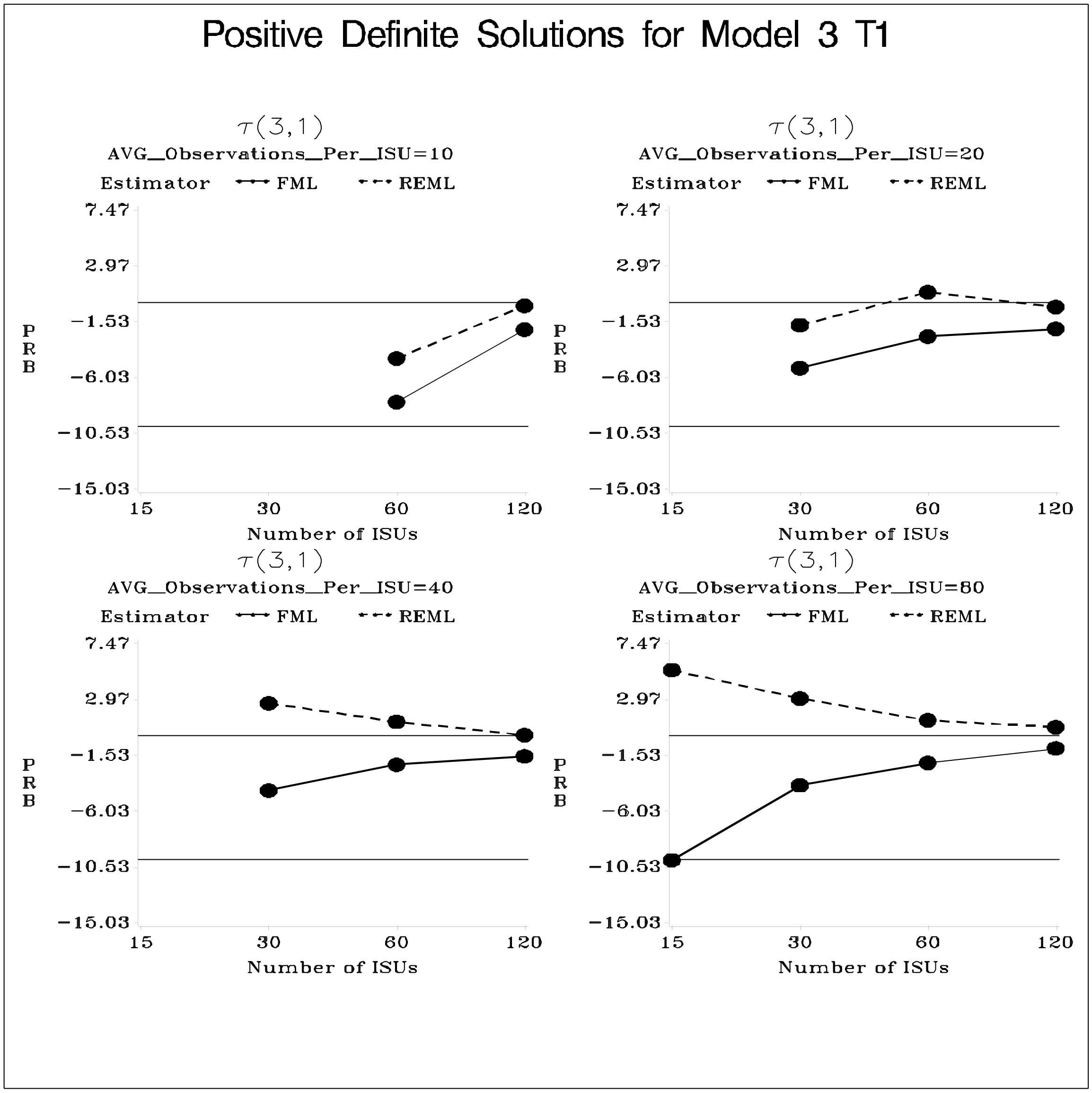

Figure 3.32: τ_{31} PRB Model 3 T1 REML & FML

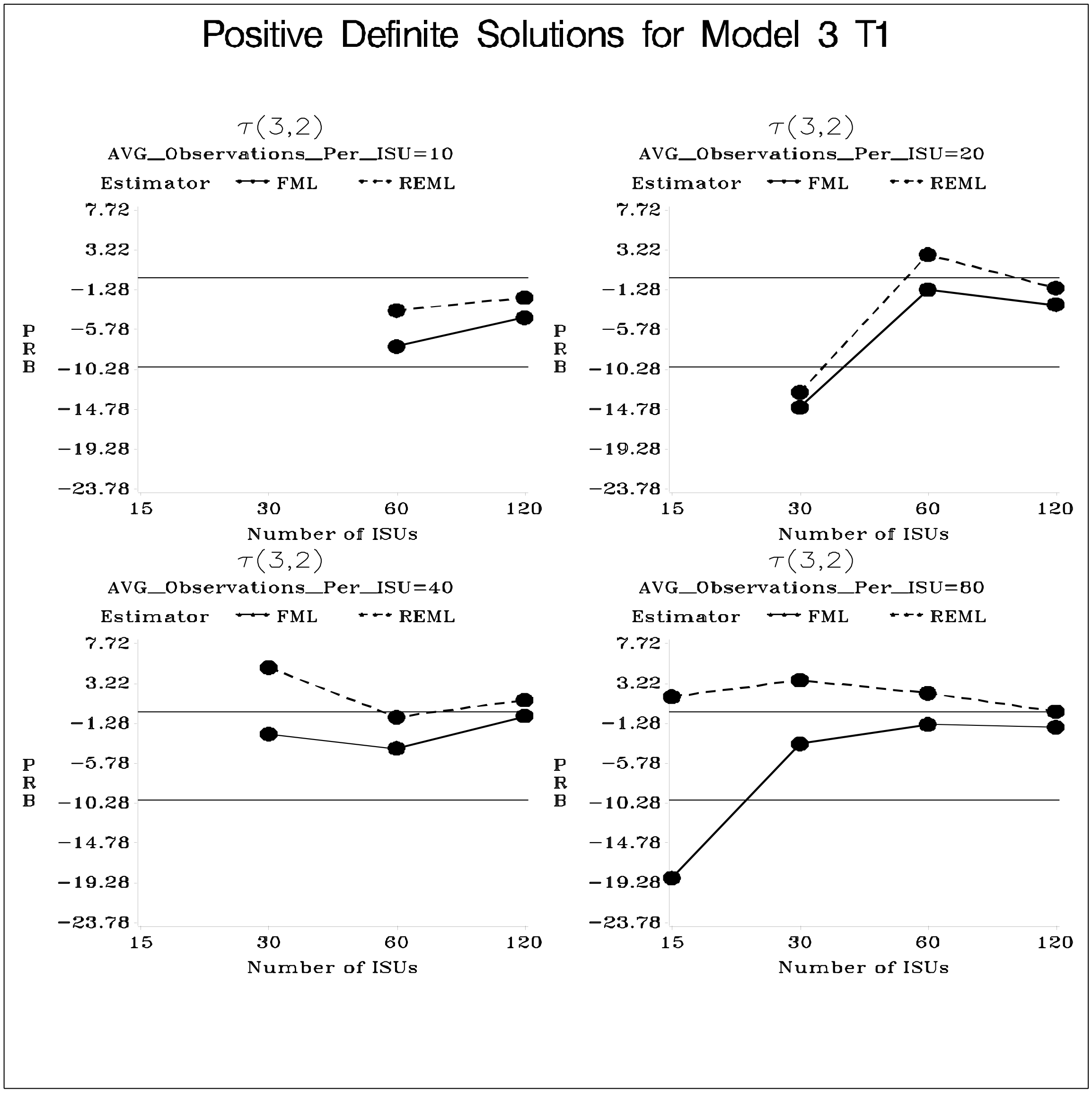

Figure 3.33: τ_{32} PRB Model 3 T1 REML & FML

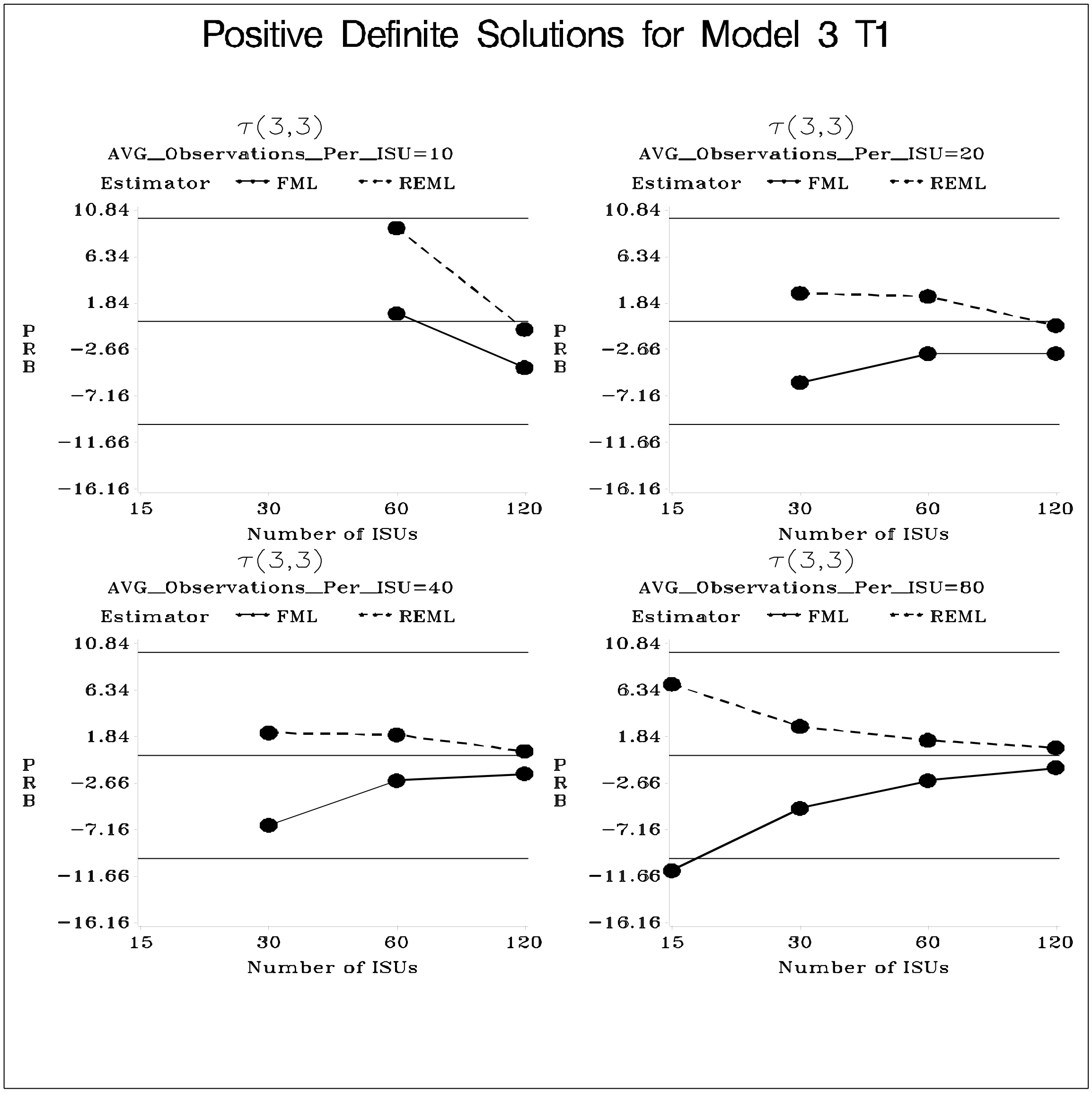

Figure 3.34: τ_{33} PRB Model 3 T1 REML & FML

Under T2, When 30 ISUs were sampled with an average 40 observations per ISU, FML bias for $\tau_{11}, \tau_{21}, \tau_{22}$, & τ_{32} exceeded -10%. When 30 ISUs were sampled with an average 80 observations per ISU, FML bias for τ_{21} & τ_{32} exceeded -10%. When 60 ISUs were sampled with an average of 10 or 20 observations per ISU, FML bias for τ_{11} & τ_{32} exceeded -10%. When 60 ISUs were sampled, no matter how many observations were sampled per ISU (whether an average of 10, 20,40, or 80 observations were sampled per ISU), FML bias for τ_{21} exceeded 10%. FML bias for τ_{31} exceeded 10% when 60 ISUs were sampled with an average of 10 observations per ISU. When 120 ISUs were sampled with an average of 10 observations per ISU, FML bias for τ_{11}, τ_{21}, & τ_{32} exceeded -10%. When 30 ISUs were sampled with an average of 40 observations per ISU, REML bias for τ_{32} exceeded -10%. REML bias for $\tau_{21}, \tau_{31}, \tau_{32}$ & τ_{33} exceeded 10%, but only when 60 ISUs were sampled with an average of 10 observations per ISU. When 60 ISUs were sampled with an average of 20 observations per ISU, REML bias exceeded 10% for τ_{33} & τ_{21}. When 120 ISUs were sampled with an average of 10 observations per ISU, REML bias for τ_{32} exceeded -10%.

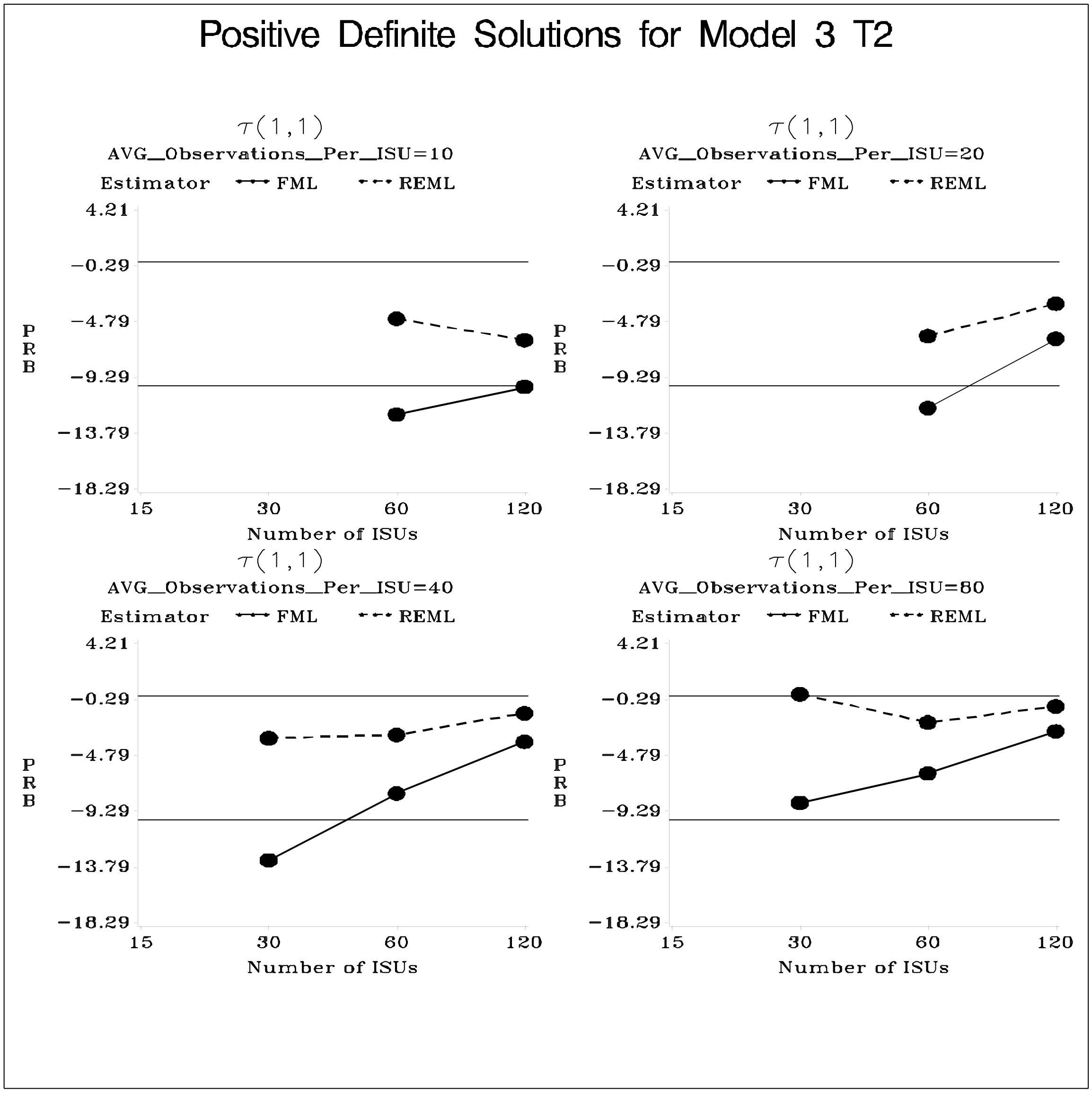

Figure 3.35: τ_{11} PRB Model 3 T2 REML & FML

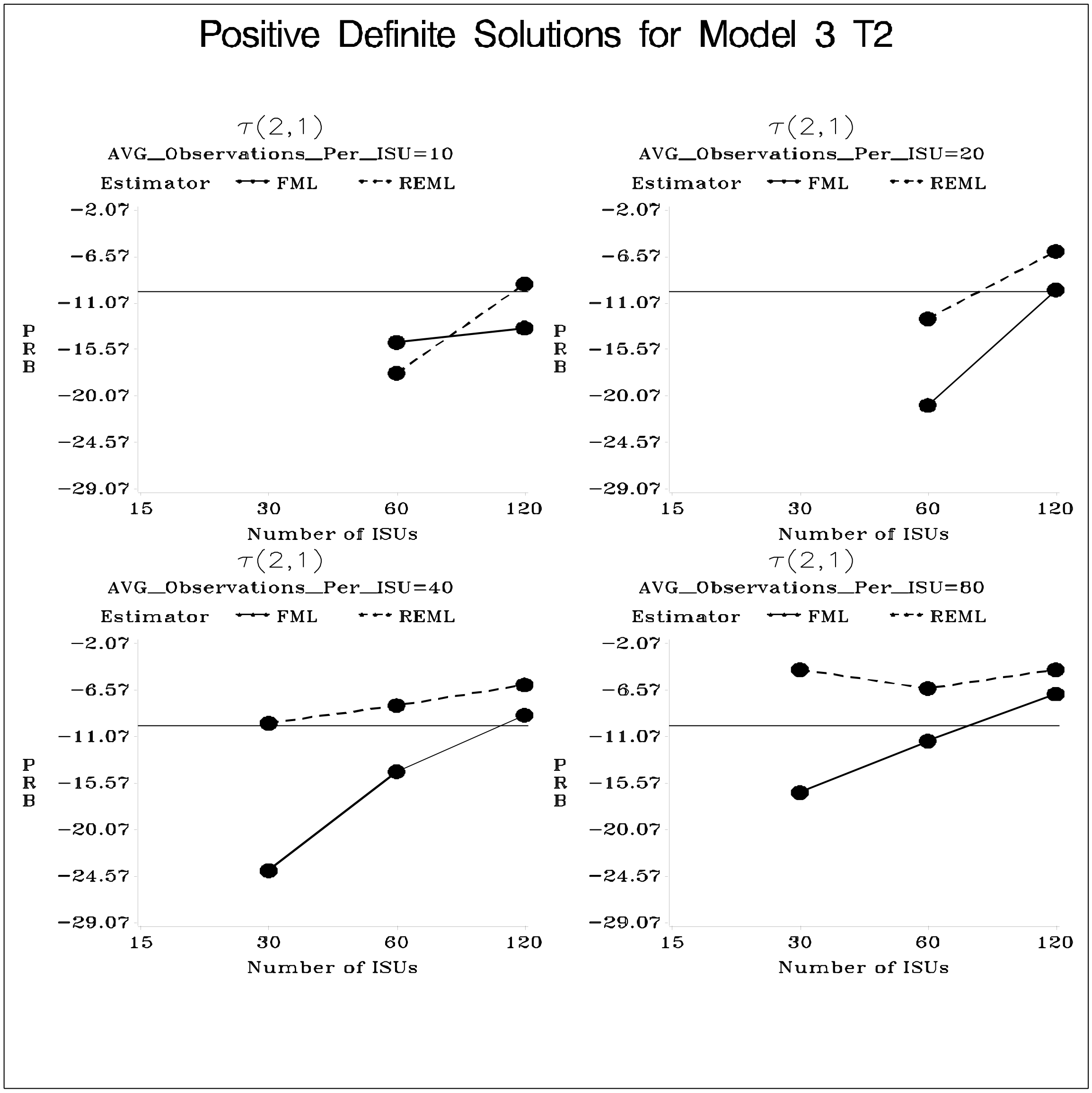

Figure 3.36: τ_{21} PRB Model 3 T2 REML & FML

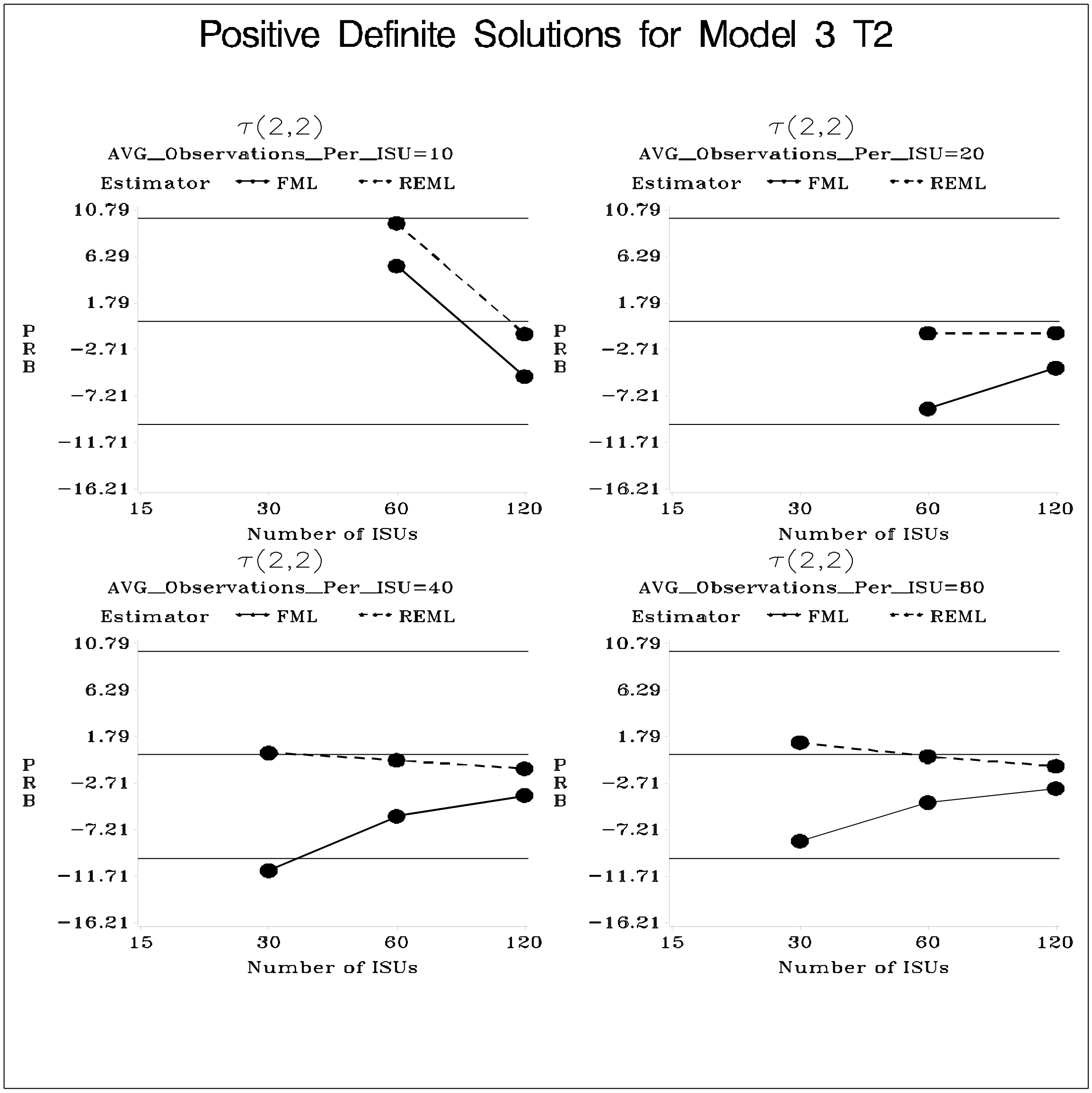

Figure 3.37: τ_{22} PRB Model 3 T2 REML & FML

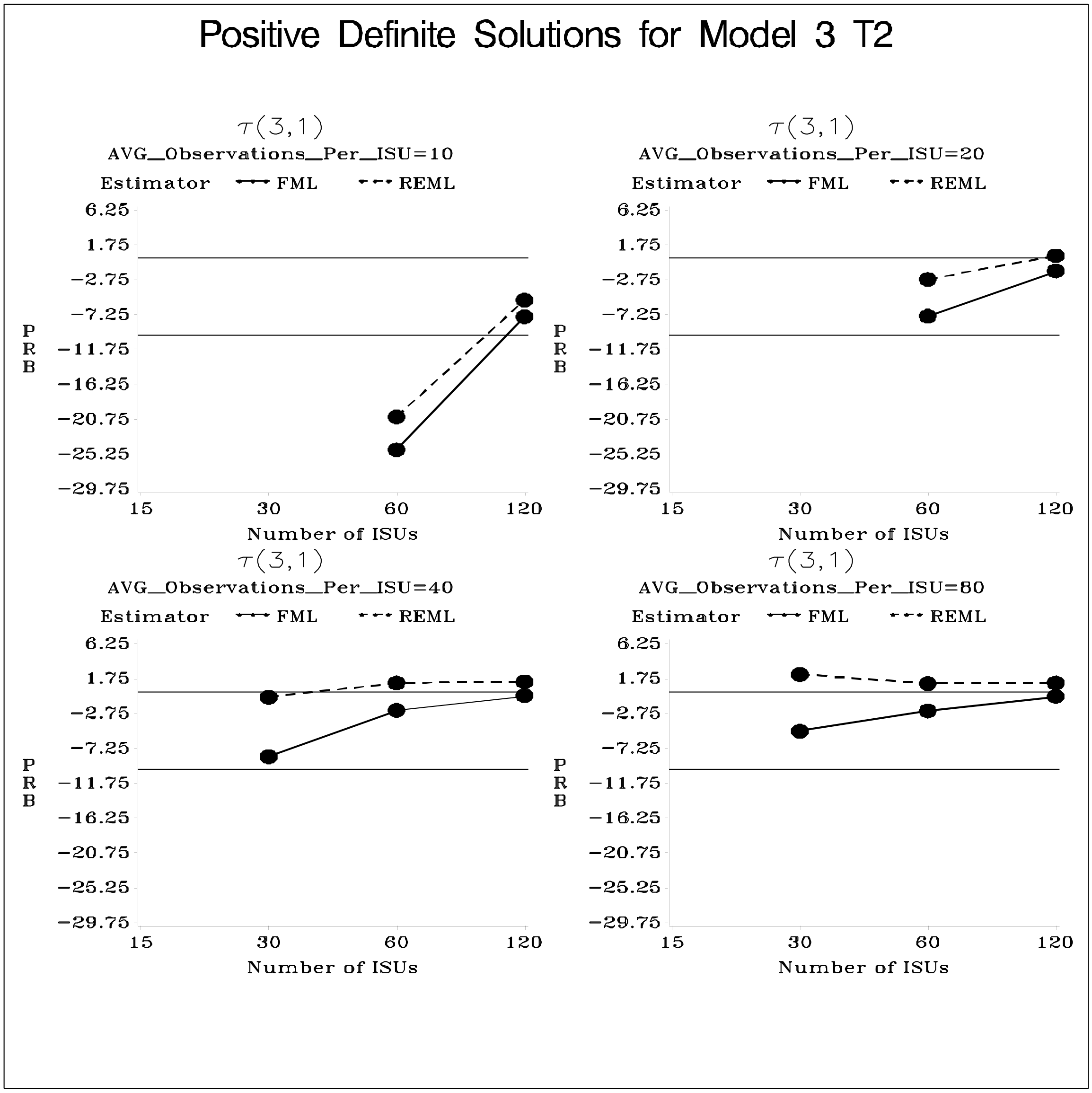

Figure 3.38: τ_{31} PRB Model 3 T2 REML & FML

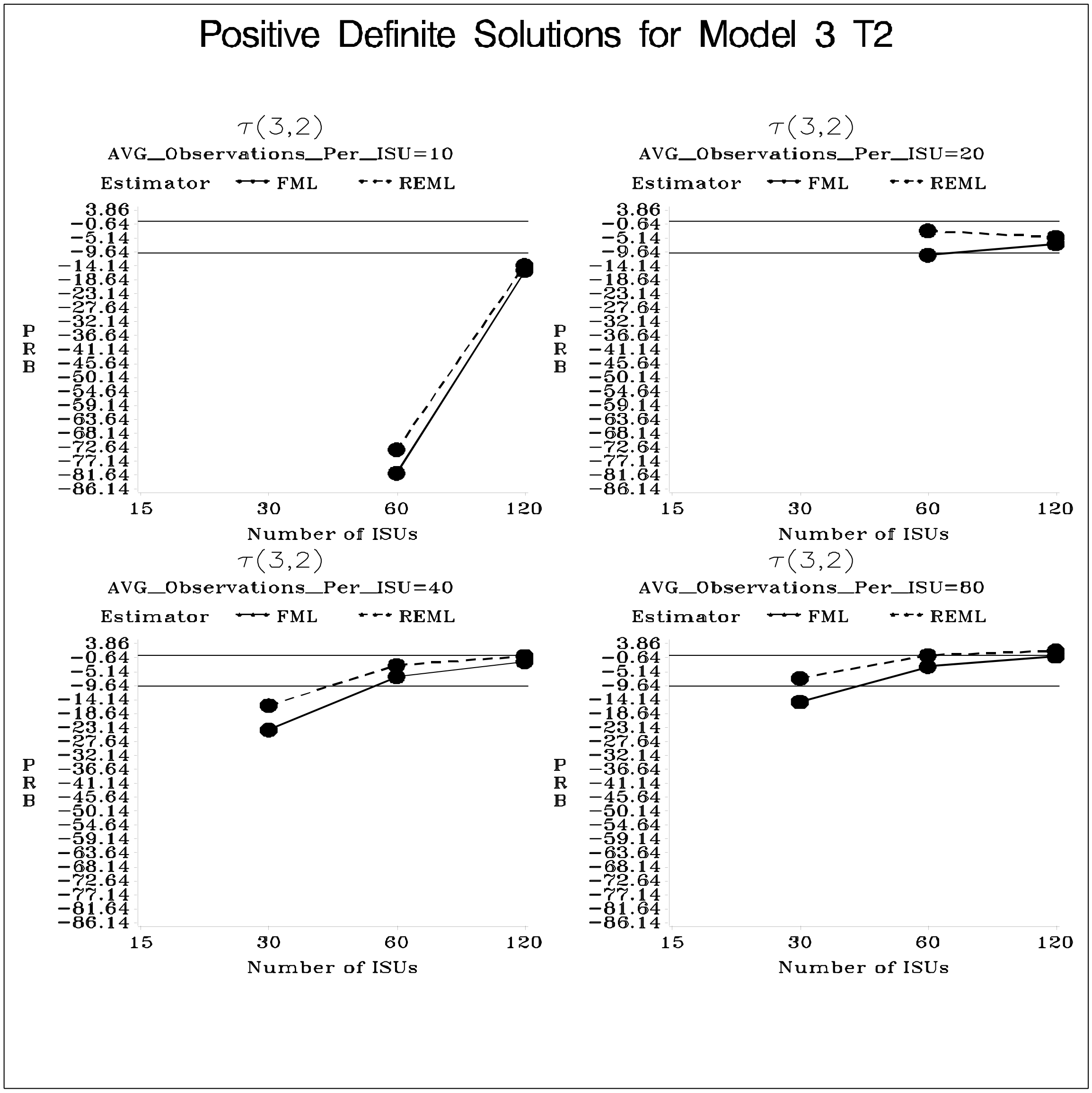

Figure 3.39: τ_{32} PRB Model 3 T2 REML & FML

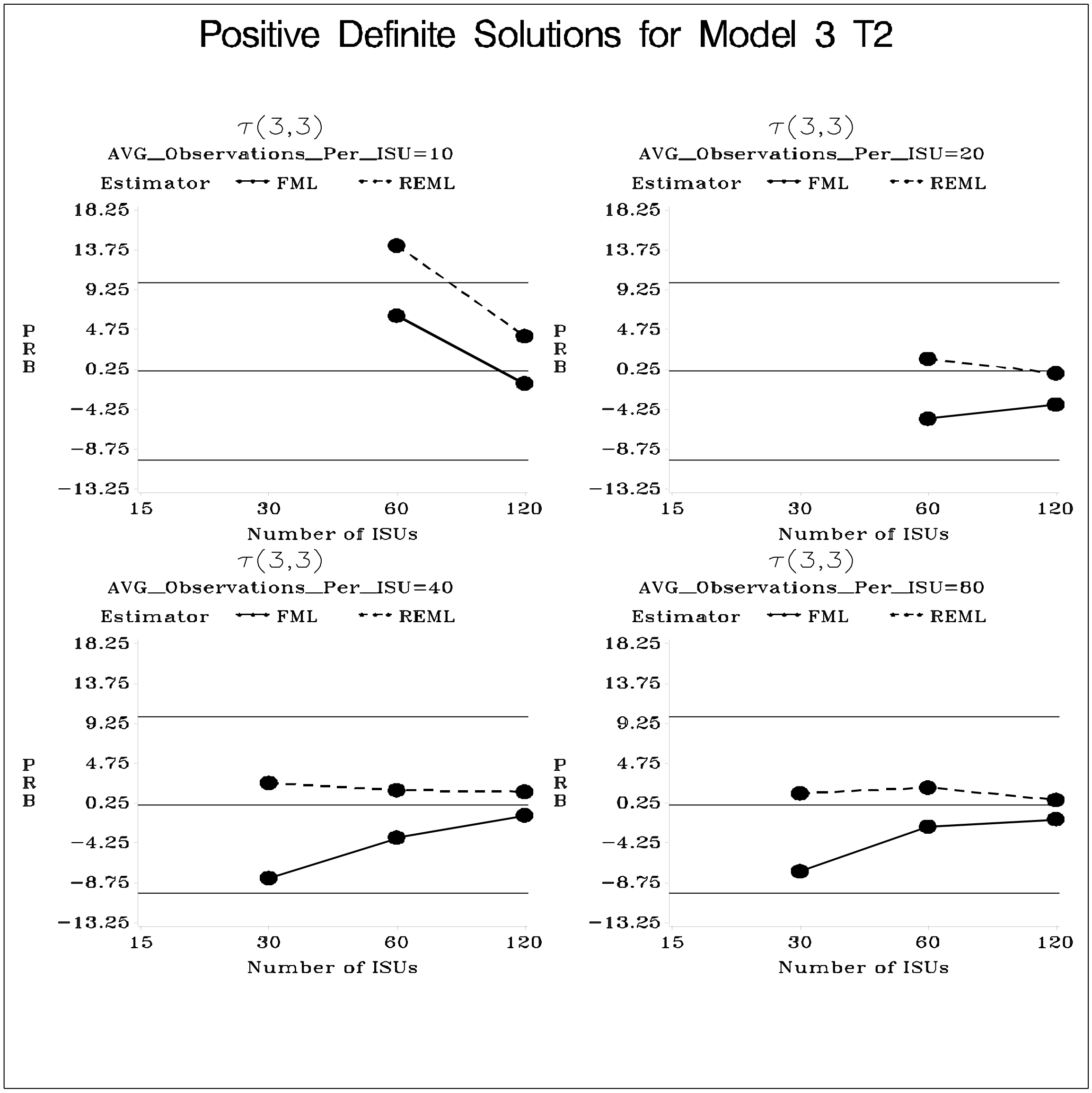

Figure 3.40: τ_{33} PRB Model 3 T2 REML & FML

3.6.3 Summary

Model 1

In model 1 when the generating covariance matrix was composed of large elements (i.e. T1), excessive bias was only observed in the smallest samples for FML estimates, and never for REML estimates. When the generating covariance matrix was composed of small elements (T2), excessive bias was not restricted to the smallest sample sizes, and could be observed in moderate to large sample sizes (i.e. FML estimates of τ_{11} when 60 ISUs were sampled with an average of 80 observations per ISU). In contrast, REML estimates remained unbiased except for the smallest of sample sizes (i.e. when 15 ISUs were sampled with an average of 10 or 20 observations per ISU, or 30 ISUs were sampled with an average of 10 observations per ISU). As observed in the FML bias results, when few ISUs were sampled (fifteen in this case), no matter how many observations were sampled per ISU, bias remains a problem. These results are consistent with the simulation findings of Mok (1995) and the theoretical work of Demidenko (2004).

Model 2

When the generating covariance matrix of random effects was composed of large elements, T1, results were similar to model 1. However, there was a noticeable model complexity effect: because many more parameters were estimable, many more biased estimates were observed. Specifically, FML bias for multiple parameters, mostly variances, exceeded 10%, but only in the smallest sample sizes, and REML did not exhibit any excessive bias.

When the generating covariance matrix was composed of small elements, T2, results were again similar to model 1, only more complex. FML estimates of all *covariances* were biased by 10% or more, but only one *variance*, τ_{11}, was biased by 10% or more. FML bias was mostly restricted to the second smallest sample size: when 30 ISUs were sampled with an average of 20 observations per ISU. However, even when 120 ISUs were sampled with an average of 10 observations per ISU, FML estimates of τ_{32} remained quite biased. REML bias was restricted to covariances, and specifically to the two covariances with the smallest generating values of all elements in T2: τ_{31} & τ_{32}, each having generating values less than 1. The most severe bias associated with these parameters occurred in the smallest sample size. As with FML, REML estimates of τ_{32} exhibited substantial bias even when 120 ISUs were sampled, so long as few observations were sampled per ISU.

Other than the cases described, FML and REML estimates of variances and covariances appeared well behaved, with little bias. What little bias existed consistently decreased as ISUs increased. FML PRB decreased more than REML PRB, primarily because FML PRB exceeded REML PRB, and thus had more room for improvement than did REML.

FML estimates of covariance components (variances and covariances) were uniformly more negatively biased than REML estimates. When covariance component estimates exhibited positive bias FML estimates were less biased than REML estimates. It is routinely stated in the literature (Demidenko, 2004) that REML estimates are less biased than FML estimates. It appears as though this is *only* the case for negatively biased estimates. It is, therefore, more accurate to state that REML is more positively biased than FML estimates, and when estimates are negatively biased REML appears less biased than FML, but when estimates are positively biased REML appears more biased than FML. Thus, the estimators maintain their relative ranking in bias and the better estimator, in terms of bias, varies as a function of the direction of bias associated with the estimates.

When balanced data were analyzed, and analyzed cells were equated to those analyzed under unbalanced data, bias was dramatically reduced. Under T1, neither REML nor FML exhibited bias exceeding 10%, though FML was consistently more negatively biased than REML, and REML exhibited near-zero bias; even when only 15 ISUs were sampled. Under T2, REML bias never exceeded 10%, and FML only did so for τ_{11}. No matter whether 30, 60, or 120 observations were sampled per ISU, whenever 15 ISUs were sampled, FML bias exceeded 10%,.

Model 3

As with model 1, no matter how many observations were sampled per ISU, FML estimates of every covariance component were excessively biased when 15 ISUs were sampled. Thus, with very few ISUs, increasing the number of observations sampled per ISU was insufficient to offset the bias induced in the FML covariance component estimates. Though excessive bias was observed in larger sample sizes, consistent with simpler models, the majority of the problematic bias was restricted to the smaller sample size cells. In fact, excess bias occured for only one parameter, τ_{21}, when 60 ISUs were sampled, and then, only when an average of 10 or 20 observations were sampled per ISU.

Consistent with model 2 findings, excess bias in REML estimates was restricted to covariances, τ_{32}, and this bias only appeared in a single cell of the design. Thus, even in complex models, REML was a robust estimator of covariance components.

Under T2, in contrast to simpler models, excessive bias was not restricted to smaller sample sizes, and was observed across a wide range of sample sizes, many involving large numbers of ISUs as well as many observations per ISU. Whereas under simpler models, FML bias was generally restricted to conditions in which few ISUs (15 or 30) were sampled, under model 3, excess FML bias was routinely observed in several parameters when 60 ISUs were sampled. Moreover, FML bias exceeded the threshold of 10% for all parameters, save τ_{33}. Thus, as model complexity increased, excess FML bias was more pervasive and less easily remedied by sampling large but *reasonable* numbers of ISUs.

Whereas FML estimates of nearly all variances and covariances exhibited bias exceeding 10% for at least one sample size, REML estimates exhibited bias exceeding 10% for only one variance, τ_{33}, at only one sample size. Other than τ_{33}, REML estimates exhibiting substantial bias under T2 were restricted to covariances, as was observed for model 2. However, under model 3, as with FML, the range of sample sizes at which REML bias exceeded 10% was much wider, with many bias values exceeding 10% when 60 and 120 ISUs were sampled, so long as few observations were sampled per ISU (an average of 10 per). This effect was unique to model 3, and most salient when covariance component generating values were small, and only under the relative bias metric.

3.7 Covariance Component RMSE

In this section the root mean squared error (RMSE) of the estimators is contrasted across covariance components, covariance matrices, sample sizes, and models. Prior simulation and theoretical work has demonstrated that for some models, REML, though uniformly less biased than FML, may exhibit greater RMSE than FML for certain models as model complexity increases (Corbeil & Searle, 1976). This is consistent with theoretical work by Demidenko (2004) demonstrating that REML is not a true likelihood, and thus does not possess the asymptotic property of efficiency that FML does. RMSE is a function of the squared bias and the sampling variance of the estimator. A necessary consequence of these facts is that for two equally biased estimates, RMSE is a measure of efficiency, upon which we would expect FML to outperform REML. As will be seen, for most models this is the case, but only slightly, and only for complex models.

Plots presented in the following section plot REML RMSE and FML RMSE against one another. REML RMSE is plotted along the abscissa, and FML RMSE is plotted along the ordinate. A 45° line is overlaid, and points falling on the line indicate when REML RMSE and FML RMSE are equivalent. Points falling below the line indicate when FML RMSE exceeds REML RMSE, points falling above the line indicate when REML RMSE exceeds FML RMSE. Plots for the sample size effect are presented in appendix 3 and are not discussed here. Discussion of the sample size effect on RMSE is omitted because there was a relatively simple and consistent pattern in the results: REML RMSE and FML RMSE values generally coincided, deviations from equality were relatively small, and only occur with a magnitude of interest when 15 ISUs were sampled.

3.7.1 Model 1 RMSE

As can be seen in figure 3.41, under T1, when FML RMSE and REML RMSE values departed from equality, it was FML that had higher values. However, this was only for τ_{11}, and for only a subset of the design cells. For virtually all cells of the design, RMSE, for estimates of σ^2, coincided between estimators; the same was true for estimates of τ_{11} when 30 or more ISUs were sampled.

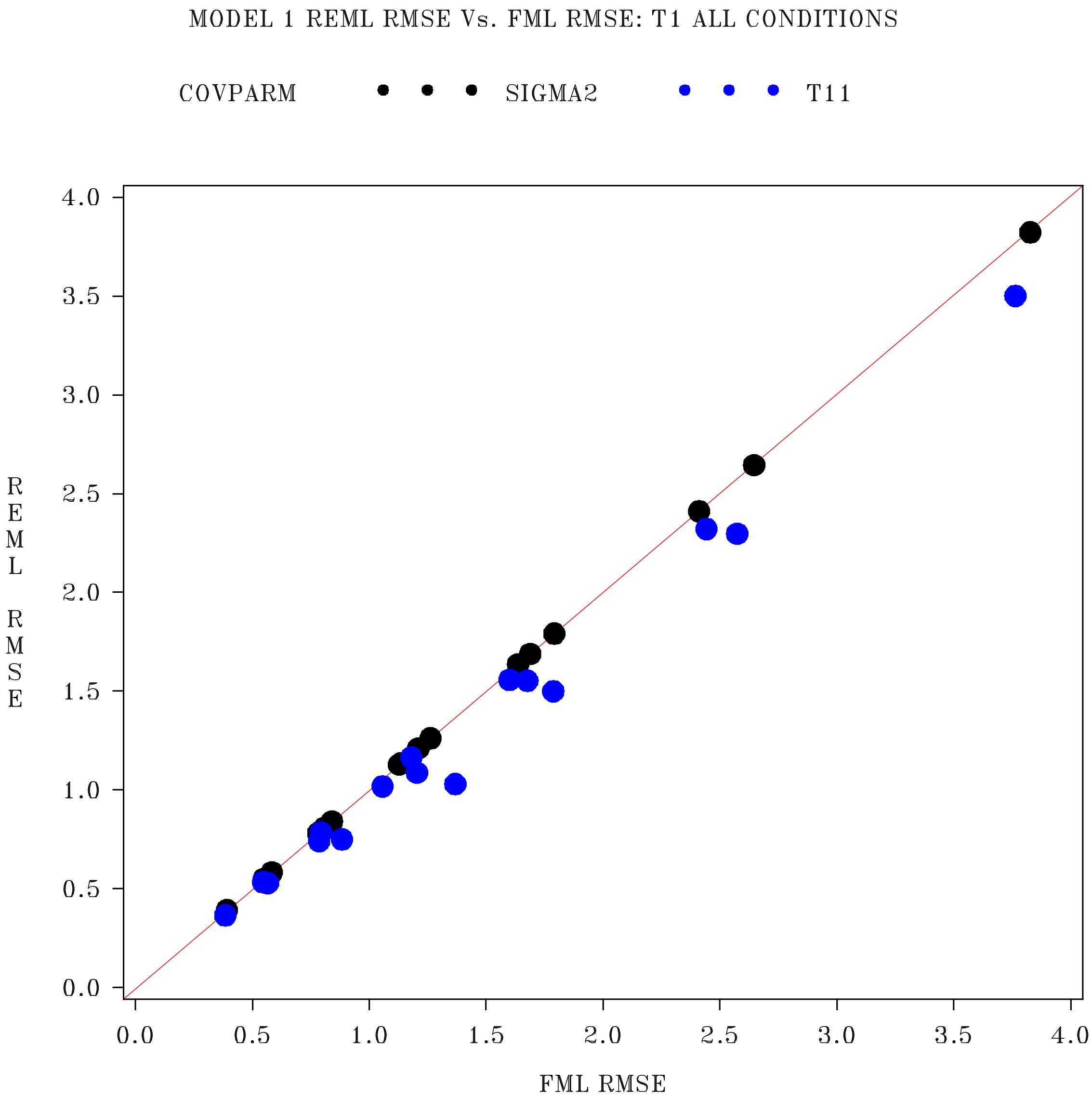

Figure 3.41: Random Effect RMSE Model 1 T1 REML & FML

Results presented in figure 3.42 for T2, are identical to those observed in figure 3.41, except that the magnitude of the observed RMSE was shrunken toward zero, and few values deviated from equality. However, as with figure 3.41, when REML RMSE and FML RMSE deviated from equality, it was FML RMSE that exceeded REML RMSE.

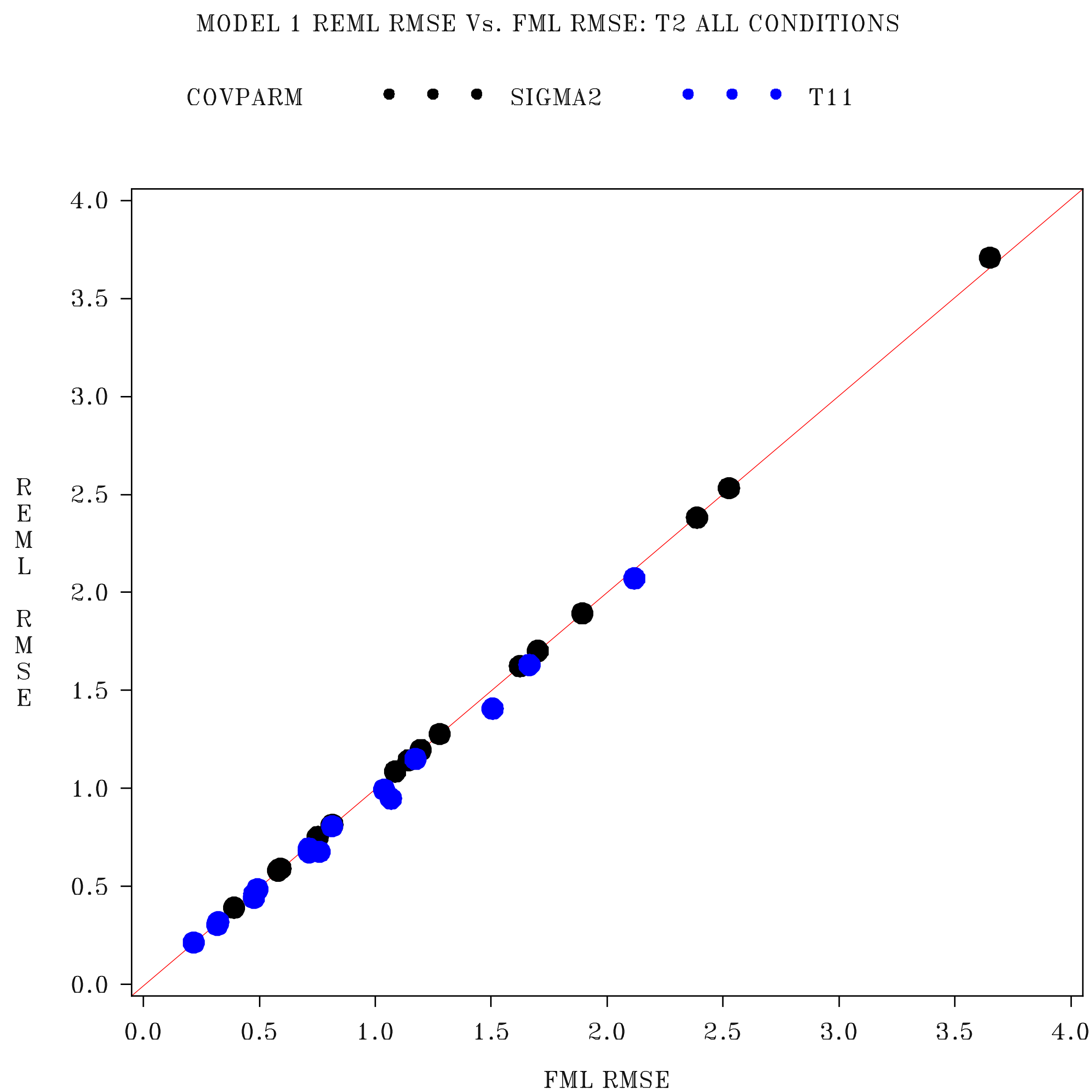

Figure 3.42: Random Effect RMSE Model 1 T2 REML & FML

3.7.2 Model 2 RMSE

Under T1 (see figure 3.43), REML RMSE and FML RMSE values were rather coincident. Though departures from equality occurred in both directions (REML exceeding FML and vice versa), generally, REML RMSE exceeded FML RMSE. Thus, the effect of estimator observed under model 1 was reversed in model 2. The inconsistency of the estimator effect on RMSE was not a new discovery,(see parameters τ_{11} & τ_{22}), exhibiting substantial RMSE. In the bias results, covariances tended to be most biased of all parameters, however, variances exhibited greater levels of RMSE than did covariances.

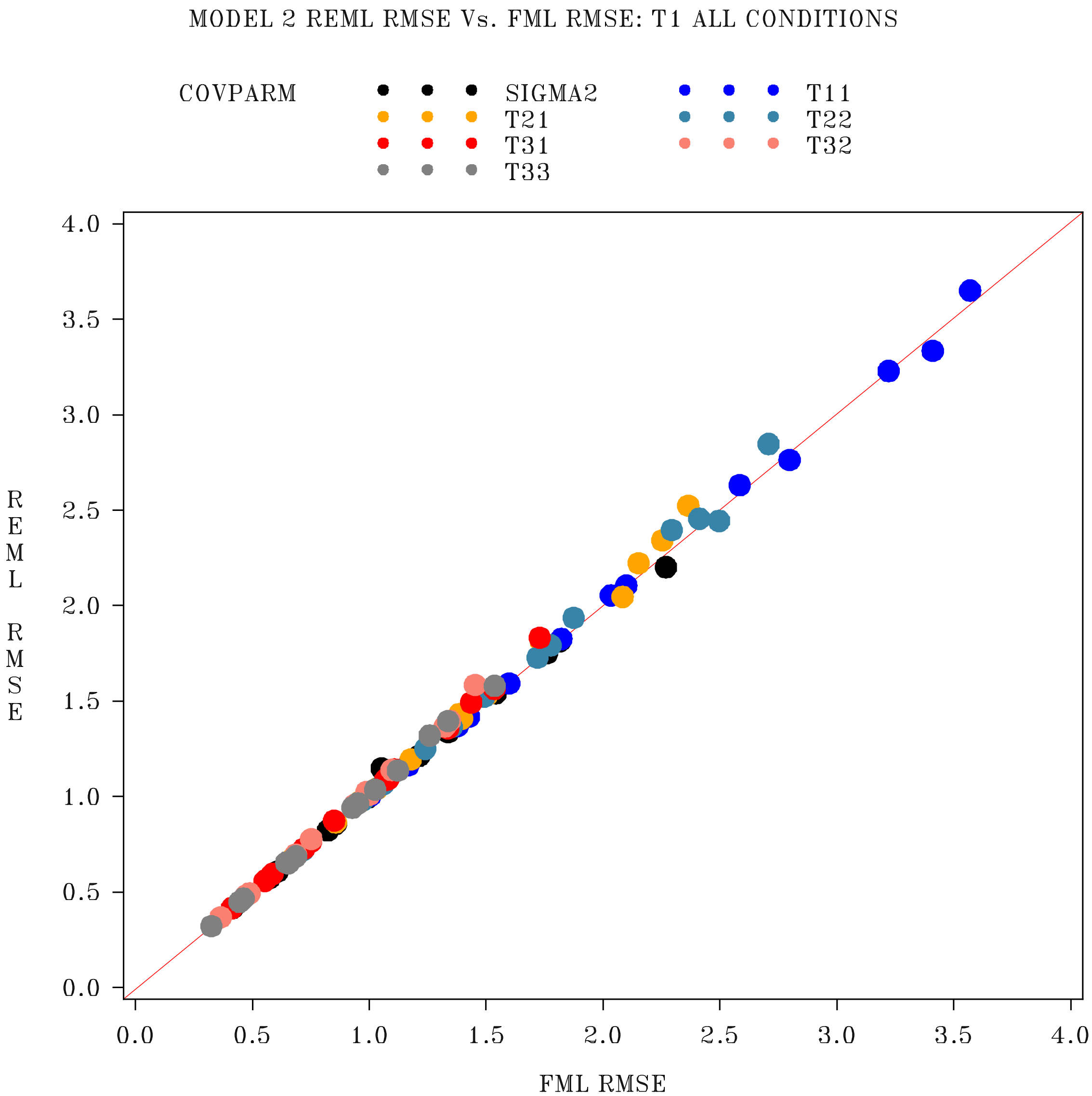

Figure 3.43: Random Effect RMSE Model 2 T1 REML & FML

Similar to the results observed under model 1, figure 3.44 demonstrates that when the generating matrix of random effect covariances was composed of small elements, RMSE values were much less dispersed than they were when the generating matrix was composed of large values. Observed maximum values under T2 were nearly half the maximum values observed under T1. In addition to lower dispersion, departures from equality were less frequent and substantial across estimators.

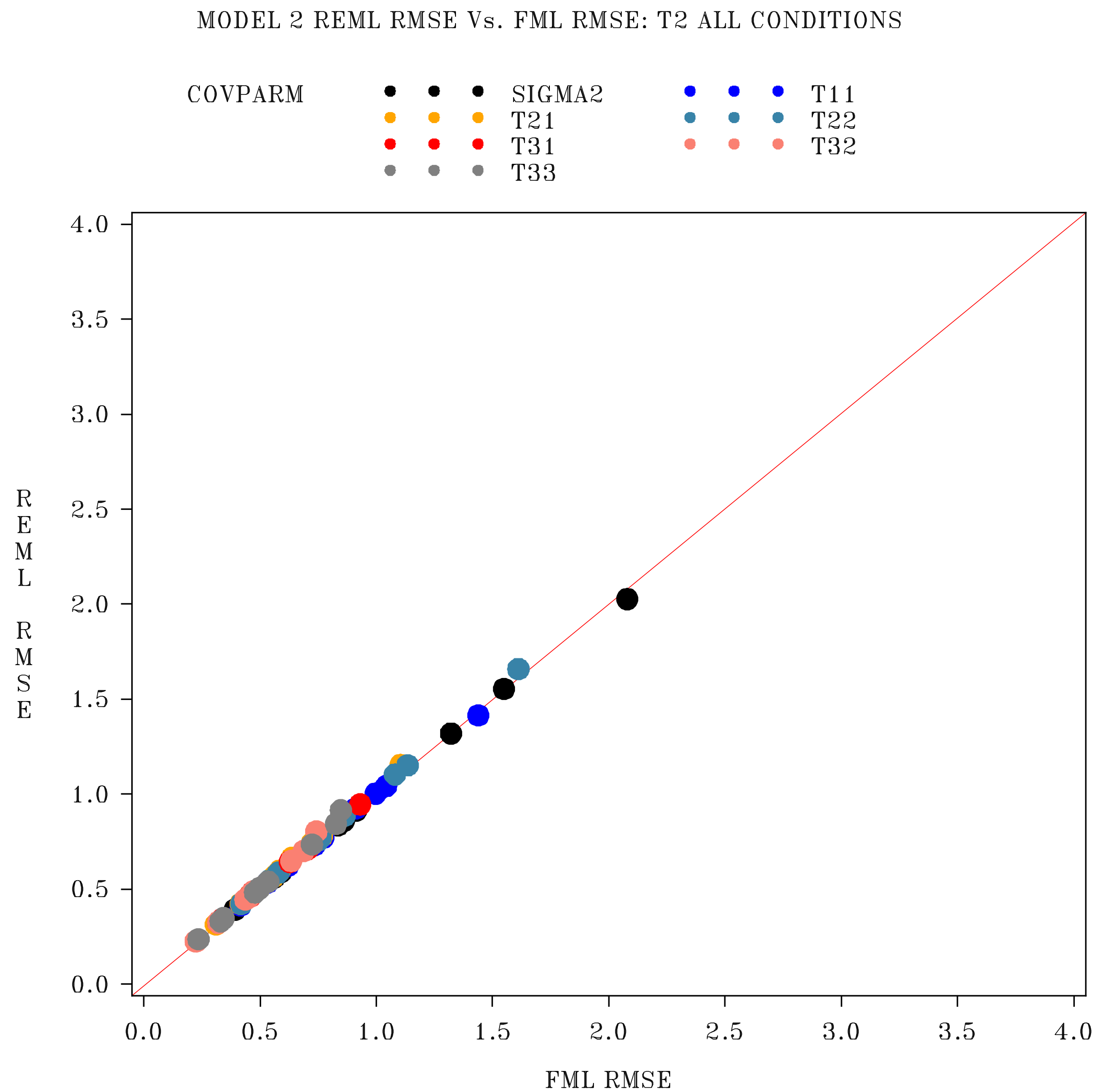

Figure 3.44: Random Effect RMSE Model 2 T2 REML & FML

3.7.3 Model 3 RMSE

Values of RMSE obtained under T1 are displayed in figure 3.45. Trends observed in RMSE were similar to those observed in model 2. REML RMSE and FML RMSE values were highly correlated, and though FML RMSE sometimes exceeded REML RMSE, it was much more common for REML RMSE to exceed FML RMSE. Another trend observed in model 3 RMSE under T1, that was consistent with model 2 RMSE obtained under T1, was the difference between variances and covariances. As in model 2, variances exhibited the largest RMSE, particularly estimates of τ_{11} & τ_{22}.

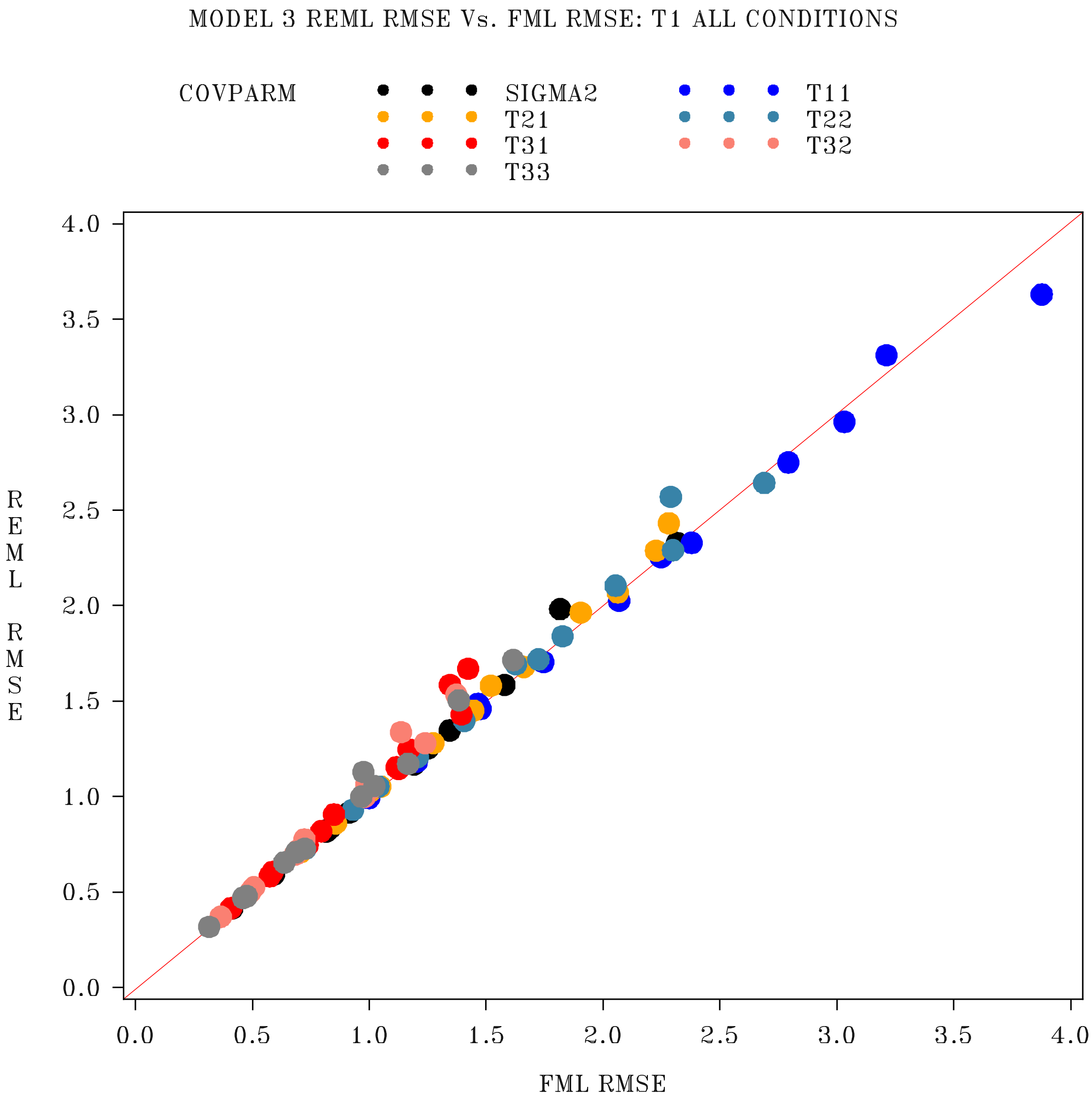

Figure 3.45: Random Effect RMSE Model 3 T1 REML & FML

As in model 2, figure 3.46 demonstrates that model 3 RMSE values observed under T2 were much less dispersed than those observed under T1. Maximum RMSE values under T2 were approximately half the maximum values observed under T1.

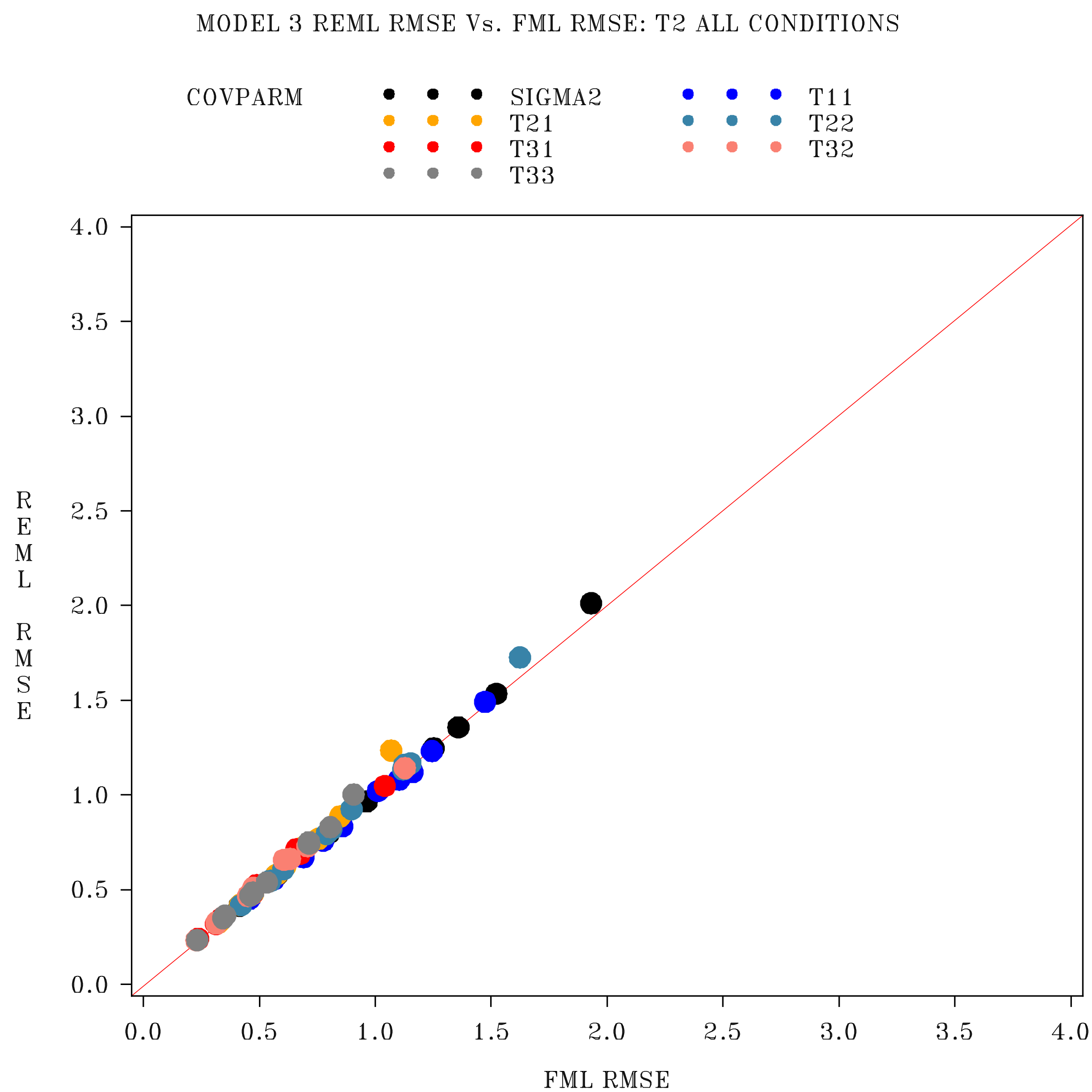

Figure 3.46: Random Effect RMSE Model 3 T2 REML & FML

3.7.4 Summary

The RMSE effect can be interpreted more succinctly than the bias effect. Estimators differed in RMSE only at the smallest sample sizes, otherwise estimators could not be differentiated on RMSE. When the estimators differed in RMSE, the most substantial differences were observed when REML RMSE exceeded FML RMSE. Consistent with previous research (Corbeil & Searle, 1976), the estimator effect varied as a function of model complexity. In the case of model 1, FML RMSE exceeded REML RMSE, but under model 2 and model 3, REML RMSE generally exceeded FML RMSE. When population covariance parameters were large (T1) RMSE values were much larger than when population covariance parameters were small (T2) for both estimators. In both model 2 and model 3, variances exhibited higher RMSE values than did covariances. When data were balanced, lower dispersion was observed in RMSE for both estimators than when data were unbalanced. However, REML and FML differed in the magnitude of RMSE for τ_{11} when data were balanced, such that FML RMSE exceeded REML RMSE.

CHAPTER 4

Conclusions

The goal of this study was to provide researchers, both applied and quantitative, with information on the behavior of the two most common estimators for linear mixed effect model parameters under realistic data conditions. Heretofore, simulation work has focussed exclusively on unrealistically simple models and balanced data. Both of these facets have limited the generalizability of previous findings because researchers often fit complex models and rarely, if ever, have access to balanced or complete data. Criticism of preceding studies must be qualified by the fact that only one of the cited simulation studies, Hox and Maas (2002), was completed after the development of standard software routines for estimating complex models. Thus, the ability to test complex models under realistic data conditions was limited by the state of the art. While at the time these studies provided valuable information on models that were estimable and estimated then, advances in software have allowed researchers to fit more complex models, thus rendering the findings less applicable to current practice. However, to the extent that applied researcher's models conform to the conditions examined in the preceding studies, information contained in those studies is useful.

Two effects were observed for sample sizes in this study. The first relates to convergence: when very few ISUs (15) were sampled and model complexity was moderate (model 2) or substantial (model 3), rates of non-converged and improper solutions were so high that bias was of little concern given that estimates worth interpreting were never likely to be observed. Doubling the sampled ISUs to 30, permitted assessment of the second sample size effect: consistent with the findings of Mok (1995), results indicated that bias was most problematic when few ISUs were sampled. Even so, there was a noticeable effect for the number of observations sampled per ISU in moderating the degree of bias. However, sampling few ISUs resulted in high degrees of bias, in most cases, irrespective of the number of observations sampled per ISU.

Model complexity also impacted the effects of ISUs. As model complexity increased, the number of ISUs required before bias ceased to be problematic, increased. An anomaly observed in the results involved inconsistencies across models in the effect of sampling many observations per ISU when few ISUs were sampled. Models 1 and 3, but not model 2, had parameters for which, when a certain number of ISUs were sampled, excessive bias was observed, no matter how many observations were sampled per ISU. Given that model 2 was more complex than model 1 and model 3 was more complex than model 2, one would have expected model 2 to exhibit the same effect. Preferably there would have been some monotonic relationship between model complexity and the number of ISUs sampled at which, no matter how many observations were sampled per ISU, bias remained substantial. In all likelihood, it is not that the phenomenon did not occur for model 2, but rather that the number of ISUs for which the phenomenon would be observed was not sampled in this study. For model 1, 15 ISUs were sufficiently low to observe the phenomenon; for model 3, 60 ISUs were sufficient to observe the phenomenon; for model 2, given that the phenomenon was not observed at 30 ISUs, as might have been expected, the number of ISUs required to observe the phenomenon was likely somewhere between 15 and 30.

As previously stated, the impact of sample size on RMSE was relatively straightforward. RMSE values were highest when very few ISUs were sampled, but decreased rather quickly as increasing numbers of ISUs were sampled. REML RMSE and FML RMSE were coincident for the most part, but when few ISUs were sampled, REML tended to exhibit slightly higher values of RMSE. The small amount by which REML RMSE exceeded FML RMSE, and the few cells in which this occurred was insufficient to require qualifying the endorsement of REML estimation in finite samples. Taken together, the substantial gains in bias reduction obtained from REML when few ISUs were sampled, and the rare and negligible increase in RMSE associated with REML when few ISUs were sampled, suggested that in finite samples REML may be the preferred estimator.

As with sample size, the covariance matrix effect can be decomposed into two main effects: the impact on convergence and the impact on bias. As Tables 3.1 and 3.3 demonstrate, rates of non-convergence tended to be higher under T2 than under T1. Under model 2, T2 had 2.3 times more cells excluded from analysis because of excessive non-convergence rates than did T1. Under Model 3, T2 had 1.5 times more cells excluded from analysis because of excessive non-convergence rates than did T1. In addition, the results of this study elucidated an interesting phenomenon associated with the relative bias metric for T1 and T2. In the raw bias metric, T2 bias exhibited less dispersion than did T1 bias, however, in the relative bias metric, T2 PRB exhibited greater dispersion than did T1 PRB. The phenomenon was generally associated with covariances, which, under T2, had small generating values (only one of the three generating values was larger than 1, and then, only slightly). Use of the relative bias metric when parameters have small generating values can make bias effects appear more severe than trends observed in raw bias. For cases in which concern existed about the potential misleading effect of the relative bias metric, raw bias results were presented. Generally, there was no difference in the relative ranking of the estimators, and the main effect of the relative metric was to render more salient the existing effects for parameters.

Irrespective of model complexity, if few ISUs were sampled, FML PRB could exceed 10% even with many observations per ISU, as many as an average of 80 per ISU. Thus, as far as covariance components were concerned, no matter how many observations were sampled per ISU, when few ISUs were sampled, point estimates could be severely biased. These findings were consistent with those of Mok (1995) in the case of balanced data.

On the other hand, REML estimates rarely exceeded 10% bias, even when few ISUs were sampled, especially when covariance components were large (T1). When covariance components were small (T2) REML was less robust when few ISUs were sampled. For Model 1, REML estimates never exceeded 10% under T1, whereas under T2 REML estimates of τ_{11} exceeded 10%, but only under the three smallest sample size conditions: when 15 ISUs were sampled with an average of 10 or 20 observations per ISU, and when 30 ISUs were sampled with an average of 10 observations per ISU. For Model 2, REML estimates never exceeded 10% except for estimates of τ_{31} and τ_{32}, but only under T2. For model 3, REML estimates never exceeded 10% except for T1 estimates of τ_{32}, and T2 estimates of τ_{21}, τ_{31}, τ_{32}, and τ_{33}. Thus REML PRB was problematic, but this was primarily isolated to covariances, and generally only in the smallest sample sizes. The incidence of both problematic REML and FML PRB values increased with model complexity. Lastly, the incidence of problematic PRB was much lower in REML than it was in FML.

REML estimates were uniformly less biased than FML estimates so long as estimates exhibited negative bias (as covariance components tend to be). In addition, REML estimates exhibited only slightly more RMSE than did FML estimates, but only when 15 ISUs were sampled and only for complex models. Bias and RMSE measure distinct aspects of estimators. Bias measures the average discrepancy between an estimator and the population value over repeated samples. Thus, researchers committed to a cumulative science, in which sequences of studies replicate a given design in order to determine the stability theoretically meaningful effects, may emphasize bias more than RMSE when selecting estimators. RMSE is a function of the squared bias and the sampling variance of the estimator, and measures the dispersion about the population value for a given estimator. Thus researchers interested in using an estimator that will, in a given replication, likely provide estimates close to the population values should use RMSE as their criterion for estimator selection. To the extent that variance across studies is great in both design and analysis in psychological applications, bias may be the less optimal measure when selecting estimators. Fortunately, of the linear mixed model estimators considered in this study, both bias and RMSE generally suggested that REML was the optimal estimator. When bias and RMSE disagreed, they did so only slightly. REML as nearly always favored by bias, and in the few cases where RMSE favored FML, it did not do so by much. In those cases of disagreement, combining the overwhelming advantage of REML in terms of bias with the negligible decrements in RMSE lead to the same conclusion, REML was the better estimator in finite samples for linear mixed models where data were consistent with model assumptions. However, given the excess within-cell variability observed in the meta-model results, the difference in REML and FML may not be meaningful in a statistical sense. Therefore, no definitive or strong endorsement of one estimator over another can be made based upon the results presented in this study.

A consistent trend observed in the bias results was the reversal of effects as a function of changes in metric. Specifically, in the raw bias metric, T2 bias estimates exhibited less dispersion than did T1 bias estimates. However, under the relative bias metric, T2 PRB estimates exhibited greater dispersion than did T1 PRB estimates. The greater dispersion, some cases qualifying as extreme cases, in the T2 PRB estimates were universally associated with covariances and not variances in model2 and model 3, but for model 1, even the random intercept variance exhibited greater dispersion under T2 than under T1. The most likely cause of this phenomenon was that the T2 generating values were all smaller than the T1 generating values. Under model 1, the random intercept variance generating value for T2 was $\frac{1}{3}$ of the T1 generating value. Under model 2 and model 3, covariance generating values under T2 were all 1 or less than 1, roughly $\frac{1}{4}$ of the T1 generating values. Nonetheless, It was clear from comparisons of figures 3.1, 3.5, and 3.9 and comparisons of figures 3.2, 3.6, and 3.10 that increasing model complexity was associated with increased rates of problematic PRB. Comparisons of the same figures reveal that REML was uniformly less biased than FML, FML was consistently negatively biased, and REML PRB was consistently evenly distributed about zero.

In more complex models covariances tended to be more severely biased than variances. This difference was particularly salient in REML estimates, where under model 2, only covariances were substantially biased, and under model 3, all covariances were biased but only one variance was substantially biased. Coupling the high rates of bias observed in covariances with the rarity with which covariances are interpreted in psychological applications begs the question: why estimate unstructured covariance matrices. If in fact, variances are the sole parameters of interest to substantive researchers, and covariances are biased, would it not behoove researchers to simply eliminate covariances from estimation. Rates of non-convergence would also likely be aided by such a shift in parameterization. Moreover, this model is a testable model, whereas the unstructured matrix is not. Thus applied researchers could test whether they were justified in excluding covariances from estimation. It is likely the case that under such a variance component model, REML estimates for models with many random effects would exhibit even less bias than was observed in this simulation – simply because the parameters most likely to be biased would be eliminated from estimation.

Though specific hypotheses were posed and tested, the goal of the study was not to provide rules of thumb or make strong statements about the minimum sample size required in analyses using the linear mixed model. Though applied researchers often seek such guidance, and questions regarding minimum sufficient sample size to fit a model are often of singular and primary interest, there are far too many nuances involved in model fitting; from measurement error and distributional violations, to unknowable missing data mechanisms and sample selection problems to permit any meaningful or generalizable statement on minimally sufficient numbers of ISUs and observations per ISU required to obtain accurate point estimates. Applied researchers must keep these considerations in mind when applying these findings to their data or design, and should realize that these results are incapable of validating or canonizing a specific design or sample size. Rather these results provide researchers with information on what, over repeated sampling, the expected bias is across several feasible sample sizes, models, estimators, and data conditions.

With these caveats in mind, clear recommendations can be made to applied researchers whose data or designs correspond closely to those considered in this study. Use of restricted maximum likelihood for point estimation of linear mixed model parameters may yield dividends in finite samples that are not available under full maximum likelihood. Variances are generally easy to estimate, so long as the population values are large. Covariance are generally difficult to estimate, exhibiting higher degrees of bias; when population values are small, bias can be extreme. Based on the findings for covariances, if there is no compelling reason to estimate covariances, applied researchers may be well served by either not estimating or ignoring covariances. For simple models like the random effect ANOVA employed in model 1, primarily when REML is employed, researchers can obtain accurate point estimates of variance components with as few as 15 ISUs with an average of 10 observations per ISU, but only when population variance components are large. When population variance components are small, 15 ISUs are sufficient when an average of 40 or 80 observations are sampled per ISU, but 60 ISUs are required when an average of 10 observations are sampled per ISU, and 30 ISUs when an average of 20 observations are sampled per ISU.

For moderately complex models like the random effects regression model with saturated covariance structure considered in model 2, the minimally sufficient number of ISUs required before minimal bias is observed varies as a function of rates of convergence. For designs with reasonable convergence rates and large population covariance components (an untestable condition in applications), REML estimates of all parameters display negligible bias at the minimum sample sizes considered. When an average of 10 observations are sampled per ISU, 60 ISUs are required to obtain adequate point estimates. When an average of 20 observations are sampled per ISU, 30 ISUs are required to obtain adequate point estimates. When an average of 40 or 80 observations are sampled per ISU, 15 ISUs are required to obtain adequate point estimates. When population covariance components are small (again, an untestable condition in applications), the sample sizes associated with reasonable convergence rates are larger, and thus, minimal bias is associated with larger sample sizes. When an average of 10 observations are sampled per ISU, 120 ISUs are required to obtain adequate point estimates. When an average of 20 observations are sampled per ISU 30 ISUs are sufficient for variance estimates, but 60 ISUs are required for covariance estimates. When an average of 40 observations are sampled per ISU, 60 ISUs are adequate. When 80 observations are sampled per ISU, 30 ISUs are required to obtain good estimates of variances and covariances. Thus, for both large and small population covariance components, minimum sample sizes for which reasonable rates of model convergence can be observed are associated with acceptably low rates of bias, though the minimally sufficient sample sizes may differ between variances and covariances.

As with model 2, for complex models like the random effects regression model with saturated covariance structure, level 2 predictor, and cross-level interactions considered in model 3, the minimally sufficient number of ISUs required before minimal bias is observed varies as a function of rates of convergence. For designs with reasonable convergence rates, REML estimates of all parameters, except τ_{32}, display negligible bias at the minimum sample sizes considered. When an average of 10 observations are sampled per ISU, 60 ISUs are required to obtain adequate point estimates. When an average of 20 observations are sampled per ISU, 30 ISUs are required to obtain adequate point estimates, except for τ_{32}, which requires 60 ISUs. When an average of 40 observations are sampled per ISU, 30 ISUs are required to obtain adequate point estimates. When an average of 80 observations are sampled per ISU, 15 ISUs are required to obtain adequate point estimates. As with model 2, when population covariance component values are small, minimally sufficient sample sizes are greater. When an average of 10 observations are sampled per ISU, 60 ISUs are required, though all covariances, and τ_{33} require 120 ISUs. When an average of 20 observations are sampled per ISU, 60 ISUs are sufficient, except for τ_{21}, which requires 120 ISUs. When an average of 40 observations are sampled per ISU, 30 ISUs are sufficient for all parameters except τ_{32}, which requires 60 ISUs. When an average of 80 observations are sampled per ISU, 30 ISUs are sufficient for all parameters.

4.1 Limitations

4.1.1 Fixed Effects

Traditionally, problems with statistical inference for fixed effects have been associated with missing or unbalanced data and complex covariance structures. Under simple covariance structures, i.e. independence or compound symmetry models, inference is quite simple (Muller & Stewart, 2006). However, inference can be quite difficult for more complex models, such as time series and unstructured covariance patterns (Kenward & Roger, 1997; Schalje & Fellingham, 2001; Fai & Cornelius, 1996). While fixed effect point estimation was considered in this study, and found to be robust in finite samples, fixed effect inference was not evaluated, as this was beyond the scope of the project. However, the generality of the design implemented in this study lends itself to an examination of problems with fixed effect inference. This study examined two models with moderately large unstructured covariance patterns (models 2 and 3), and one with a compound symmetric pattern (model 1), contrasts across these two sets would permit tests of problems of inference associated with covariance pattern complexity. Unbalanced data was another central feature of the simulation design employed in this study. The design was intended to be general enough to apply to either cluster sampling or repeated measures designs, hence the use of the design-neutral ISU and observations per ISU terminology. Thus, little effort would be required to extend this design to include a manipulation of fixed effect inference. Though a body of excellent work exists on the topic of fixed effect inference (Kackar & Harville, 1984; Kenward & Roger, 1997; Prasad & Rao, 1990; Harville & Jeske, 1992; Schalje & Fellingham, 2001; Fai & Cornelius, 1996), none of these studies examined the models typically fit in psychological applications, nor those considered here. Future research would do well to study these issues more closely.

4.1.2 Generation of Unbalanced Data

one detailed limitation of this design was the sampling design that was used for generating unbalanced designs. The manner in which observations were sampled within ISUs invoked unequal sampling probabilities. Though the data adhere to concepts like observations missing at random (MAR), this is only within a given ISU, across ISUs observations are missing with unequal probabilities. Consider the cell with 15 ISUs: for the first five of these ISUs, observations have a probability of selection of 5/15; for the second five ISUs, observations have probabilities of selection of 10/15; and for the last five ISUs, observations have probabilities of selection of 1. Probability of selection varies as a function of which ISU observations come from, thus violating the assumption of a simple random sample. Thus, while the missingness mechanism is, in principle, MAR, the MAR is conditioned upon clusters of ISUs. A well known consequence of using mixed models in the presence of complex sampling designs is bias of the variance components. An additional consequence is shrinking of the standard errors of the fixed effects, which results in higher type I error rates (Kovacevic & Rai, 2003; Pfefferman, Skinner, Holmes, Goldstein, & Rasbash, 1998; Rabe-Hesketh & Skrondal, 2005). While the bias rates of the covariance components may have been affected by this, the impact is not necessarily quantifiable, given that expected bias rates for such models in the conditions examined do not exist. On the other hand, the impact of this potential bias would be obvious in the departure from nominal alpha rates of the fixed effect tests, had they been examined.

4.2 Future Directions

As previously stated, treatment of fixed effect inference was beyond the scope of this study. Fixed effect inference is integral to the use and importance of the linear mixed effect model. A logical and advantageous complement to this study would be the examination of fixed effect inference under the general models considered here. Such a study would likely benefit from the addition of a contrast between the performance of inference procedures under generalized covariance patterns – both classical time series and the unstructured patterns typically fit in psychological applications. Such a study would either need to use a different procedure for generating unbalanced data, or use two procedures, one of which was the current method. Use of the method used in this study along with another one would permit a contrast of the effect of complex sampling probabilities on inference for the fixed effects when compared to simple random sampling.

This study focussed on a properly specified linear mixed model conforming to the assumptions of the model. In practice, models fit in a sample rarely conform to a/the population generating process which produced the observed sample data. Data can be from an unknowable distribution, which we approximate with the normal distribution, or be misspecified in some way. Model misspecification is a complex issue. Traditionally, misspecification has been manipulated by either omission of parameters used to generate data, often referred to parametric misspecification. However, this procedure assumes that there is a model which, if fit, would correspond exactly to the population generating model. In reality, misspecification can be a function of any number of causes: nonlinear relationships, distributional violations, sampling complexities, informative missingness, parametric misspecification, etc, as well as all possible combinations of these factors. Unfortunately, positing that a generating model *could* be observed in a sample realization seems like a rather convoluted contrivance. Rather, it seems more consistent with what we believe about models (Box, 1979), to generate data under misspecifications where the misspecification is induced by non-parametric methods.

This work has been addressed in the covariance structure modeling framework (Cudeck & Browne, 1992). However, implementing the procedure proposed by Cudeck and Browne (1992) requires the development of two components established in covariance structure modeling but currently undefined for the linear mixed model. The Cudeck and Browne (1992) procedure requires a function for defining the discrepancy between a fitted and saturated model, which requires the definition of a saturated model; neither of which have been defined in the linear mixed model. I am currently working on the issue of saturated models and discrepancy function analogs for the linear mixed effect model. Results are promising but are restricted to testable structures in the covariance parameters, which necessarily excludes unstructured models – usually the models of interest in psychological applications. A logical future direction for this work would be to examine how findings change for point estimation under non-parametric misspecification. Results for such a study would be of greatest interest to researchers focussed on intensive longitudinal or time-series designs.

In order to maintain accurate statistical inference for the fixed effects and point estimation of the variance components, the conditional distribution of the response given the predictors must conform to the gaussian distribution. Though the Cudeck and Browne (1992) procedure may be useful for testing a wide array of unspecified model misspecifications, or a broadly defined model misspecification, it may not be useful in addressing the issue of deviations from distributional assumptions. In order to test deviations from normality, explicit manipulations of the degree of conformation to the gaussian distribution may be preferred to use of the Cudeck and Browne (1992) method. In order to determine the impact of violations of the gaussian assumption in fixed effect inference and variance component point estimation, future studies should consider such manipulations as an additional interesting facet for manipulation in the simulation design.

In sum, the linear mixed model (LMM) is an elegant and flexible method for estimating regression parameters adjusted for complex dependencies in data of both balanced and unbalanced or mistimed types. As with all models, the LMM is not without limitations. However, it is our view that, when the limitations are understood, the model's utility can be maximized. This study has attempted to elucidate the limitations of the model. Results indicate that applied researchers designing a cluster sampling or repeated measures study design will maximize the accuracy of covariance component estimates by sampling large numbers of ISUs, and that the minimally sufficient number of ISUs required to obtain good point estimates vary as a function of expected convergence rates for models, and parameter (variances or covariances). If balanced data can be collected, researchers are encouraged to do so, as this permits greater accuracy in variance estimates at smaller sample sizes. Thus, researches whose budgets would not permit sampling numbers of ISUs, could sample fewer ISUs with fewer observations per ISU if they can implement procedures to guarantee collected data will be balanced. Regardless of sampling design, researchers should exclusively employ REML in model estimation.

CHAPTER 5

Appendices

5.1 Appendix 1: Covariance Component PRB Tables

5.1.1 Model 1

Table 5.1: Positive Definite Solutions for Model 1 Comparing Percent Relative Bias for REML and FML Estimates of Covariance Parameters Across T1 and T2

					T1		**T2**	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
σ^2	1	1	48.86	48.86	2.80	2.81	2.57	2.40
σ^2	2	1	48.86	48.86	1.02	1.03	0.78	0.76
σ^2	3	1	48.86	48.86	0.75	0.75	0.51	0.52
σ^2	4	1	48.86	48.86	0.17	0.17	0.27	0.27
σ^2	1	2	48.86	48.86	0.98	0.98	1.07	1.09
σ^2	2	2	48.86	48.86	0.75	0.75	0.68	0.68
σ^2	3	2	48.86	48.86	0.38	0.38	0.31	0.31
σ^2	4	2	48.86	48.86	0.14	0.14	0.15	0.15
σ^2	1	3	48.86	48.86	0.80	0.80	0.66	0.66
σ^2	2	3	48.86	48.86	0.40	0.40	0.35	0.35
σ^2	3	3	48.86	48.86	0.06	0.06	0.22	0.22
σ^2	4	3	48.86	48.86	0.07	0.07	0.05	0.05

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Table 5.1 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
σ^2	1	4	48.86	48.86	0.37	0.37	0.26	0.26
σ^2	2	4	48.86	48.86	0.15	0.15	0.20	0.20
σ^2	3	4	48.86	48.86	0.08	0.08	0.11	0.11
σ^2	4	4	48.86	48.86	0.06	0.06	0.00	0.00
τ_{11}	1	1	12	4	-8.01	-17.24	-18.74	-30.32
τ_{11}	2	1	12	4	-4.34	-9.04	-10.99	-17.92
τ_{11}	3	1	12	4	-1.90	-4.28	-6.24	-9.94
τ_{11}	4	1	12	4	-1.12	-2.32	-2.83	-4.70
τ_{11}	1	2	12	4	-4.71	-12.64	-11.31	-21.61
τ_{11}	2	2	12	4	-2.72	-6.74	-6.24	-11.59
τ_{11}	3	2	12	4	-0.94	-2.98	-3.58	-6.29
τ_{11}	4	2	12	4	-0.34	-1.36	-1.67	-3.04
τ_{11}	1	3	12	4	-2.20	-9.50	-8.47	-16.87
τ_{11}	2	3	12	4	-1.41	-5.09	-3.85	-8.20
τ_{11}	3	3	12	4	-0.70	-2.55	-2.05	-4.25
τ_{11}	4	3	12	4	-0.25	-1.18	-0.79	-1.90
τ_{11}	1	4	12	4	-1.20	-8.18	-3.41	-11.03
τ_{11}	2	4	12	4	-0.75	-4.26	-1.74	-5.60
τ_{11}	3	4	12	4	-0.12	-1.89	-0.98	-2.92
τ_{11}	4	4	12	4	-0.22	-1.10	-0.29	-1.27

5.1.2 Model 2

Table 5.2: Positive Definite Solutions for Model 2 Comparing Percent Relative Bias for REML and FML Estimates of Covariance Parameters Across T1 and T2

					T1		**T2**	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
σ^2	15	$\bar{4}0$	46.58	.	0.77	0.72	.	.
σ^2	15	$\bar{8}0$	46.58	.	0.47	0.50	.	.
σ^2	30	$\bar{2}0$	46.58	46.58	0.74	0.78	0.67	0.59
σ^2	30	$\bar{4}0$	46.58	.	0.41	0.41	.	.
σ^2	30	$\bar{8}0$	46.58	46.58	0.13	0.14	0.14	0.15
σ^2	60	$\bar{1}0$	46.58	.	0.77	0.88	.	.
σ^2	60	$\bar{2}0$	46.58	46.58	0.50	0.50	0.31	0.29
σ^2	60	$\bar{4}0$	46.58	46.58	0.19	0.20	0.18	0.19
σ^2	60	$\bar{8}0$	46.58	46.58	0.01	0.01	0.15	0.16
σ^2	120	$\bar{1}0$	46.58	46.58	0.34	0.34	0.25	0.24
σ^2	120	$\bar{2}0$	46.58	46.58	0.15	0.15	0.25	0.26
σ^2	120	$\bar{4}0$	46.58	46.58	0.05	0.05	0.13	0.13
σ^2	120	$\bar{8}0$	46.58	46.58	0.05	0.05	0.07	0.07
τ_{11}	15	$\bar{4}0$	12	.	-4.70	-12.52	.	.
τ_{11}	15	$\bar{8}0$	12	.	-0.36	-10.52	.	.
τ_{11}	30	$\bar{2}0$	12	4	-2.03	-7.27	-7.20	-13.51
τ_{11}	30	$\bar{4}0$	12	.	0.14	-4.49	.	.
τ_{11}	30	$\bar{8}0$	12	4	0.21	-4.01	-0.54	-5.49
τ_{11}	60	$\bar{1}0$	12	.	-0.82	-4.22	.	.
τ_{11}	60	$\bar{2}0$	12	4	-0.83	-3.41	-1.92	-5.36
τ_{11}	60	$\bar{4}0$	12	4	-0.64	-2.92	-1.43	-4.29
τ_{11}	60	$\bar{8}0$	12	4	-0.48	-2.55	-0.29	-2.75
τ_{11}	120	$\bar{1}0$	12	4	-0.27	-1.86	-1.63	-4.11

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Table 5.2 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{11}	120	$\bar{2}0$	12	4	-1.06	-2.35	-1.96	-3.73
τ_{11}	120	$\bar{4}0$	12	4	-0.46	-1.59	-0.06	-1.50
τ_{11}	120	$\bar{8}0$	12	4	-0.13	-1.16	-0.53	-1.76
τ_{21}	15	$\bar{4}0$	4	.	-3.03	-14.85	.	.
τ_{21}	15	$\bar{8}0$	4	.	0.43	-9.86	.	.
τ_{21}	30	$\bar{2}0$	4	1	-0.86	-8.37	-4.78	-11.95
τ_{21}	30	$\bar{4}0$	4	.	2.94	-3.27	.	.
τ_{21}	30	$\bar{8}0$	4	1	0.82	-4.51	1.98	-6.03
τ_{21}	60	$\bar{1}0$	4	.	2.35	-2.80	.	.
τ_{21}	60	$\bar{2}0$	4	1	-0.05	-3.58	1.68	-4.95
τ_{21}	60	$\bar{4}0$	4	1	-0.38	-3.37	1.11	-3.75
τ_{21}	60	$\bar{8}0$	4	1	-0.41	-2.98	2.34	-1.57
τ_{21}	120	$\bar{1}0$	4	1	-0.30	-2.54	3.46	-0.94
τ_{21}	120	$\bar{2}0$	4	1	-0.08	-1.87	0.01	-3.08
τ_{21}	120	$\bar{4}0$	4	1	0.39	-1.10	1.66	-0.75
τ_{21}	120	$\bar{8}0$	4	1	0.05	-1.24	0.65	-1.29
τ_{22}	15	$\bar{4}0$	7	.	-1.52	-12.55	.	.
τ_{22}	15	$\bar{8}0$	7	.	-0.83	-7.70	.	.
τ_{22}	30	$\bar{2}0$	7	3	-1.03	-7.60	3.53	-2.54
τ_{22}	30	$\bar{4}0$	7	.	1.63	-3.59	.	.
τ_{22}	30	$\bar{8}0$	7	3	0.60	-3.94	0.36	-4.87
τ_{22}	60	$\bar{1}0$	7	.	-0.89	-4.73	.	.
τ_{22}	60	$\bar{2}0$	7	3	-0.89	-3.96	1.08	-3.06
τ_{22}	60	$\bar{4}0$	7	3	-0.25	-2.80	0.64	-2.51

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Table 5.2 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{22}	60	$\bar{80}$	7	3	-0.19	-2.42	0.45	-2.12
τ_{22}	120	$\bar{10}$	7	3	-0.73	-2.74	1.68	-1.12
τ_{22}	120	$\bar{20}$	7	3	0.46	-1.09	0.42	-1.63
τ_{22}	120	$\bar{40}$	7	3	0.51	-0.76	0.70	-0.87
τ_{22}	120	$\bar{80}$	7	3	-0.03	-1.14	0.43	-0.86
τ_{31}	15	$\bar{40}$	3	.	-0.85	-8.62	.	.
τ_{31}	15	$\bar{80}$	3	.	1.60	-7.00	.	.
τ_{31}	30	$\bar{20}$	3	0.9	0.46	-2.76	-12.23	-18.69
τ_{31}	30	$\bar{40}$	3	.	-0.84	-4.30	.	.
τ_{31}	30	$\bar{80}$	3	0.9	0.40	-3.04	-0.18	-3.64
τ_{31}	60	$\bar{10}$	3	.	0.37	0.82	.	.
τ_{31}	60	$\bar{20}$	3	0.9	1.14	-0.64	0.07	-2.67
τ_{31}	60	$\bar{40}$	3	0.9	-0.05	-1.79	2.32	0.43
τ_{31}	60	$\bar{80}$	3	0.9	0.14	-1.56	-1.82	-3.54
τ_{31}	120	$\bar{10}$	3	0.9	-0.40	-1.44	-3.19	-4.16
τ_{31}	120	$\bar{20}$	3	0.9	0.07	-0.85	-1.02	-1.98
τ_{31}	120	$\bar{40}$	3	0.9	0.57	-0.31	1.22	0.30
τ_{31}	120	$\bar{80}$	3	0.9	0.19	-0.66	1.38	0.49
τ_{32}	15	$\bar{40}$	1	.	5.86	-6.61	.	.
τ_{32}	15	$\bar{80}$	1	.	0.09	-9.99	.	.
τ_{32}	30	$\bar{20}$	1	0.3	-2.68	-6.95	55.20	38.83
τ_{32}	30	$\bar{40}$	1	.	-1.10	-4.74	.	.
τ_{32}	30	$\bar{80}$	1	0.3	0.46	-3.13	-5.79	-9.30
τ_{32}	60	$\bar{10}$	1	.	-0.91	-7.36	.	.

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Table 5.2 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{32}	60	$\bar{2}0$	1	0.3	6.32	4.13	-6.08	-8.92
τ_{32}	60	$\bar{4}0$	1	0.3	-3.80	-5.60	-1.98	-4.07
τ_{32}	60	$\bar{8}0$	1	0.3	0.99	-0.77	-5.74	-7.49
τ_{32}	120	$\bar{1}0$	1	0.3	-0.95	-2.14	-10.89	-13.92
τ_{32}	120	$\bar{2}0$	1	0.3	0.99	-0.04	-0.90	-2.04
τ_{32}	120	$\bar{4}0$	1	0.3	2.50	1.54	-0.48	-1.51
τ_{32}	120	$\bar{8}0$	1	0.3	1.41	0.52	0.39	-0.55
τ_{33}	15	$\bar{4}0$	4	.	1.27	-7.10	.	.
τ_{33}	15	$\bar{8}0$	4	.	-0.46	-7.63	.	.
τ_{33}	30	$\bar{2}0$	4	2	-1.59	-6.90	3.07	-4.62
τ_{33}	30	$\bar{4}0$	4	.	-0.27	-4.85	.	.
τ_{33}	30	$\bar{8}0$	4	2	-0.57	-4.51	-0.89	-5.40
τ_{33}	60	$\bar{1}0$	4	.	3.40	1.59	.	.
τ_{33}	60	$\bar{2}0$	4	2	-0.64	-3.44	-0.21	-3.92
τ_{33}	60	$\bar{4}0$	4	2	0.72	-1.58	0.25	-2.61
τ_{33}	60	$\bar{8}0$	4	2	0.26	-1.71	-0.79	-3.03
τ_{33}	120	$\bar{1}0$	4	2	1.39	-0.71	2.88	0.29
τ_{33}	120	$\bar{2}0$	4	2	-1.09	-2.54	0.55	-1.45
τ_{33}	120	$\bar{4}0$	4	2	0.50	-0.64	1.04	-0.38
τ_{33}	120	$\bar{8}0$	4	2	-0.68	-1.66	0.11	-1.02

5.1.3 Balanced Model 2

Table 5.3: Balanced Positive Definite Solutions for Model 2 Comparing Percent Relative Bias (PRB) for REML and FML Estimates of Covariance Parameters Across T1 and T2

					T1 PRB		**T2 PRB**	
Parm	**OBS**	**ISU**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
σ^2	2	1	46.58	46.58	1.61	1.59	1.12	1.23
σ^2	3	1	46.58	46.58	0.95	0.95	0.63	0.57
σ^2	4	1	46.58	46.58	0.43	0.43	0.4	0.4
σ^2	1	2	46.58	46.58	1.58	1.56	1.53	1.53
σ^2	2	2	46.58	46.58	0.77	0.77	0.81	0.8
σ^2	3	2	46.58	46.58	0.36	0.36	0.39	0.39
σ^2	4	2	46.58	46.58	0.23	0.23	0.24	0.24
σ^2	1	3	46.58	46.58	0.88	0.88	0.81	0.81
σ^2	2	3	46.58	46.58	0.45	0.45	0.4	0.4
σ^2	3	3	46.58	46.58	0.18	0.18	0.2	0.2
σ^2	4	3	46.58	46.58	0.09	0.09	0.09	0.09
σ^2	1	4	46.58	46.58	0.41	0.41	0.4	0.4
σ^2	2	4	46.58	46.58	0.18	0.18	0.2	0.2
σ^2	3	4	46.58	46.58	0.09	0.09	0.1	0.1
σ^2	4	4	46.58	46.58	0.06	0.06	0.06	0.06
τ_{11}	2	1	12	4	-4.38	-8.48	-13	-17.7
τ_{11}	3	1	12	4	-2.27	-4.35	-5.87	-8.51
τ_{11}	4	1	12	4	-1.04	-2.09	-3.6	-5.07
τ_{11}	1	2	12	4	-4.64	-11.87	-13.98	-22.48
τ_{11}	2	2	12	4	-2.16	-5.86	-6.69	-11.13
τ_{11}	3	2	12	4	-1.11	-2.98	-3.45	-5.72
τ_{11}	4	2	12	4	-0.57	-1.51	-2.19	-3.33
τ_{11}	1	3	12	4	-2.52	-9.46	-6.93	-14.46

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Table 5.3 – continued from previous page

					T1 PRB		T2 PRB	
Parm	**OBS**	**ISU**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{11}	2	3	12	4	-1.16	-4.68	-3.34	-7.22
τ_{11}	3	3	12	4	-0.59	-2.36	-1.68	-3.65
τ_{11}	4	3	12	4	-0.26	-1.15	-0.74	-1.73
τ_{11}	1	4	12	4	-1.22	-8.03	-3.41	-10.5
τ_{11}	2	4	12	4	-0.54	-3.97	-1.74	-5.34
τ_{11}	3	4	12	4	-0.26	-1.97	-0.92	-2.73
τ_{11}	4	4	12	4	-0.15	-1.01	-0.42	-1.33
τ_{21}	2	1	4	1	1.89	-1.61	-10.07	-10.46
τ_{21}	3	1	4	1	-0.48	-2.14	3.18	0.78
τ_{21}	4	1	4	1	-0.63	-1.46	0.86	0.02
τ_{21}	1	2	4	1	-1.2	-7.85	-8.69	-19.9
τ_{21}	2	2	4	1	-0.47	-3.74	0.21	-3.17
τ_{21}	3	2	4	1	0.09	-1.57	-0.58	-2.24
τ_{21}	4	2	4	1	0.37	-0.46	-0.31	-1.14
τ_{21}	1	3	4	1	-1.11	-7.7	-2.67	-9.11
τ_{21}	2	3	4	1	0.27	-3.07	-0.05	-3.39
τ_{21}	3	3	4	1	0.38	-1.29	0.68	-0.99
τ_{21}	4	3	4	1	-0.31	-1.14	0.18	-0.66
τ_{21}	1	4	4	1	-0.74	-7.36	-1	-7.6
τ_{21}	2	4	4	1	-0.13	-3.46	-1.46	-4.74
τ_{21}	3	4	4	1	0.05	-1.61	-0.41	-2.07
τ_{21}	4	4	4	1	0	-0.84	0.42	-0.41
τ_{22}	2	1	7	3	1.92	-2.87	10.33	0.67
τ_{22}	3	1	7	3	-0.75	-3.18	0.59	-2.68

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Table 5.3 – continued from previous page

					T1 PRB		T2 PRB	
Parm	**OBS**	**ISU**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{22}	4	1	7	3	-0.42	-1.64	0.89	-0.85
τ_{22}	1	2	7	3	-0.45	-8.75	1.71	-11.11
τ_{22}	2	2	7	3	0.43	-3.64	1.78	-3.48
τ_{22}	3	2	7	3	0.44	-1.62	0.18	-2.37
τ_{22}	4	2	7	3	0.33	-0.69	-0.84	-2.11
τ_{22}	1	3	7	3	-0.26	-7.66	1.41	-6.92
τ_{22}	2	3	7	3	0.47	-3.26	0.31	-3.91
τ_{22}	3	3	7	3	0.54	-1.33	-0.23	-2.33
τ_{22}	4	3	7	3	-0.2	-1.12	0.05	-1
τ_{22}	1	4	7	3	-0.44	-7.45	0.35	-7.21
τ_{22}	2	4	7	3	-0.37	-3.87	-0.19	-3.95
τ_{22}	3	4	7	3	0.11	-1.65	-0.22	-2.1
τ_{22}	4	4	7	3	0.01	-0.87	-0.18	-1.12
τ_{31}	2	1	3	0.9	1.55	-2.05	-3.21	-9.47
τ_{31}	3	1	3	0.9	0.24	-1.44	2.76	-0.07
τ_{31}	4	1	3	0.9	-0.61	-1.45	-1.57	-2.41
τ_{31}	1	2	3	0.9	0.7	-6.06	-11.06	-9.47
τ_{31}	2	2	3	0.9	1.06	-2.31	-0.45	-3.78
τ_{31}	3	2	3	0.9	0.5	-1.18	-1.21	-2.86
τ_{31}	4	2	3	0.9	0.24	-0.59	0.84	-0.01
τ_{31}	1	3	3	0.9	0.75	-5.97	1.8	-5.11
τ_{31}	2	3	3	0.9	0.19	-3.15	2.12	-1.28
τ_{31}	3	3	3	0.9	-0.37	-2.03	-1.05	-2.7
τ_{31}	4	3	3	0.9	-0.53	-1.36	1.34	0.49

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Table 5.3 – continued from previous page

					T1 PRB		T2 PRB	
Parm	**OBS**	**ISU**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{31}	1	4	3	0.9	-0.54	-7.18	-1.44	-8.02
τ_{31}	2	4	3	0.9	0.23	-3.11	1.4	-1.99
τ_{31}	3	4	3	0.9	0.52	-1.16	-0.45	-2.11
τ_{31}	4	4	3	0.9	-0.37	-1.2	-0.35	-1.18
τ_{32}	2	1	1	0.3	8.39	5.32	-18.01	-1.83
τ_{32}	3	1	1	0.3	-2.82	-4.45	5.71	4.46
τ_{32}	4	1	1	0.3	-3.92	-4.73	4.16	3.28
τ_{32}	1	2	1	0.3	-4.22	-10.57	-1.21	-29.64
τ_{32}	2	2	1	0.3	1.09	-2.18	5.01	0.16
τ_{32}	3	2	1	0.3	-2.44	-4.07	-2.66	-4.26
τ_{32}	4	2	1	0.3	0.9	0.06	4.1	3.23
τ_{32}	1	3	1	0.3	-1.82	-8.36	-1.52	-8.82
τ_{32}	2	3	1	0.3	-1.21	-4.5	-3.26	-6.5
τ_{32}	3	3	1	0.3	-0.44	-2.1	4.61	2.87
τ_{32}	4	3	1	0.3	0.32	-0.51	-2.31	-3.13
τ_{32}	1	4	1	0.3	-0.2	-6.86	0.02	-6.68
τ_{32}	2	4	1	0.3	-1.67	-4.95	-2.44	-5.71
τ_{32}	3	4	1	0.3	0.27	-1.41	-1.8	-3.44
τ_{32}	4	4	1	0.3	-0.77	-1.6	-0.23	-1.07
τ_{33}	2	1	4	2	1.39	-4.68	15.67	5.16
τ_{33}	3	1	4	2	-1.4	-4.62	1.5	-2.05
τ_{33}	4	1	4	2	0.01	-1.59	0.11	-2.21
τ_{33}	1	2	4	2	0.6	-8.54	13.33	4.5
τ_{33}	2	2	4	2	0.49	-4.27	1.09	-4.65

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Table 5.3 – continued from previous page

					T1 PRB		T2 PRB	
Parm	**OBS**	**ISU**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{33}	3	2	4	2	0.62	-1.78	-0.94	-4.01
τ_{33}	4	2	4	2	0.32	-0.88	0.46	-1.08
τ_{33}	1	3	4	2	-0.66	-8.67	1.02	-8.25
τ_{33}	2	3	4	2	-0.83	-4.82	-0.84	-5.52
τ_{33}	3	3	4	2	0.27	-1.74	-0.69	-3.02
τ_{33}	4	3	4	2	-0.15	-1.16	0.22	-0.95
τ_{33}	1	4	4	2	0.17	-7.17	0.23	-7.78
τ_{33}	2	4	4	2	-0.22	-3.88	0.6	-3.42
τ_{33}	3	4	4	2	0.31	-1.53	0.03	-1.97
τ_{33}	4	4	4	2	-0.11	-1.03	-0.06	-1.05

5.1.4 Model 3

Table 5.4: Positive Definite Solutions for Model 3 Comparing Percent Relative Bias for REML and FML Estimates of Covariance Parameters Across T1 and T2

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
σ^2	15	$\bar{8}0$	46.58	.	0.42	0.49	.	.
σ^2	30	$\bar{2}0$	46.58	.	0.82	0.92	.	.
σ^2	30	$\bar{4}0$	46.58	46.58	0.57	0.55	0.39	0.36
σ^2	30	$\bar{8}0$	46.58	46.58	0.29	0.28	0.20	0.18
σ^2	60	$\bar{1}0$	46.58	46.58	0.85	0.76	-0.35	-0.53
σ^2	60	$\bar{2}0$	46.58	46.58	0.31	0.27	0.51	0.48

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Table 5.4 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
σ^2	60	$\bar{40}$	46.58	46.58	0.31	0.29	0.27	0.25
σ^2	60	$\bar{80}$	46.58	46.58	0.14	0.13	0.08	0.07
σ^2	120	$\bar{10}$	46.58	46.58	0.56	0.48	0.17	0.08
σ^2	120	$\bar{20}$	46.58	46.58	0.18	0.15	0.26	0.23
σ^2	120	$\bar{40}$	46.58	46.58	0.08	0.06	0.14	0.13
σ^2	120	$\bar{80}$	46.58	46.58	0.07	0.07	0.07	0.06
τ_{11}	15	$\bar{80}$	12	.	3.23	-13.70	.	.
τ_{11}	30	$\bar{20}$	12	.	-3.65	-12.66	.	.
τ_{11}	30	$\bar{40}$	12	4	-1.13	-9.22	-3.45	-13.29
τ_{11}	30	$\bar{80}$	12	4	1.11	-6.59	0.11	-8.65
τ_{11}	60	$\bar{10}$	12	4	-3.77	-8.88	-4.58	-12.31
τ_{11}	60	$\bar{20}$	12	4	-2.37	-6.73	-5.98	-11.78
τ_{11}	60	$\bar{40}$	12	4	-0.90	-4.79	-3.17	-7.90
τ_{11}	60	$\bar{80}$	12	4	1.10	-2.61	-2.17	-6.27
τ_{11}	120	$\bar{10}$	12	4	-3.14	-5.58	-6.31	-10.07
τ_{11}	120	$\bar{20}$	12	4	-0.82	-2.94	-3.37	-6.19
τ_{11}	120	$\bar{40}$	12	4	-0.73	-2.62	-1.42	-3.73
τ_{11}	120	$\bar{80}$	12	4	-0.00	-1.81	-0.88	-2.88
τ_{21}	15	$\bar{80}$	4	.	-0.64	-17.86	.	.
τ_{21}	30	$\bar{20}$	4	.	-8.26	-16.56	.	.
τ_{21}	30	$\bar{40}$	4	1	-4.54	-13.89	-9.81	-24.07
τ_{21}	30	$\bar{80}$	4	1	-0.69	-9.24	-4.61	-16.51
τ_{21}	60	$\bar{10}$	4	1	-9.76	-15.79	-17.90	-14.91
τ_{21}	60	$\bar{20}$	4	1	-5.21	-10.28	-12.63	-21.02

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Table 5.4 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{21}	60	$\bar{4}0$	4	1	-4.14	-8.43	-8.09	-14.50
τ_{21}	60	$\bar{8}0$	4	1	0.30	-3.69	-6.45	-11.52
τ_{21}	120	$\bar{1}0$	4	1	-5.92	-8.76	-9.27	-13.53
τ_{21}	120	$\bar{2}0$	4	1	-2.14	-4.50	-6.10	-9.85
τ_{21}	120	$\bar{4}0$	4	1	-2.05	-4.09	-6.09	-9.02
τ_{21}	120	$\bar{8}0$	4	1	-1.17	-3.06	-4.63	-6.98
τ_{22}	15	$\bar{8}0$	7	.	2.72	-13.39	.	.
τ_{22}	30	$\bar{2}0$	7	.	-1.15	-10.29	.	.
τ_{22}	30	$\bar{4}0$	7	3	0.58	-8.61	0.18	-11.21
τ_{22}	30	$\bar{8}0$	7	3	2.23	-5.99	1.20	-8.36
τ_{22}	60	$\bar{1}0$	7	3	-2.51	-9.30	9.48	5.34
τ_{22}	60	$\bar{2}0$	7	3	-0.90	-6.13	-1.17	-8.50
τ_{22}	60	$\bar{4}0$	7	3	-1.45	-5.77	-0.53	-5.94
τ_{22}	60	$\bar{8}0$	7	3	0.81	-3.12	-0.16	-4.61
τ_{22}	120	$\bar{1}0$	7	3	-2.65	-5.90	-1.25	-5.36
τ_{22}	120	$\bar{2}0$	7	3	-0.70	-3.20	-1.15	-4.55
τ_{22}	120	$\bar{4}0$	7	3	-0.30	-2.42	-1.33	-3.93
τ_{22}	120	$\bar{8}0$	7	3	0.11	-1.81	-1.10	-3.26
τ_{31}	15	$\bar{8}0$	3	.	5.31	-10.03	.	.
τ_{31}	30	$\bar{2}0$	3	.	-1.85	-5.31	.	.
τ_{31}	30	$\bar{4}0$	3	0.9	2.63	-4.40	-0.69	-8.36
τ_{31}	30	$\bar{8}0$	3	0.9	3.01	-3.98	2.24	-5.08
τ_{31}	60	$\bar{1}0$	3	0.9	-4.54	-8.06	-20.48	-24.75
τ_{31}	60	$\bar{2}0$	3	0.9	0.81	-2.76	-2.74	-7.49

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Table 5.4 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{31}	60	$\bar{40}$	3	0.9	1.14	-2.32	1.15	-2.40
τ_{31}	60	$\bar{80}$	3	0.9	1.26	-2.17	1.06	-2.45
τ_{31}	120	$\bar{10}$	3	0.9	-0.30	-2.21	-5.42	-7.55
τ_{31}	120	$\bar{20}$	3	0.9	-0.39	-2.14	0.31	-1.63
τ_{31}	120	$\bar{40}$	3	0.9	0.07	-1.64	1.27	-0.49
τ_{31}	120	$\bar{80}$	3	0.9	0.70	-1.00	1.14	-0.59
τ_{32}	15	$\bar{80}$	1	.	1.69	-18.78	.	.
τ_{32}	30	$\bar{20}$	1	.	-12.90	-14.60	.	.
τ_{32}	30	$\bar{40}$	1	0.3	4.99	-2.54	-16.20	-24.10
τ_{32}	30	$\bar{80}$	1	0.3	3.56	-3.65	-7.45	-15.03
τ_{32}	60	$\bar{10}$	1	0.3	-3.66	-7.73	-73.54	-81.14
τ_{32}	60	$\bar{20}$	1	0.3	2.62	-1.31	-2.99	-10.82
τ_{32}	60	$\bar{40}$	1	0.3	-0.63	-4.14	-3.19	-6.94
τ_{32}	60	$\bar{80}$	1	0.3	2.09	-1.45	-0.02	-3.68
τ_{32}	120	$\bar{10}$	1	0.3	-2.22	-4.48	-14.10	-15.82
τ_{32}	120	$\bar{20}$	1	0.3	-1.15	-2.99	-5.02	-7.19
τ_{32}	120	$\bar{40}$	1	0.3	1.31	-0.47	-0.29	-2.15
τ_{32}	120	$\bar{80}$	1	0.3	0.00	-1.75	1.46	-0.35
τ_{33}	15	$\bar{80}$	4	.	6.88	-11.16	.	.
τ_{33}	30	$\bar{20}$	4	.	2.74	-5.89	.	.
τ_{33}	30	$\bar{40}$	4	2	2.17	-6.78	2.50	-8.25
τ_{33}	30	$\bar{80}$	4	2	2.79	-5.13	1.31	-7.48
τ_{33}	60	$\bar{10}$	4	2	9.05	0.78	14.21	6.28
τ_{33}	60	$\bar{20}$	4	2	2.43	-3.10	1.41	-5.36

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Table 5.4 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{33}	60	$\bar{40}$	4	2	1.99	-2.44	1.67	-3.68
τ_{33}	60	$\bar{80}$	4	2	1.45	-2.45	1.95	-2.44
τ_{33}	120	$\bar{10}$	4	2	-0.76	-4.46	3.97	-1.37
τ_{33}	120	$\bar{20}$	4	2	-0.40	-3.10	-0.22	-3.75
τ_{33}	120	$\bar{40}$	4	2	0.39	-1.79	1.49	-1.17
τ_{33}	120	$\bar{80}$	4	2	0.72	-1.21	0.57	-1.59

5.2 Appendix 1a: Fixed Effect Graphical Results

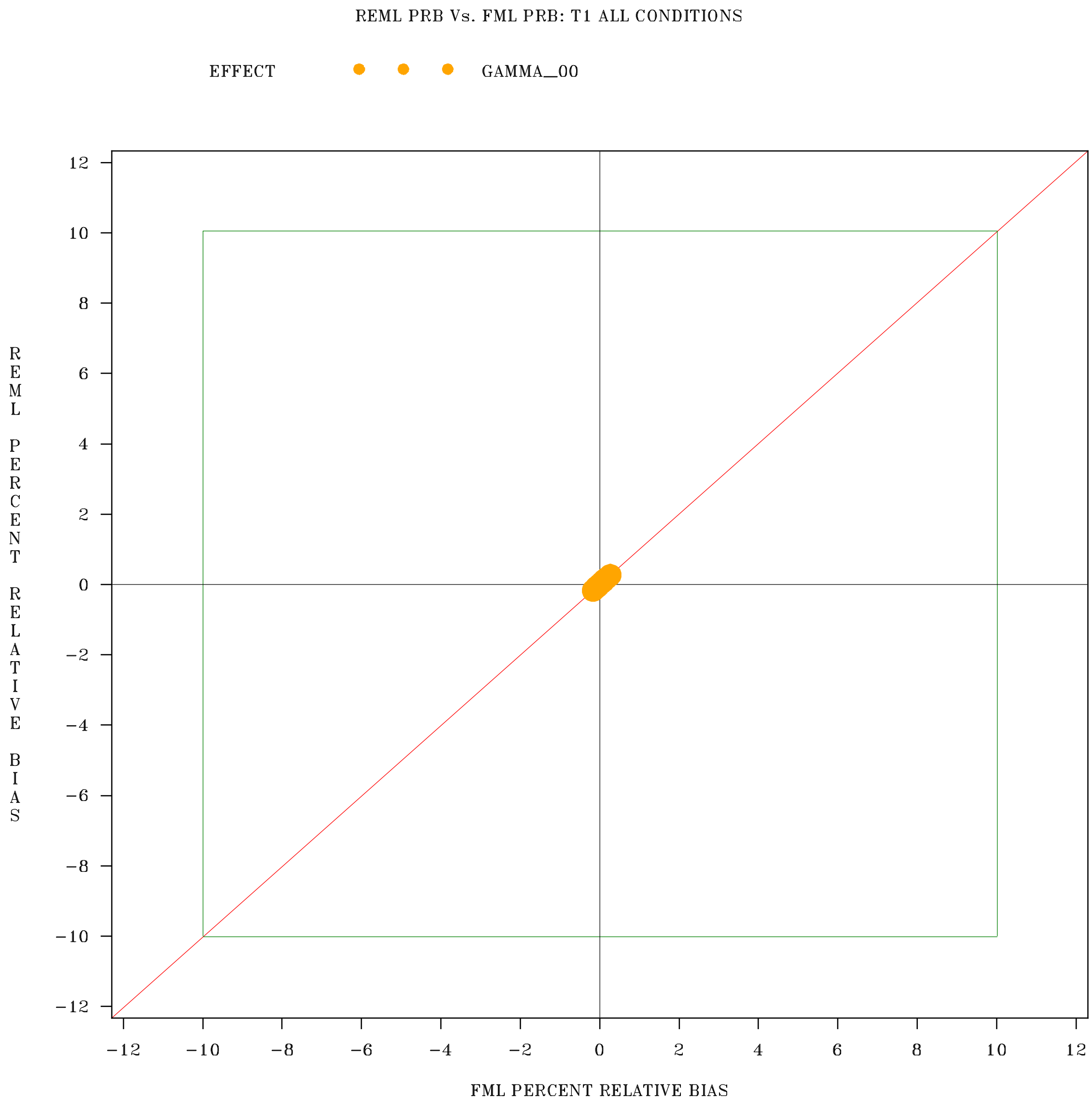

Figure 5.1: Fixed Effect PRB Model 1 T1 REML & FML

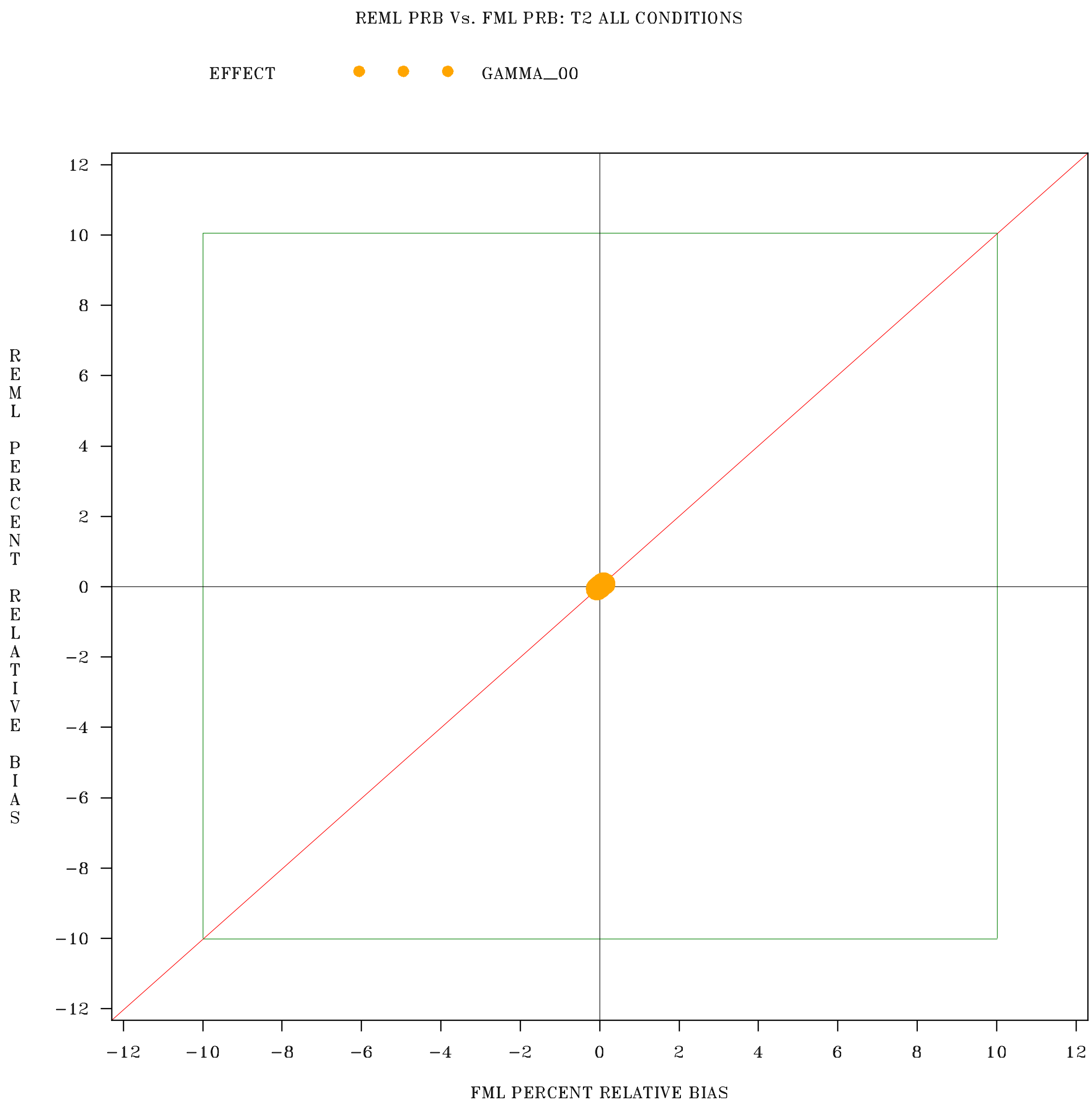

Figure 5.2: Fixed Effect PRB Model 1 T2 REML & FML

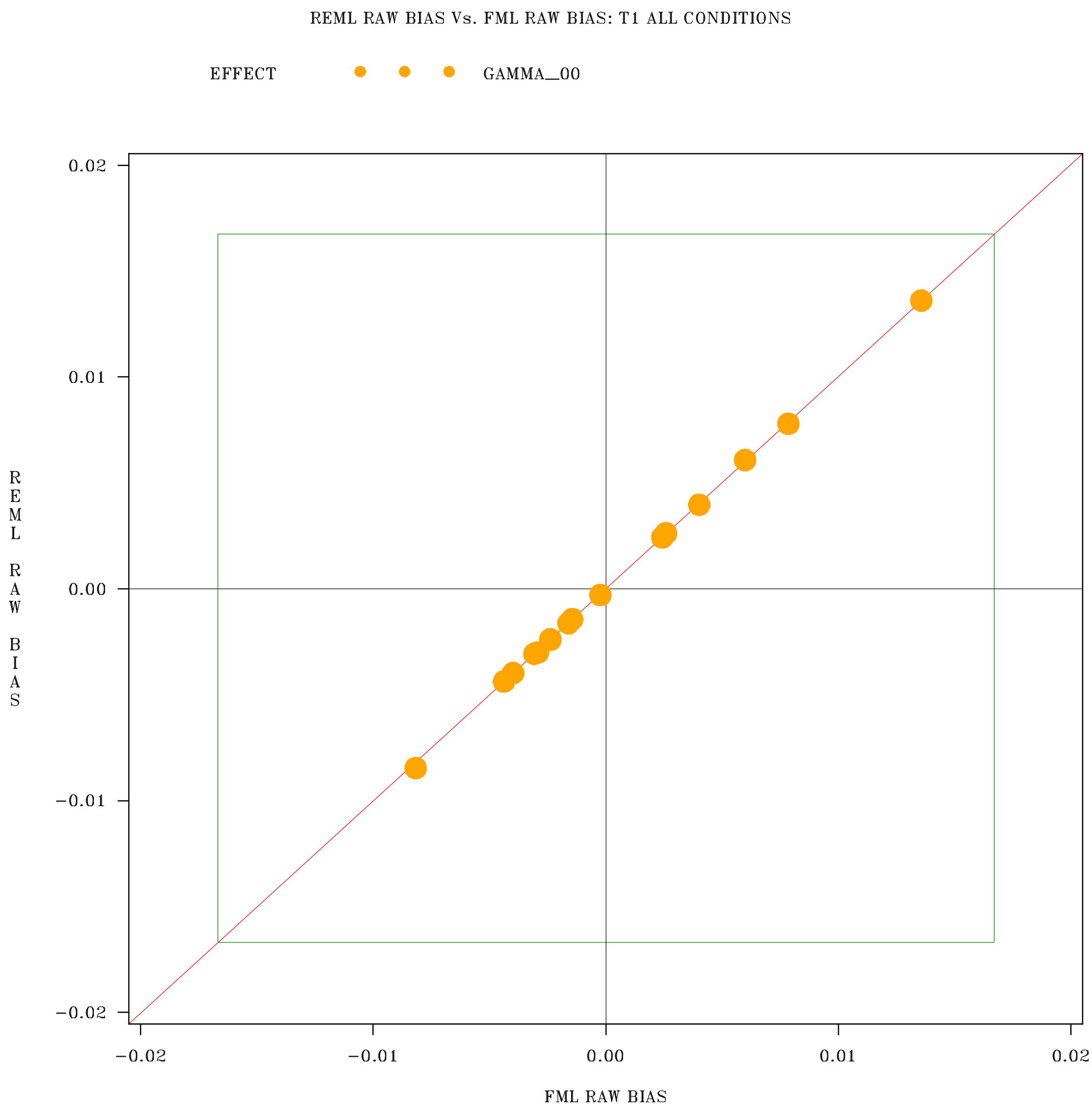

Figure 5.3: Fixed Effect RAW BIAS Model 1 T1 REML & FML

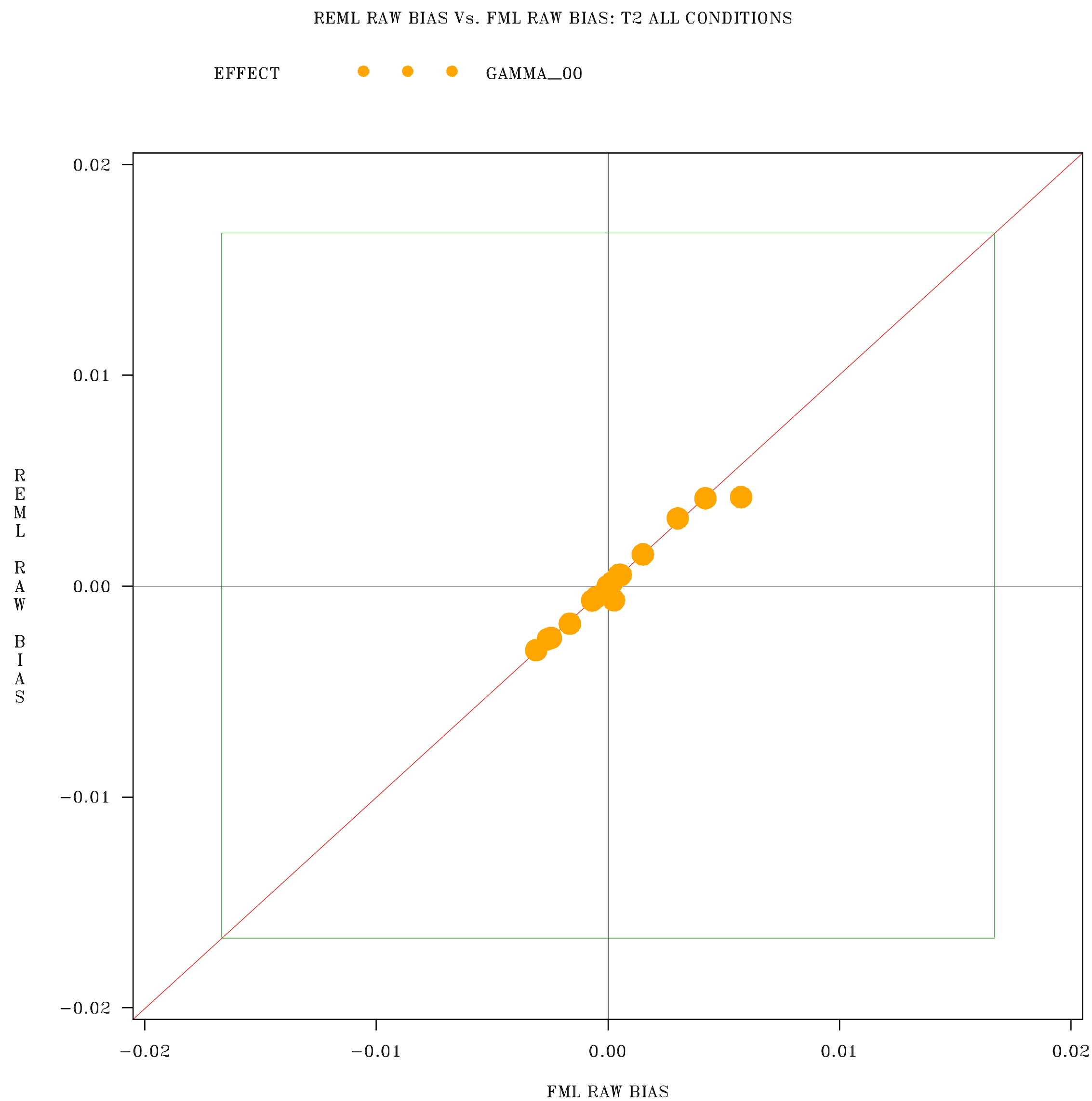

Figure 5.4: Fixed Effect RAW BIAS Model 1 T2 REML & FML

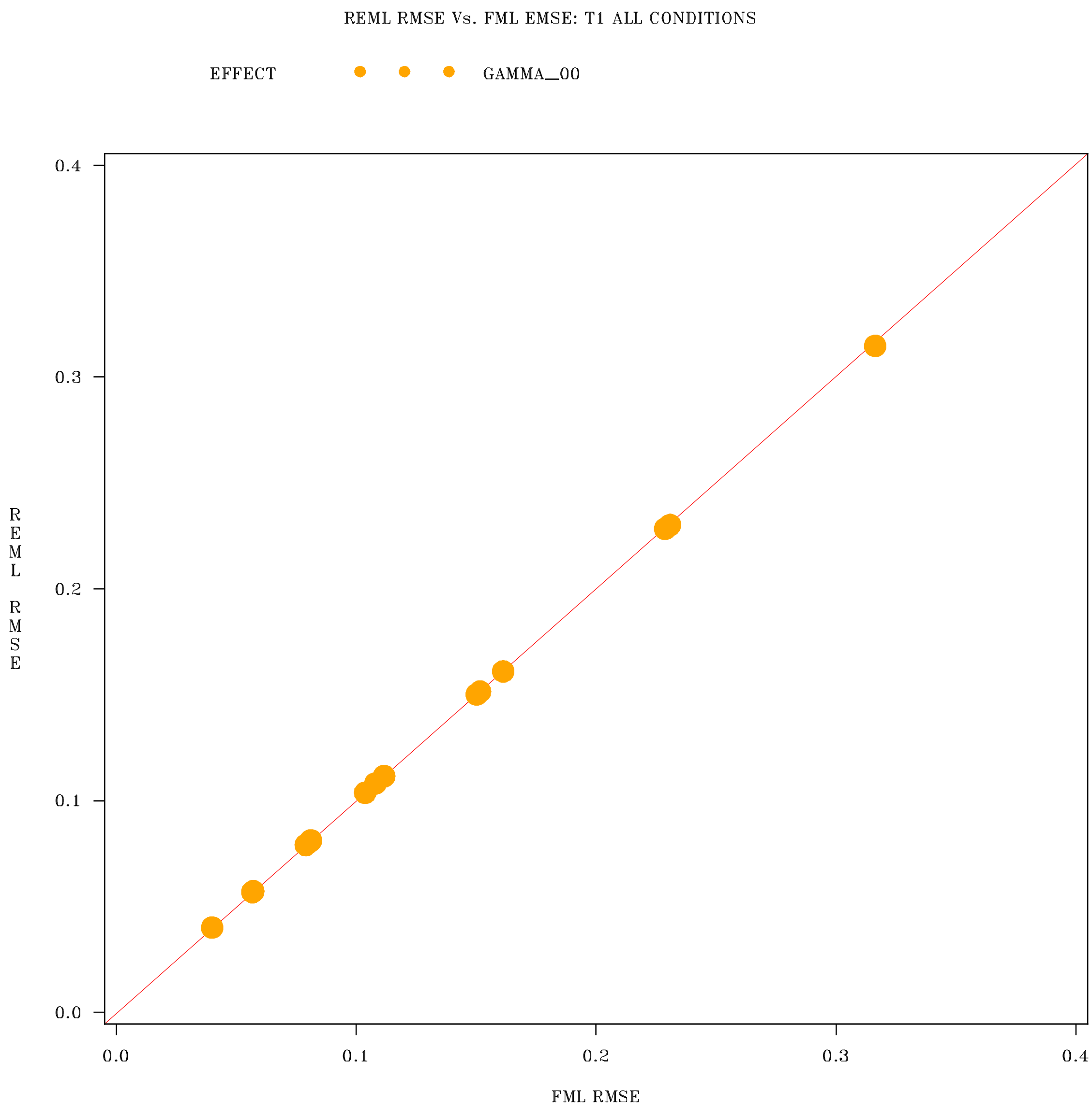

Figure 5.5: Fixed Effect RMSE Model 1 T1 REML & FML

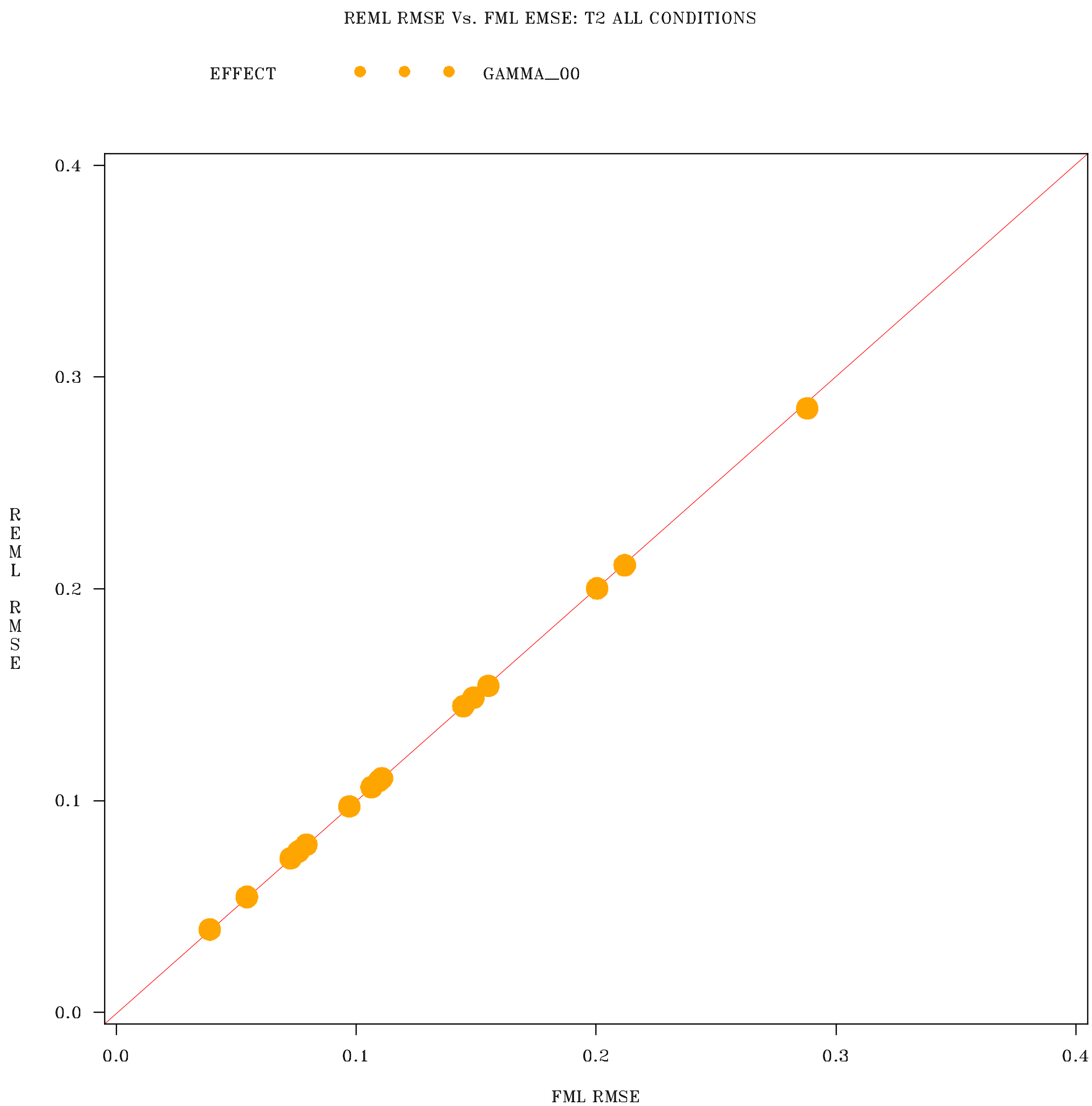

Figure 5.6: Fixed Effect RMSE Model 1 T2 REML & FML

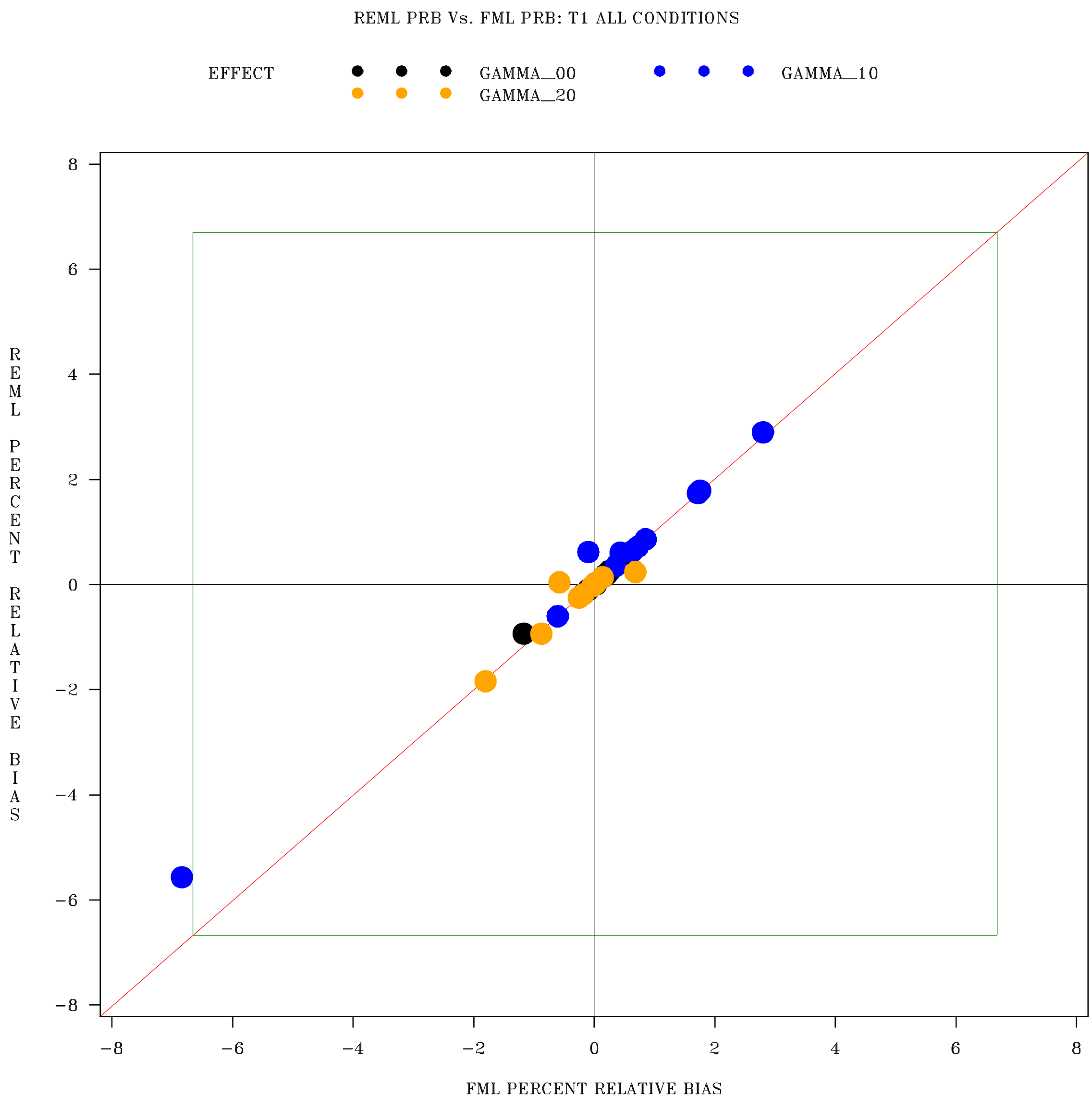

Figure 5.7: Fixed Effect PRB Model 2 T1 REML & FML

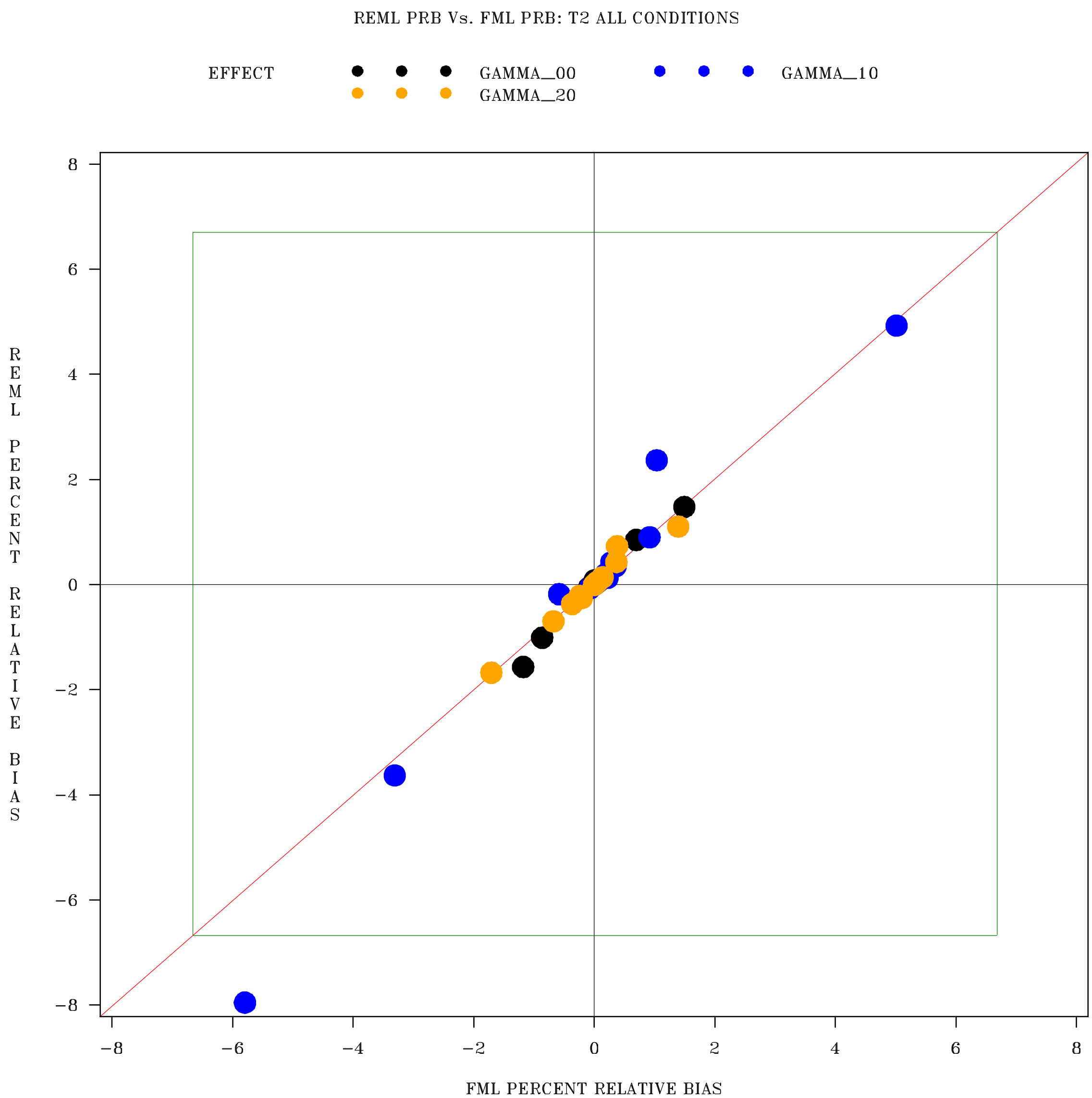

Figure 5.8: Fixed Effect PRB Model 2 T2 REML & FML

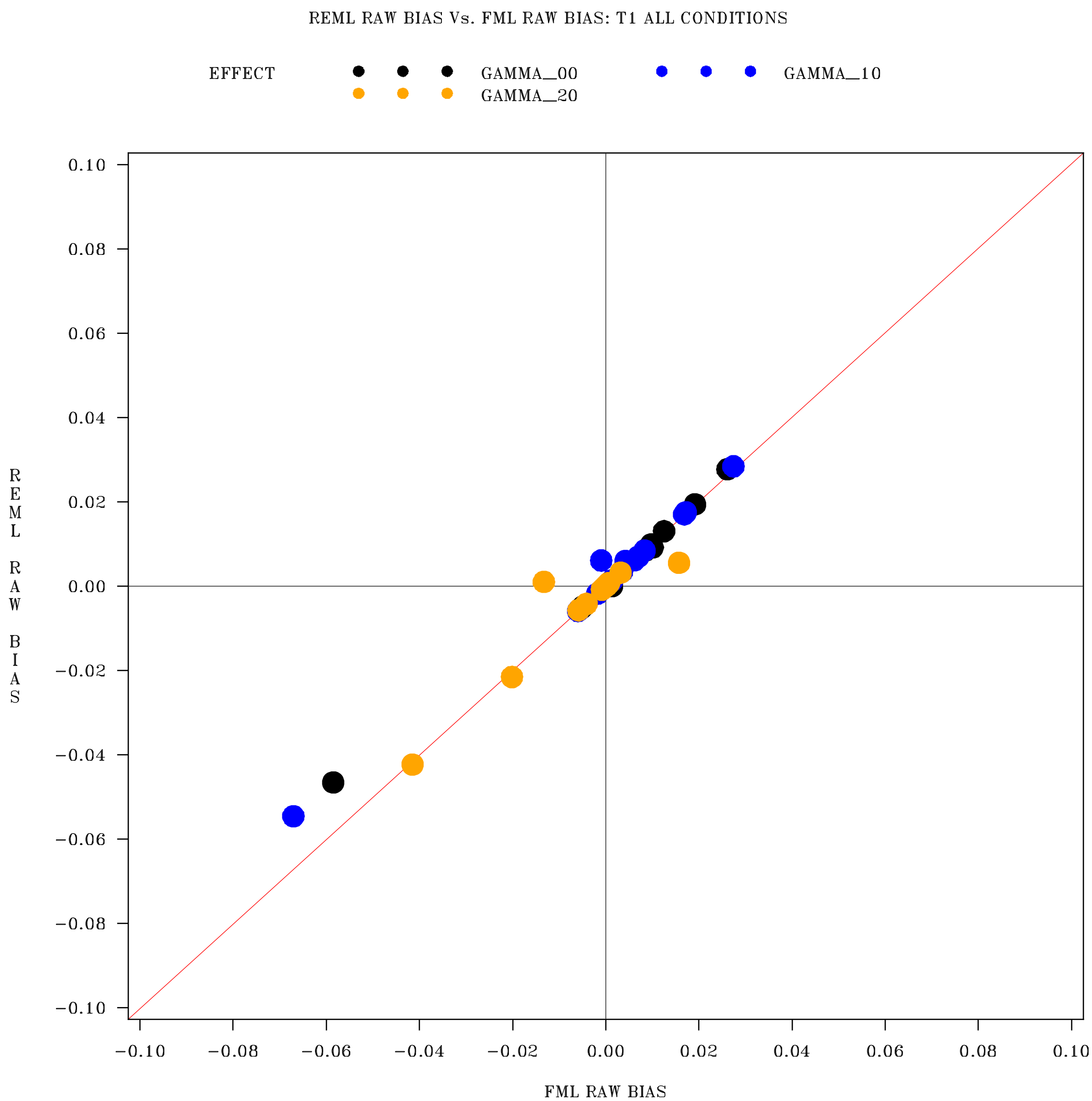

Figure 5.9: Fixed Effect RAW BIAS Model 2 T1 REML & FML

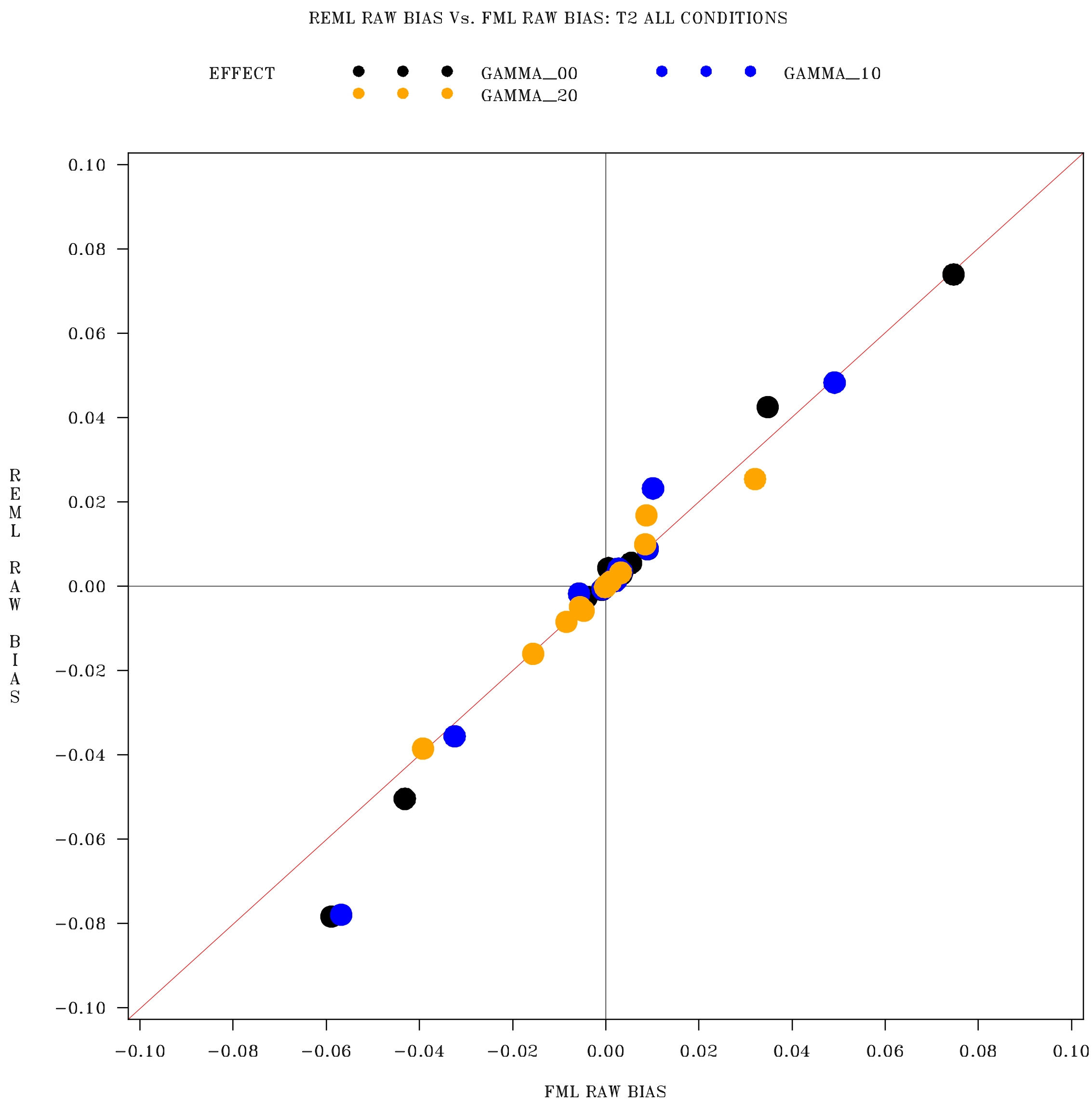

Figure 5.10: Fixed Effect RAW BIAS Model 2 T2 REML & FML

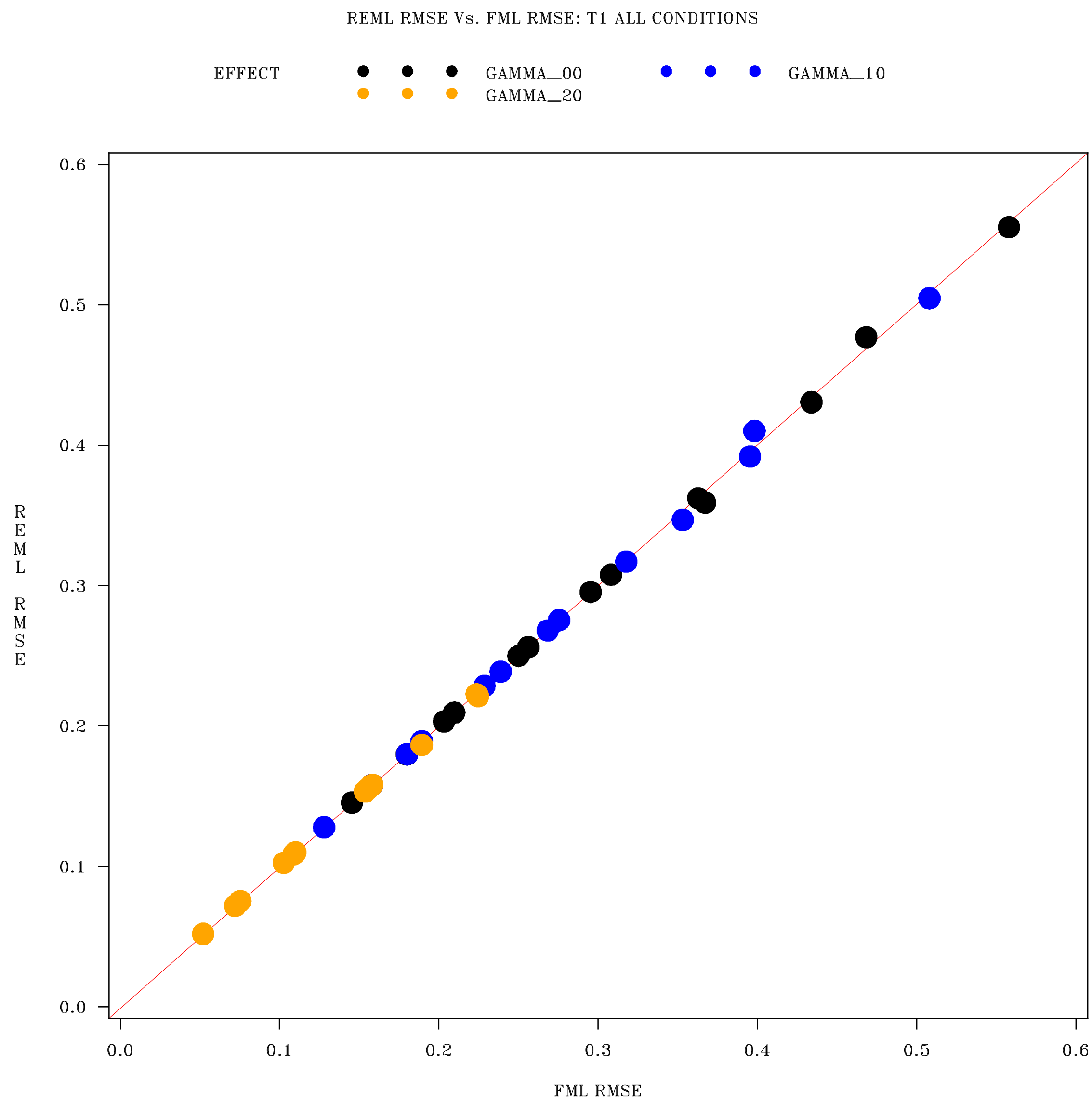

Figure 5.11: Fixed Effect RMSE Model 2 T1 REML & FML

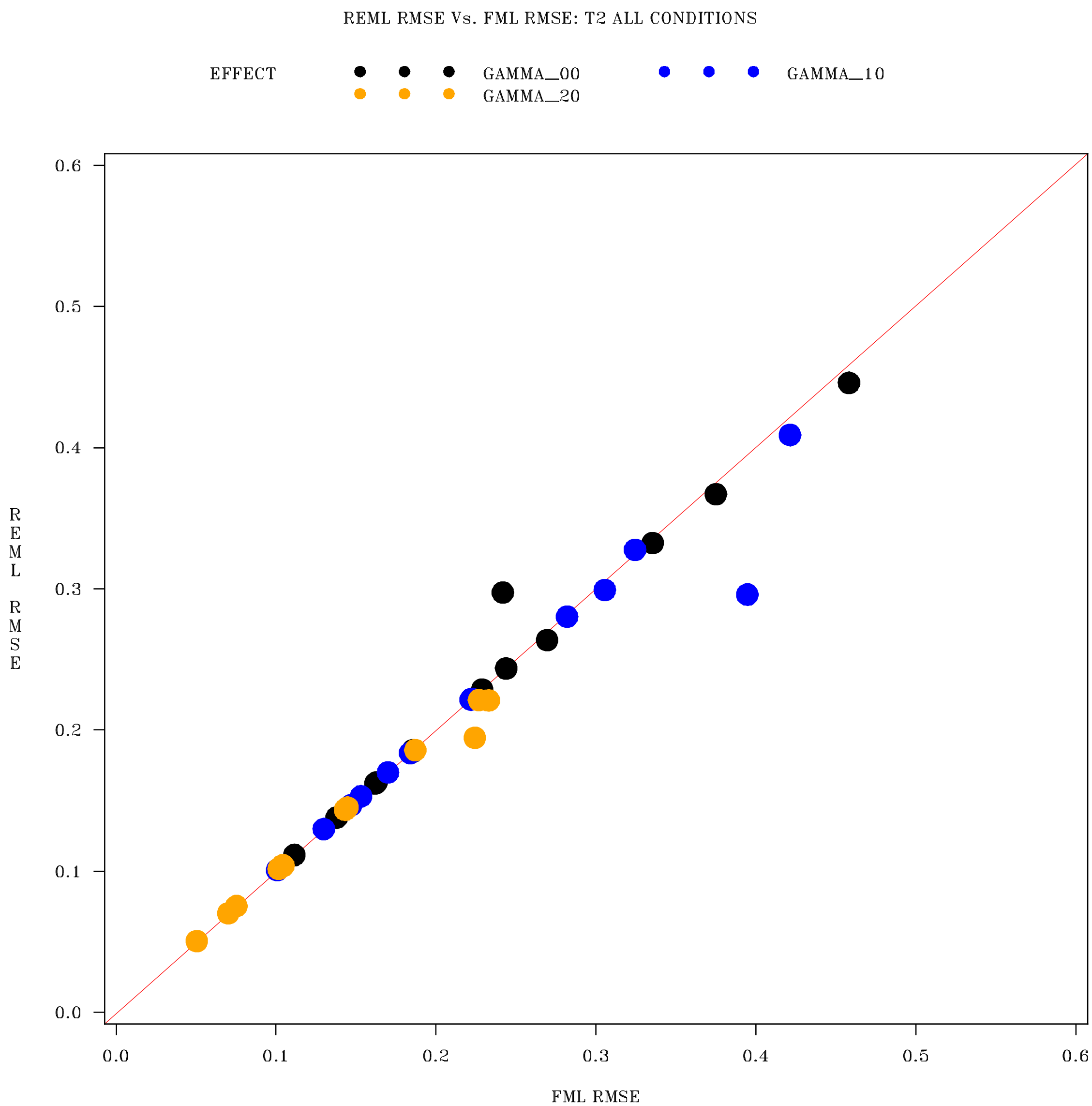

Figure 5.12: Fixed Effect RMSE Model 2 T2 REML & FML

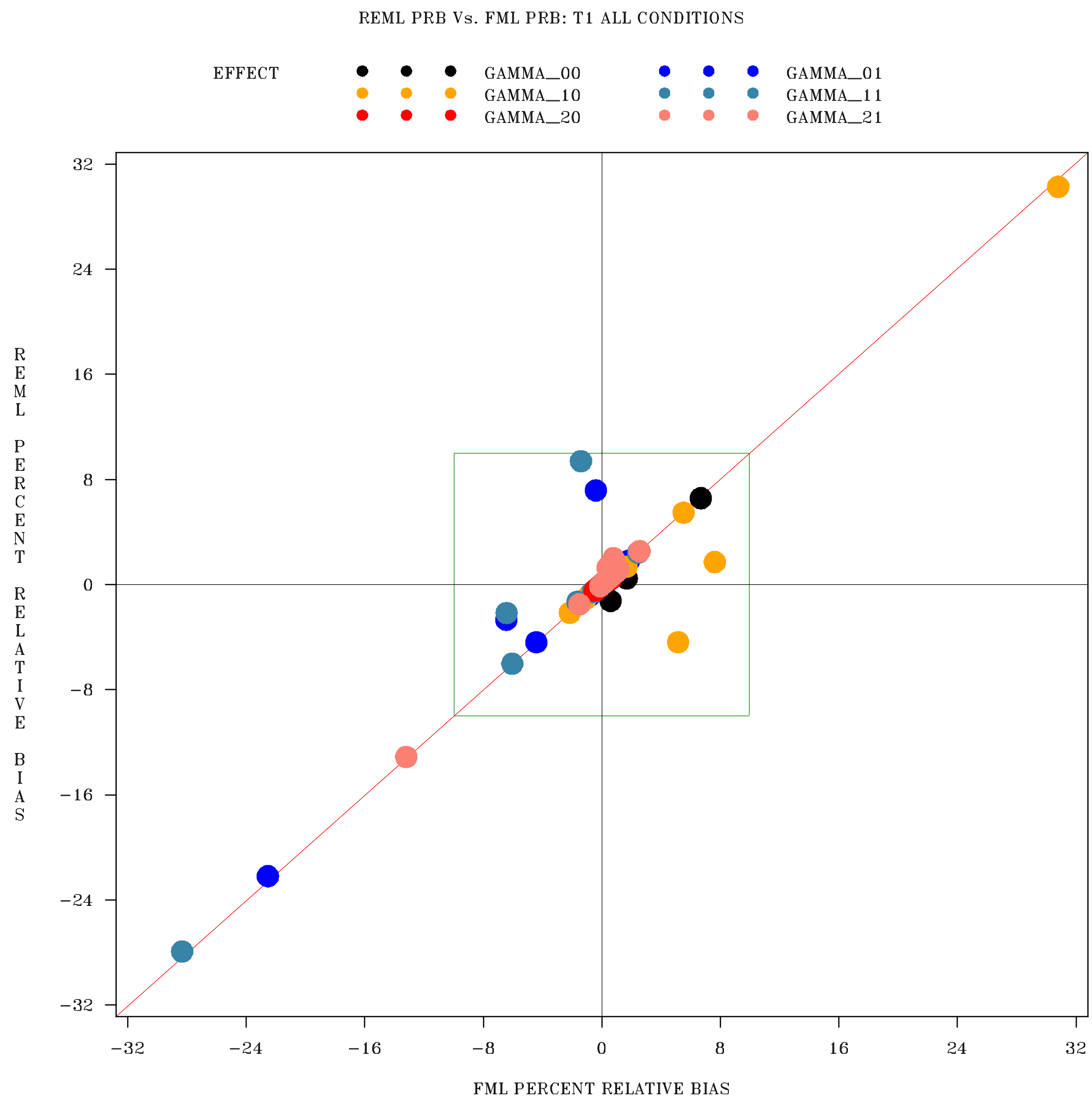

Figure 5.13: Fixed Effect PRB Model 3 T1 REML & FML

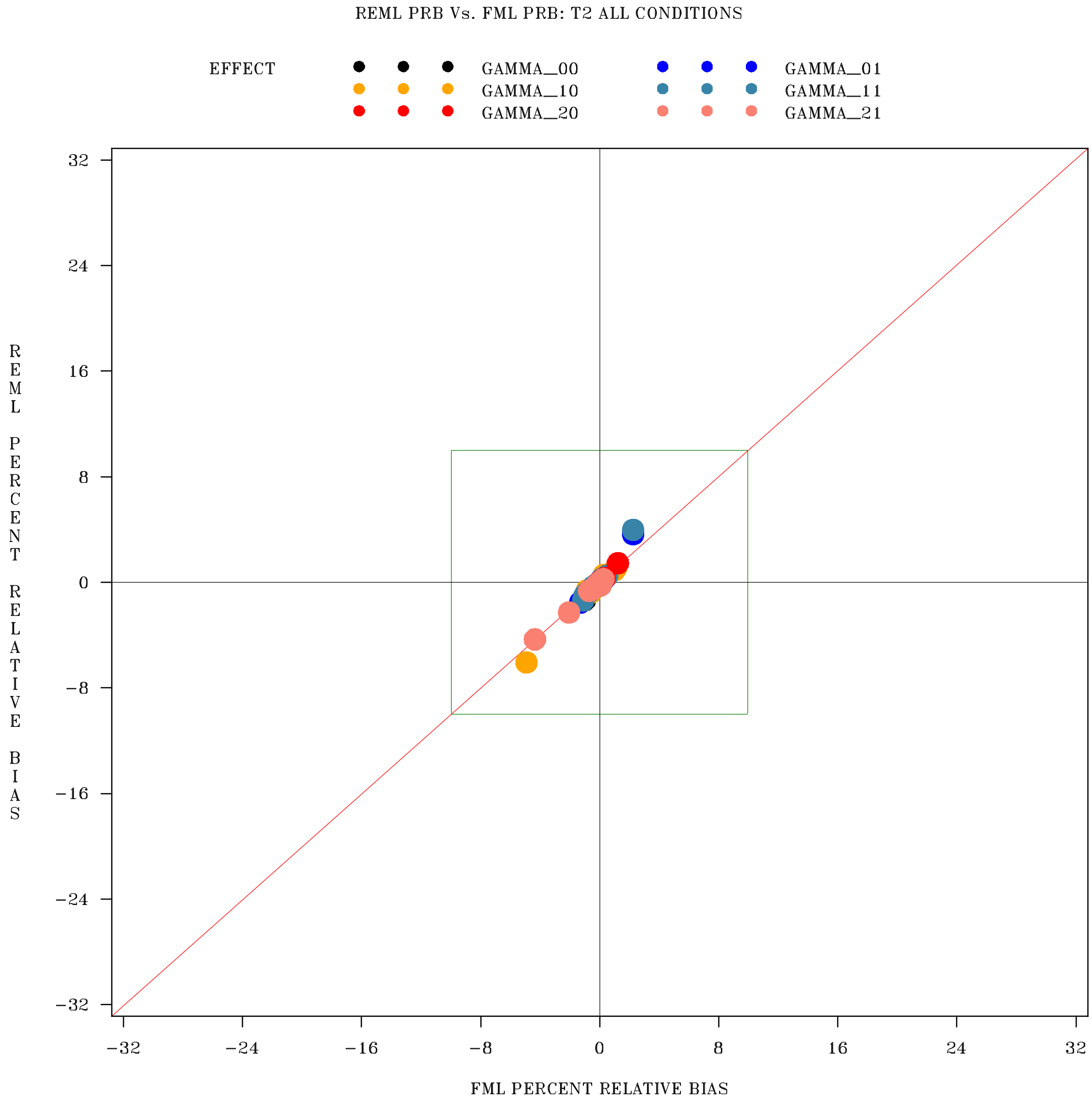

Figure 5.14: Fixed Effect PRB Model 3 T2 REML & FML

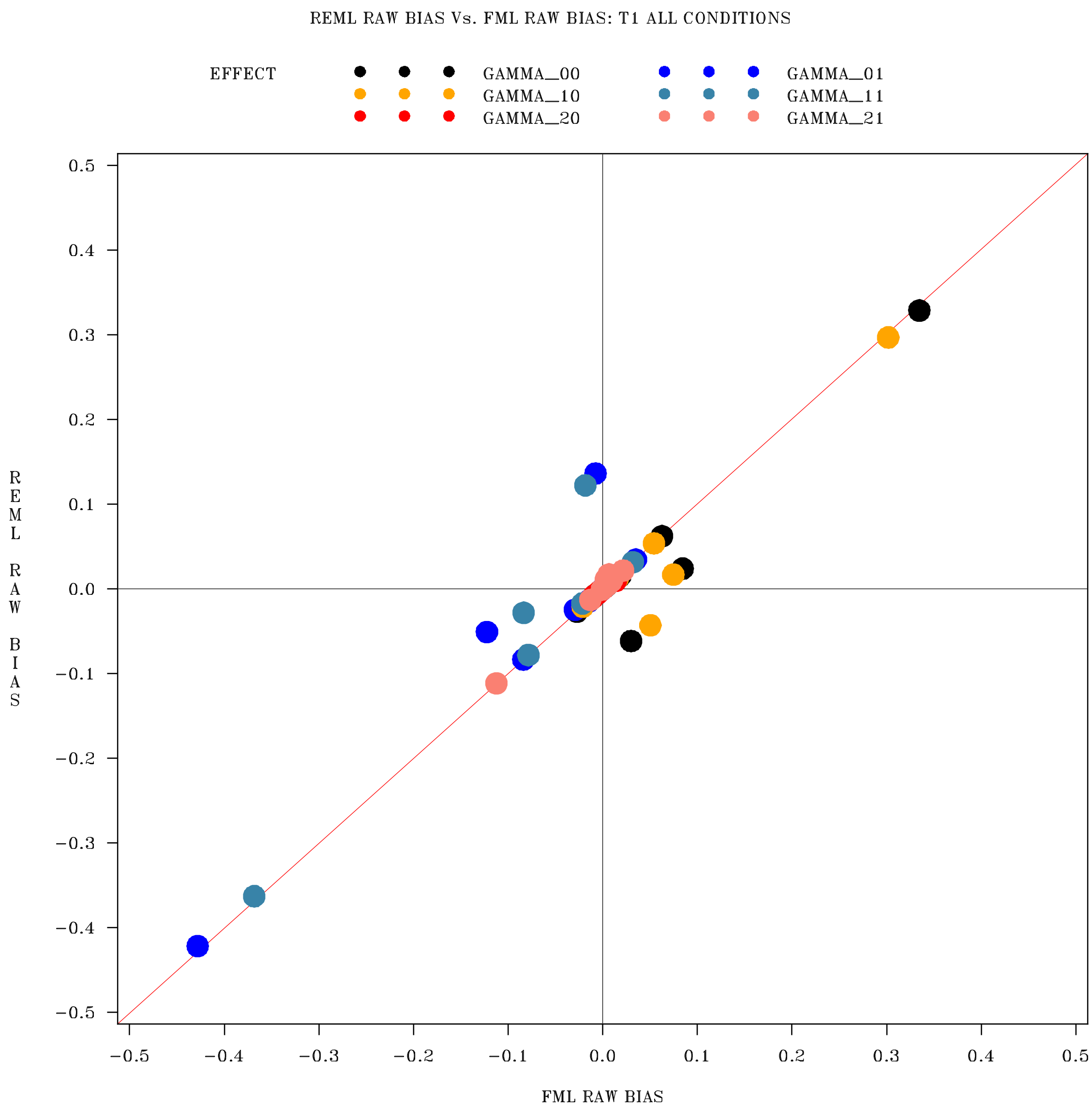

Figure 5.15: Fixed Effect Raw Bias Model 3 T1 REML & FML

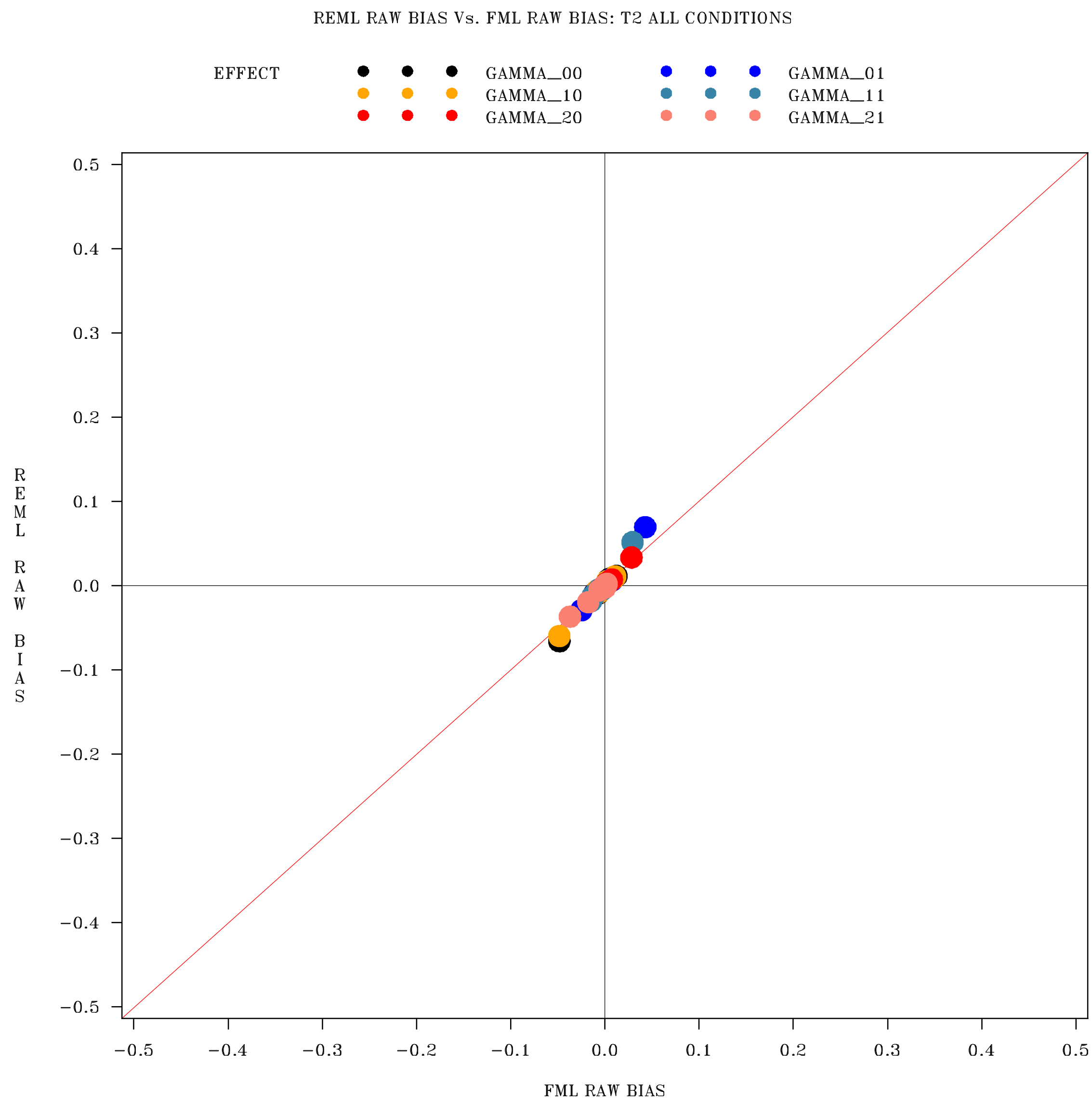

Figure 5.16: Fixed Effect Raw Bias Model 3 T2 REML & FML

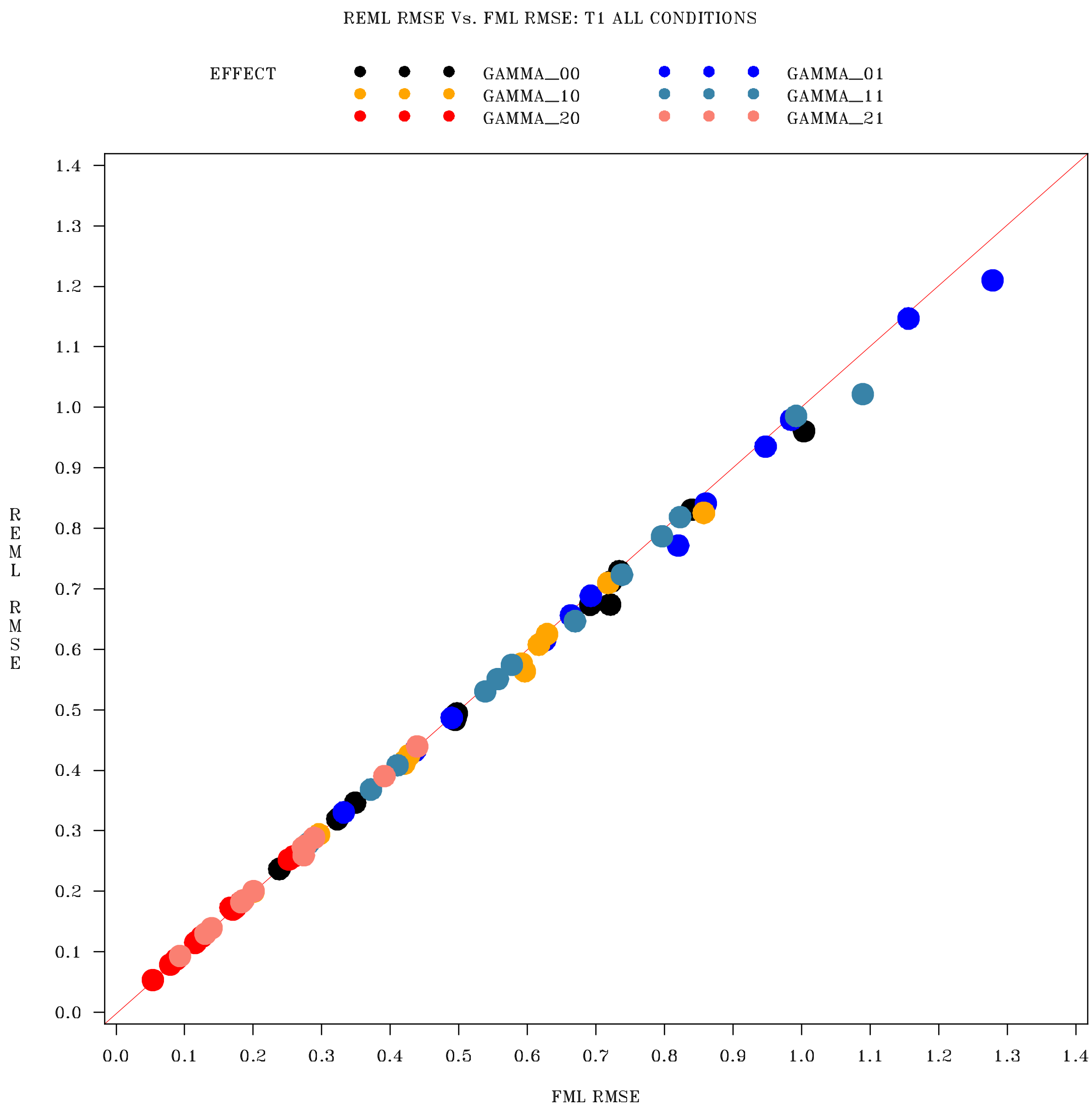

Figure 5.17: Fixed Effect RMSE Model 3 T1 REML & FML

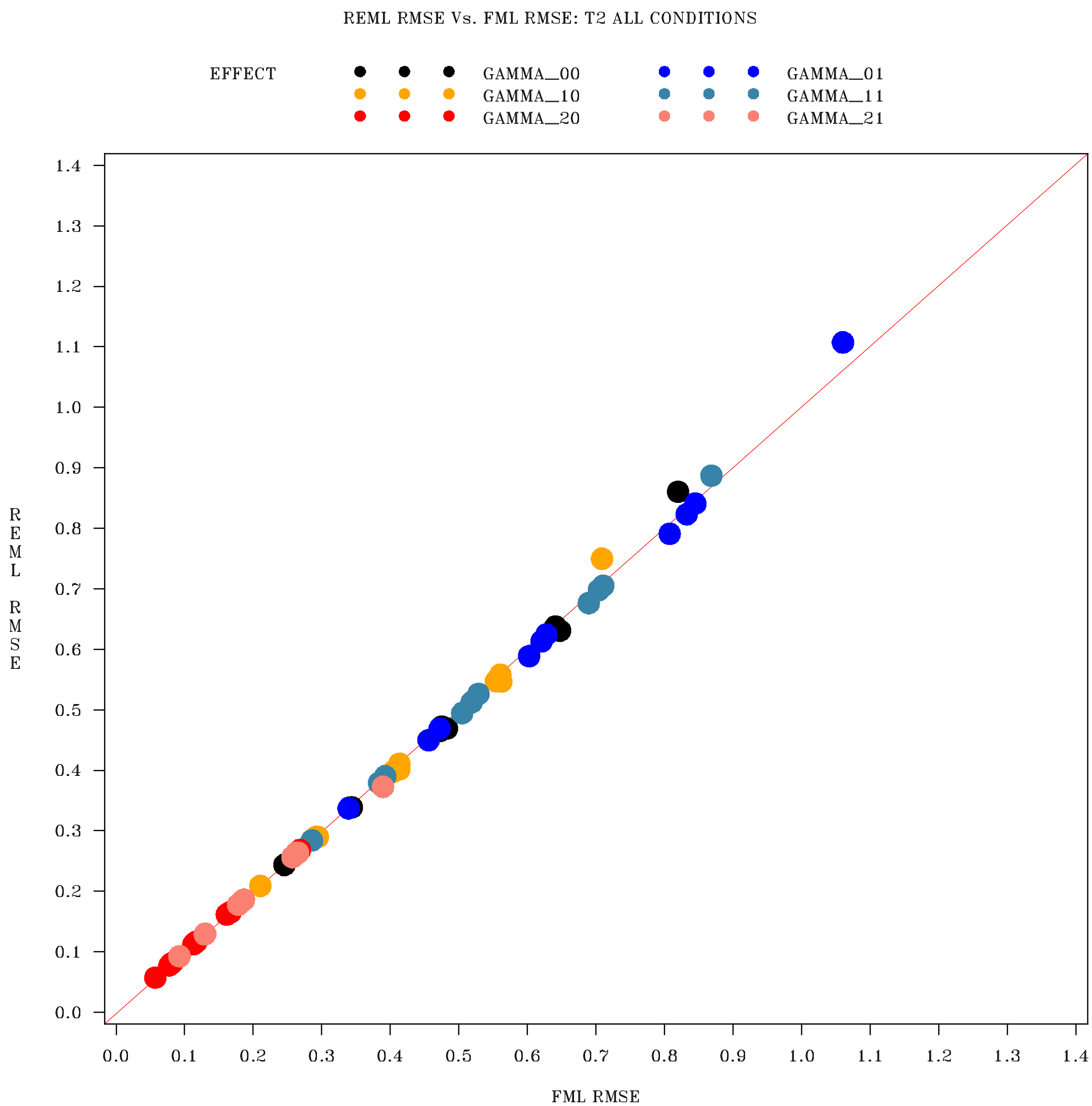

Figure 5.18: Fixed Effect RMSE Model 3 T2 REML & FML

5.3 Appendix 1b: Covariance Component PRB and RMSE for Balanced Data

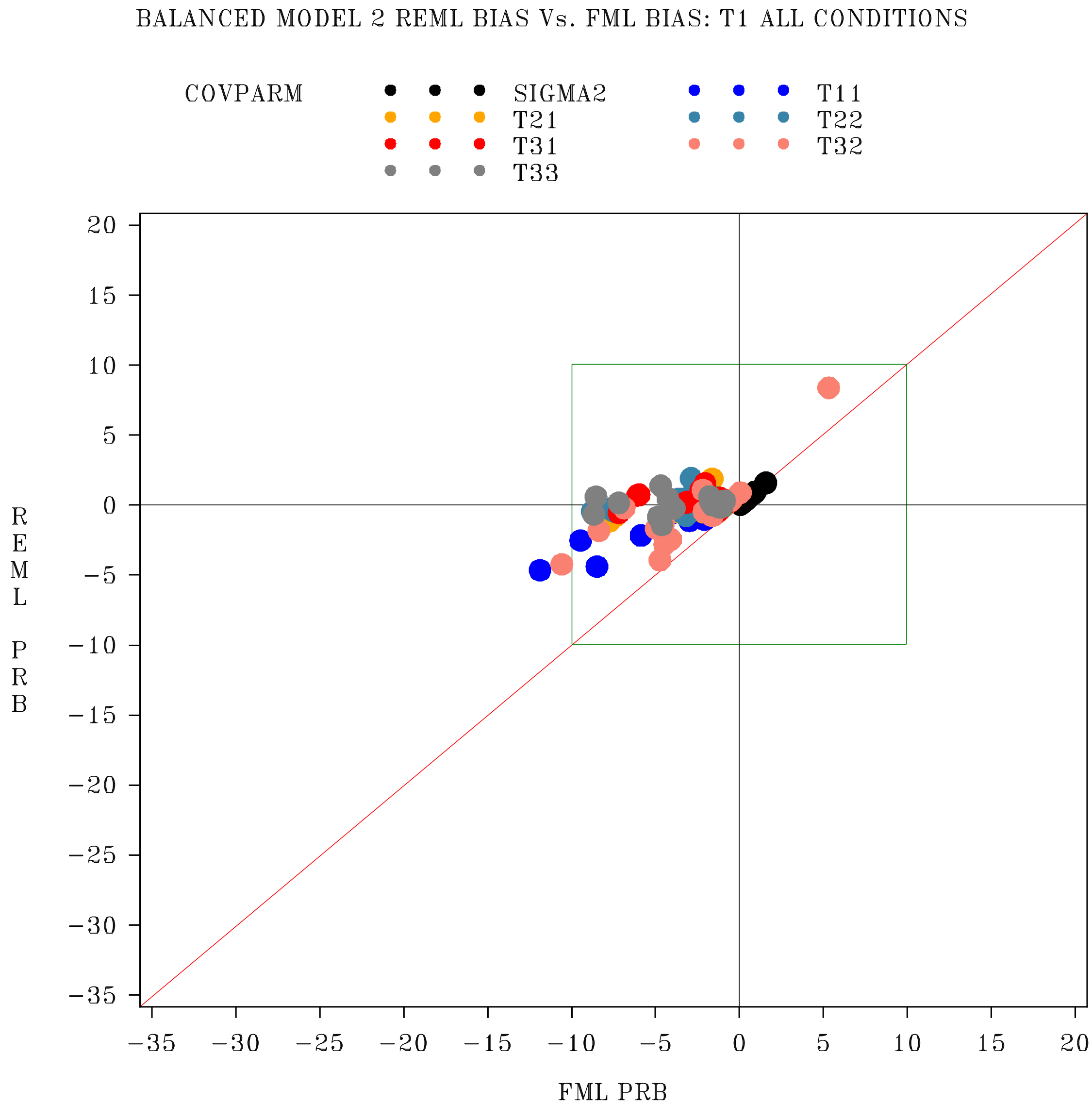

Figure 5.19: Random Effect PRB Balanced Data Model 2 T1 REML & FML

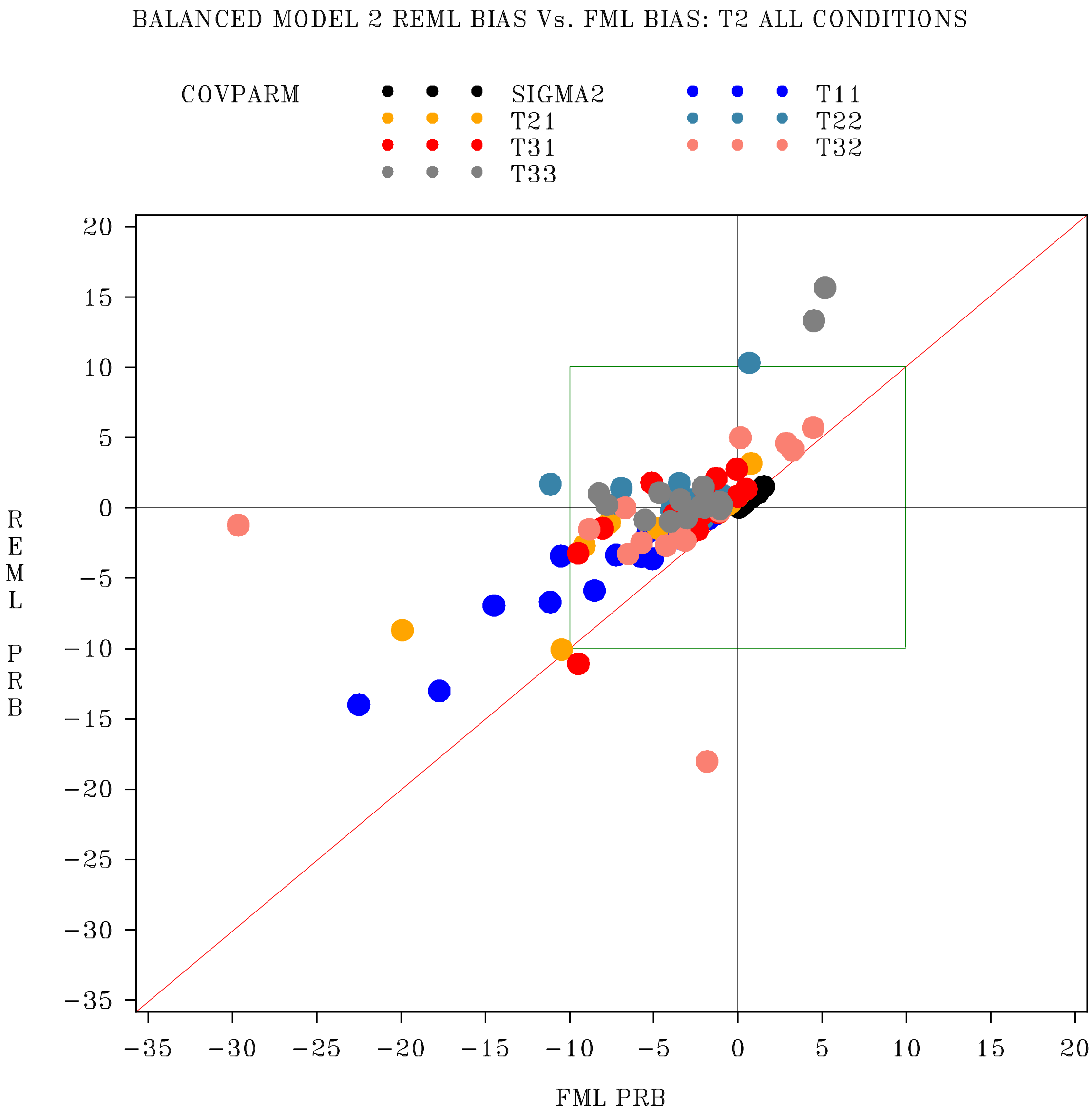

Figure 5.20: Random Effect PRB Balanced Data Model 2 T2 REML & FML

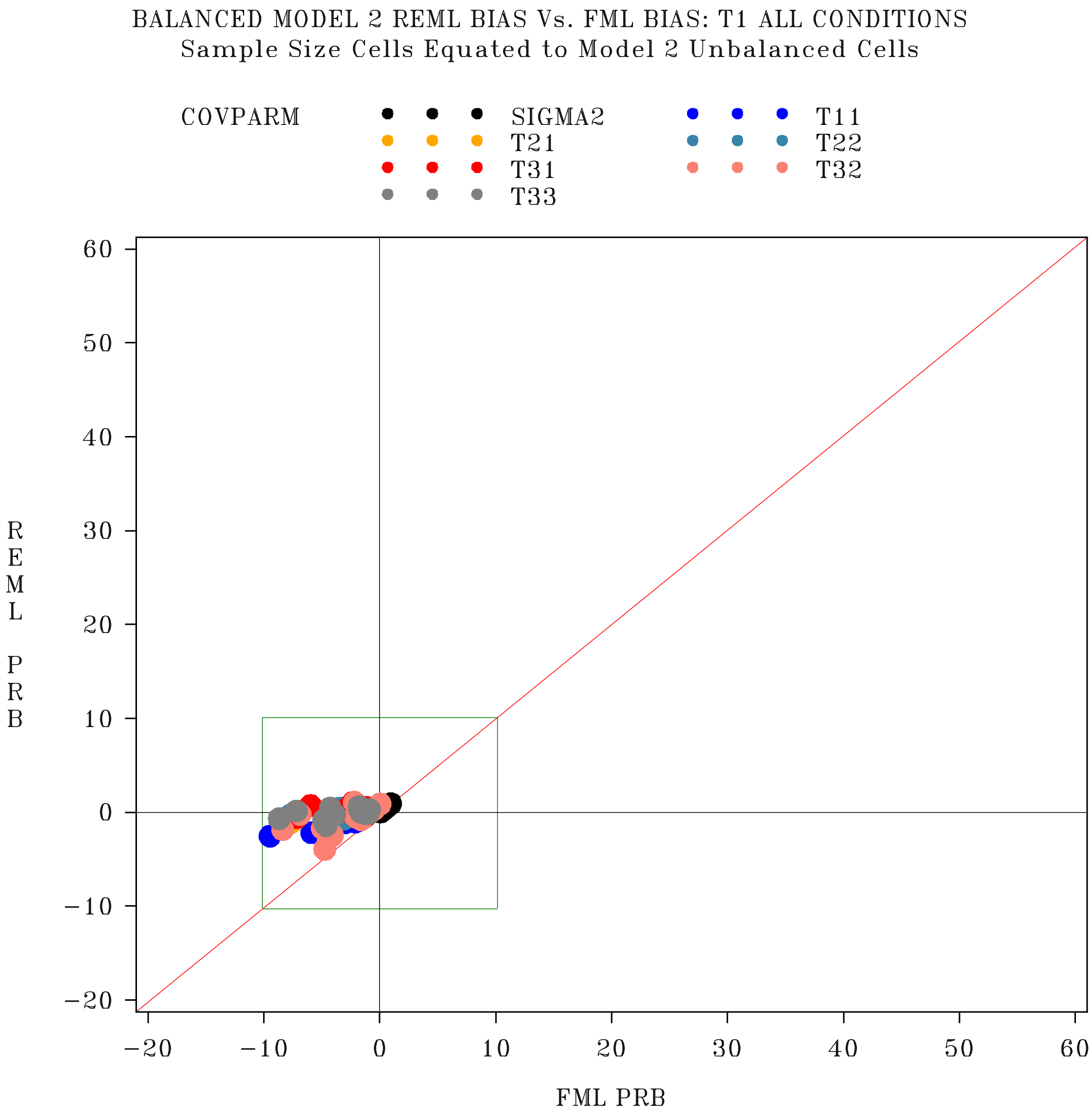

Figure 5.21: Random Effect PRB Balanced Data Restricted Cells Model 2 T1 REML & FML

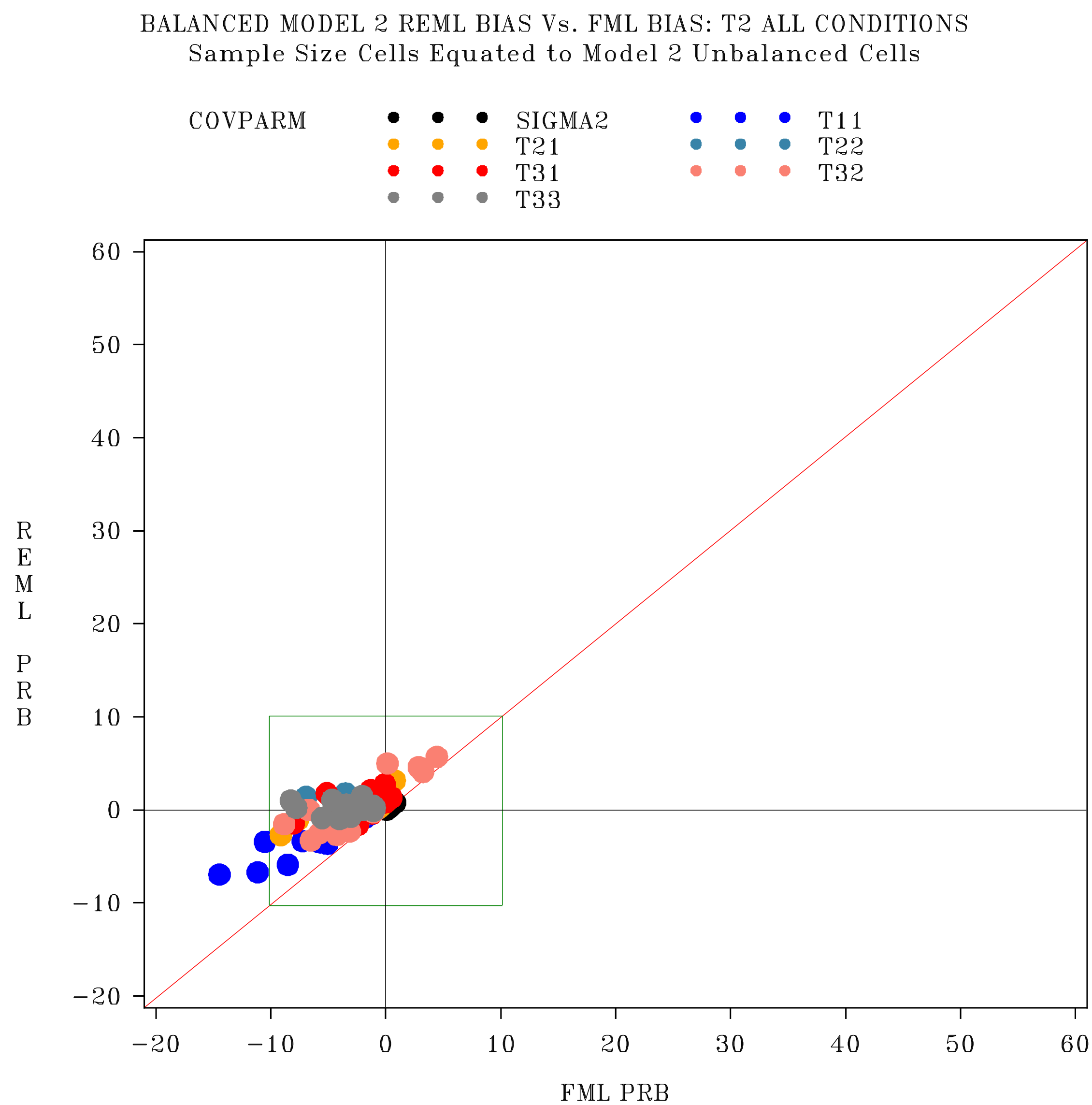

Figure 5.22: Random Effect PRB Balanced Data Restricted Cells Model 2 T2 REML & FML

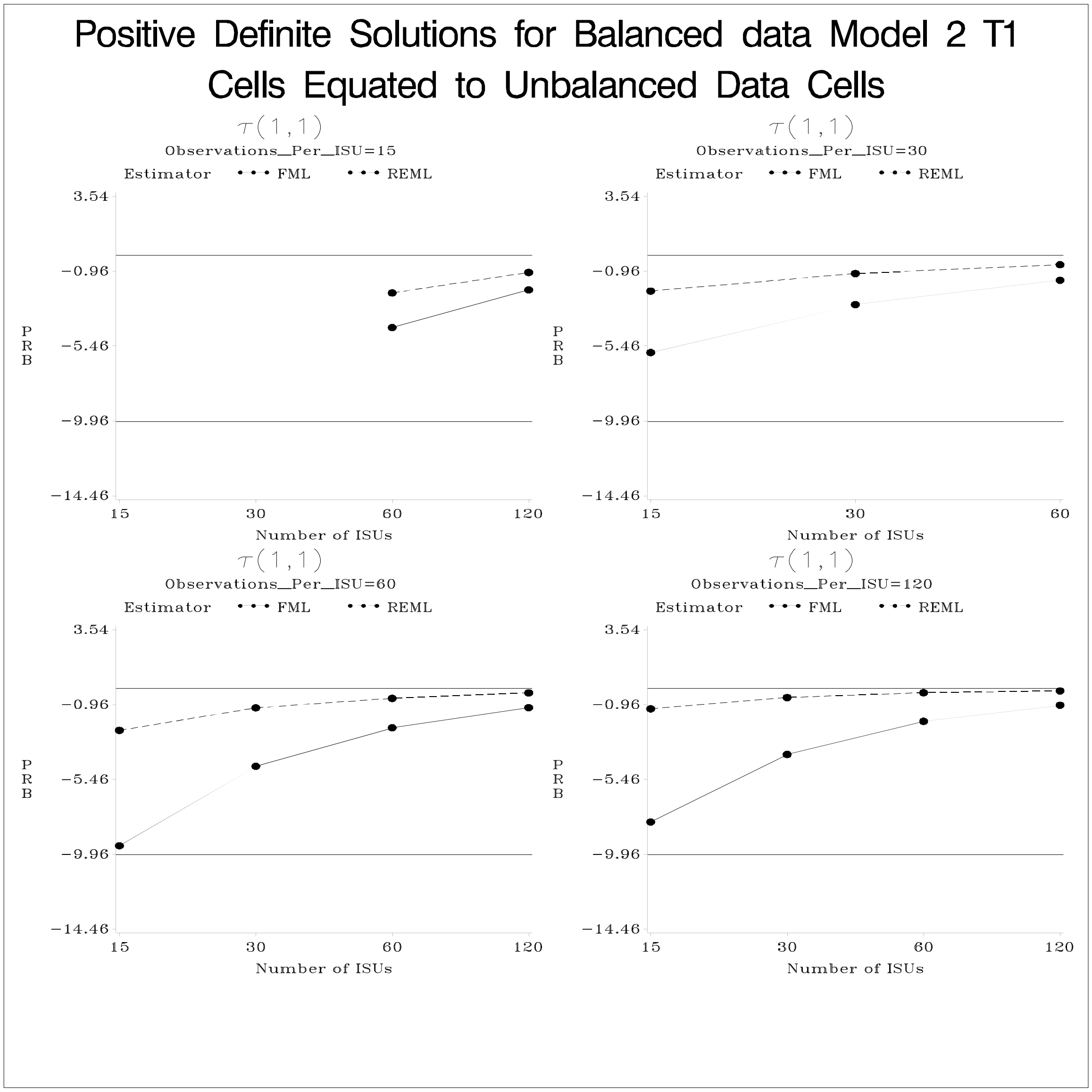

Figure 5.23: τ_{11} PRB Balance Data Cells Restricted Model 2 T1 REML & FML

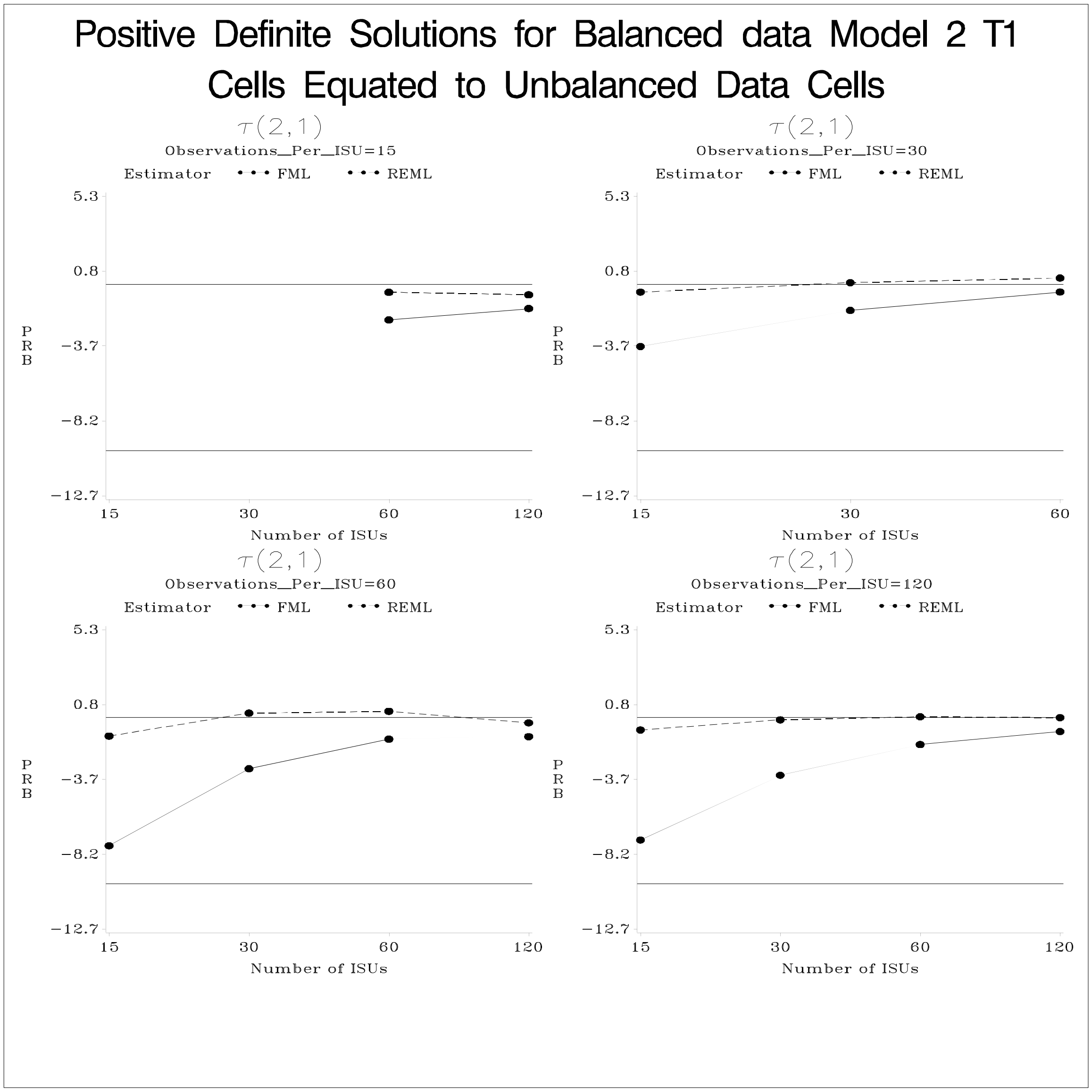

Figure 5.24: τ_{21} PRB Balance Data Cells Restricted Model 2 T1 REML & FML

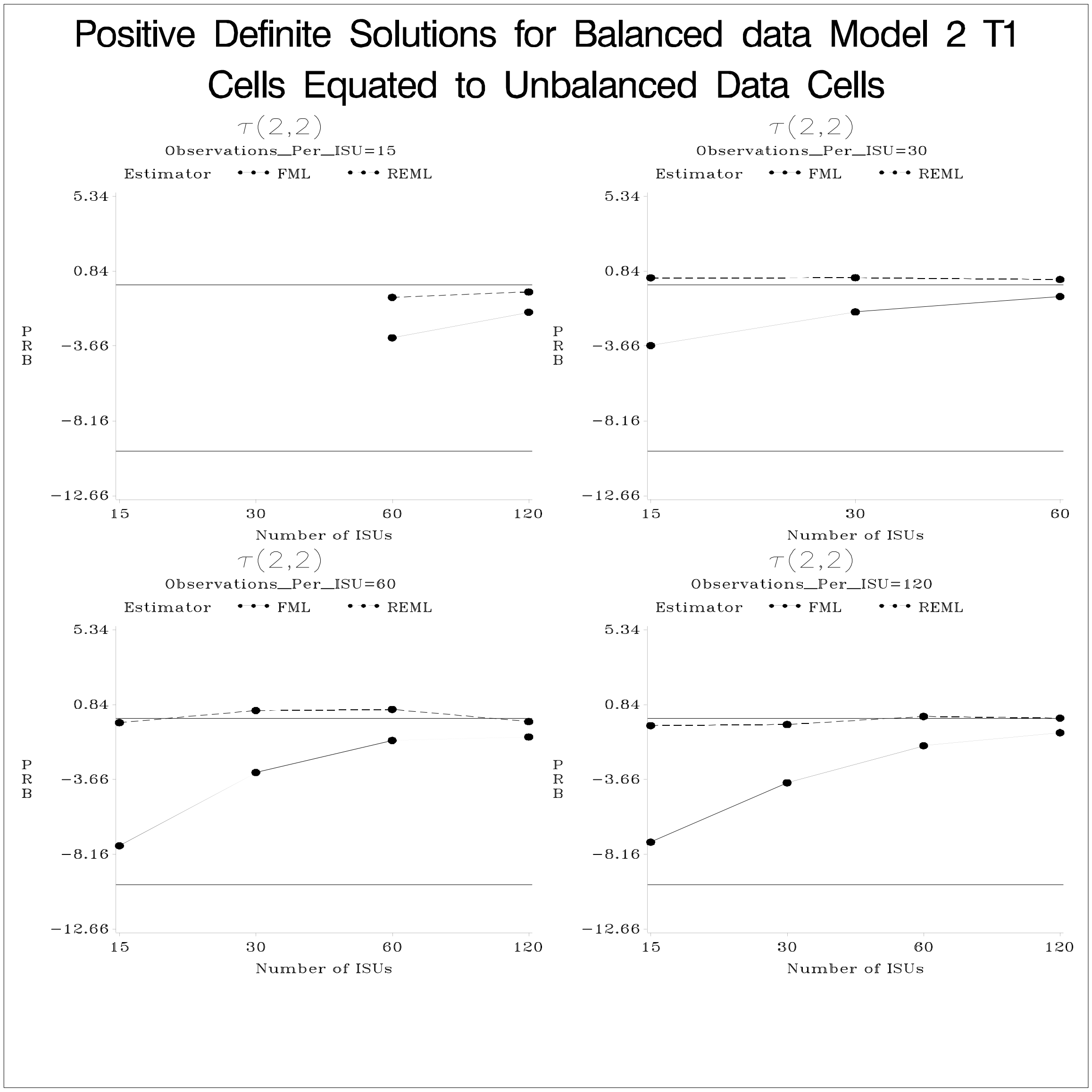

Figure 5.25: τ_{22} PRB Balance Data Cells Restricted Model 2 T1 REML & FML

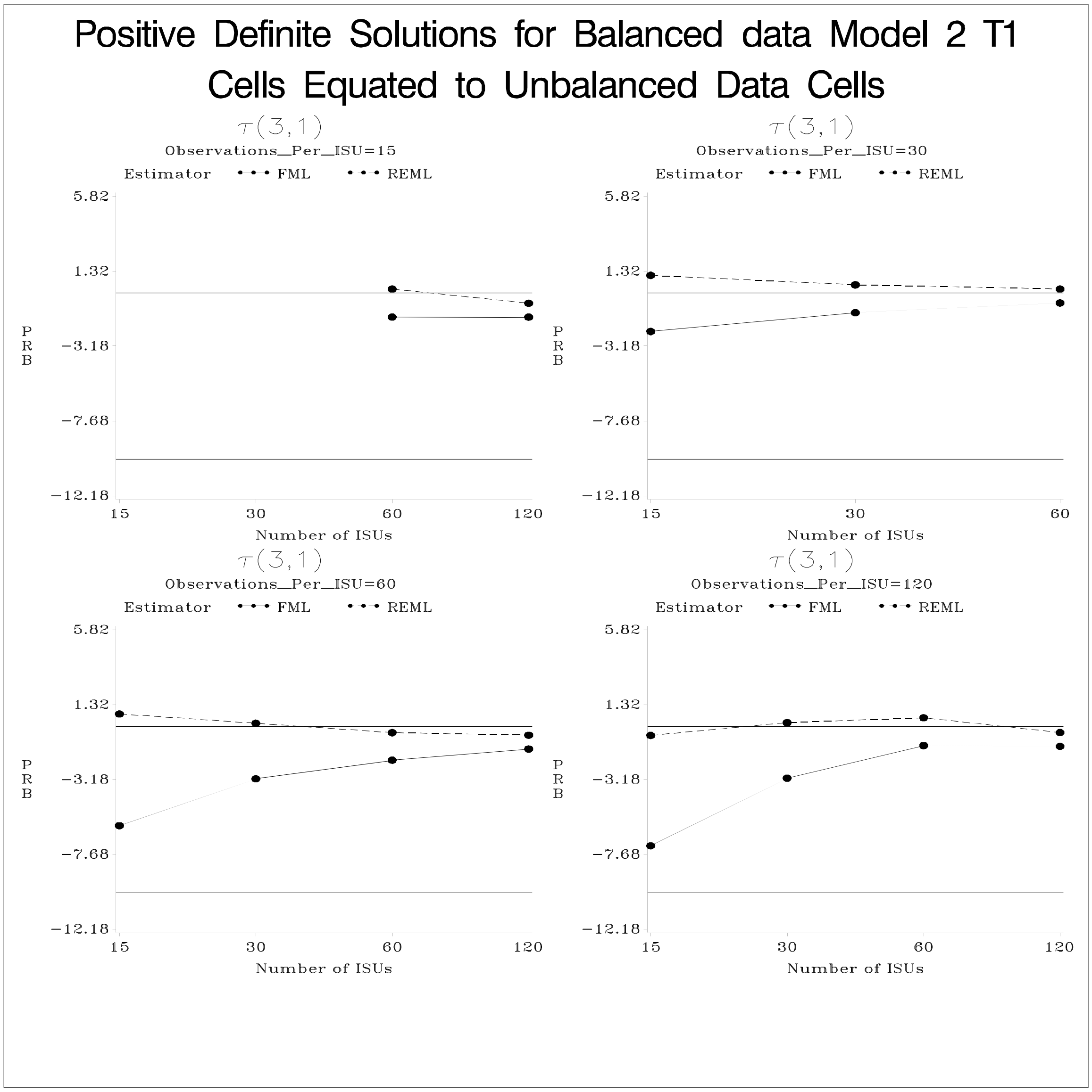

Figure 5.26: τ_{31} PRB Balance Data Cells Restricted Model 2 T1 REML & FML

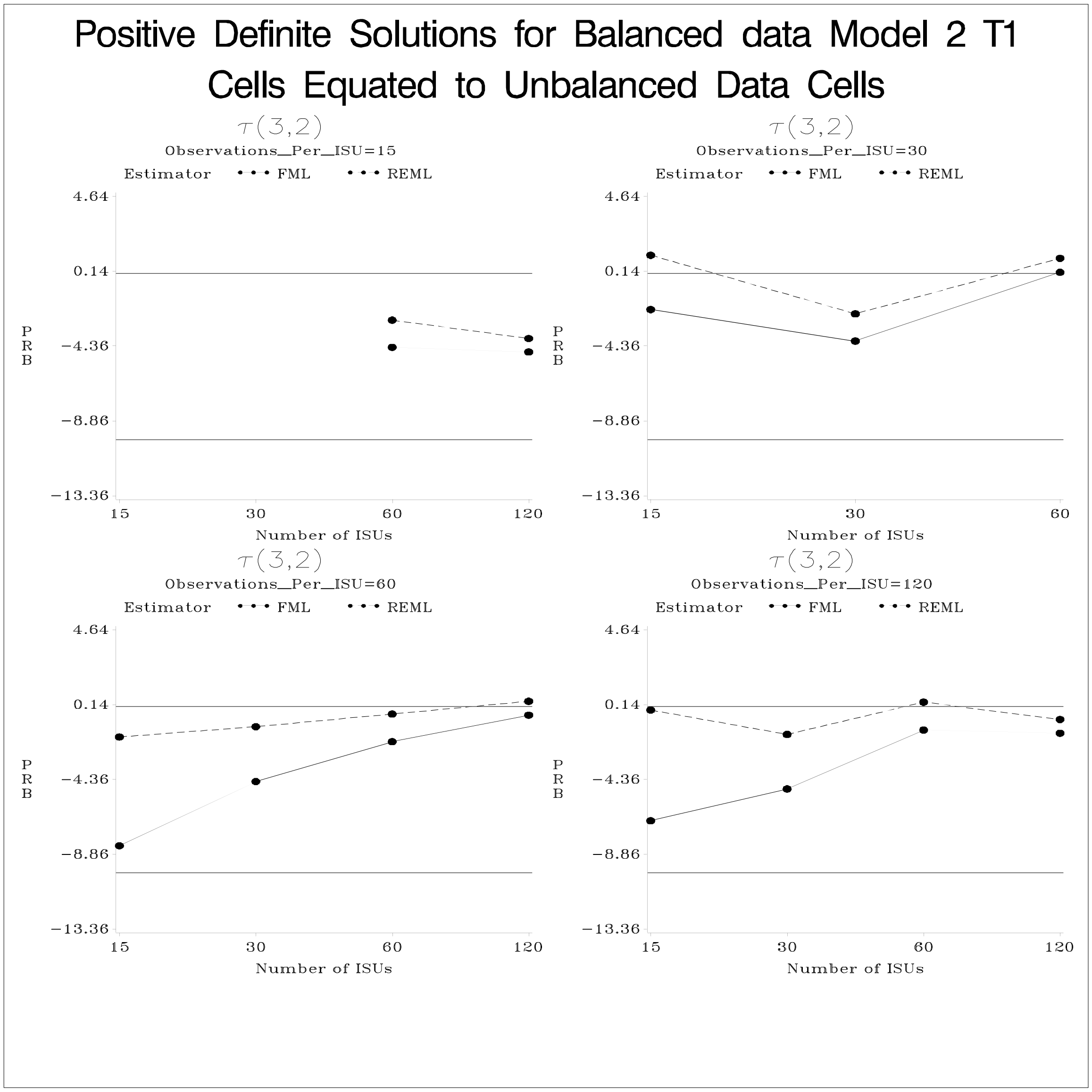

Figure 5.27: τ_{32} PRB Balance Data Cells Restricted Model 2 T1 REML & FML

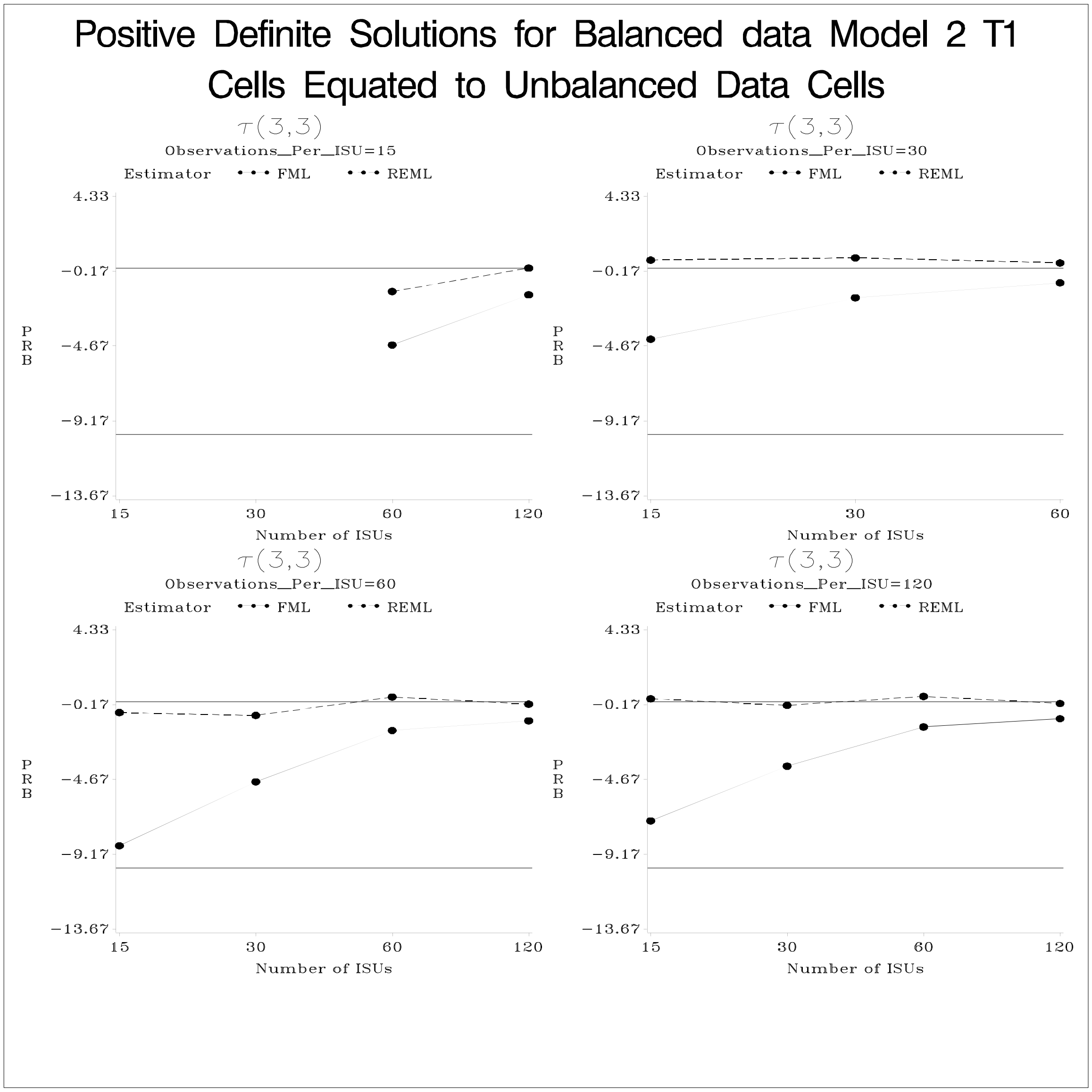

Figure 5.28: τ_{33} PRB Balance Data Cells Restricted Model 2 T1 REML & FML

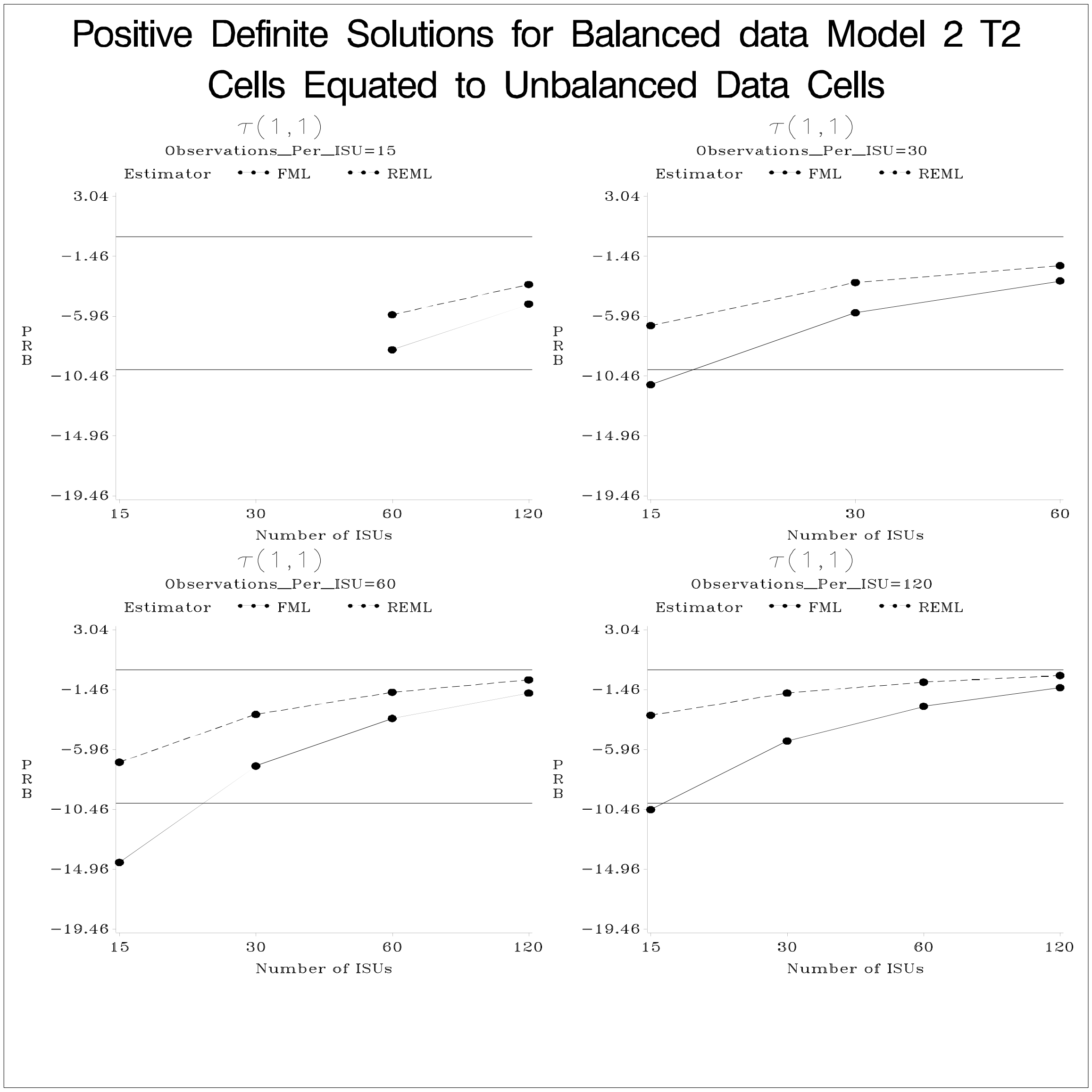

Figure 5.29: τ_{11} PRB Balance Data Cells Restricted PRB Model 2 T2 REML & FML

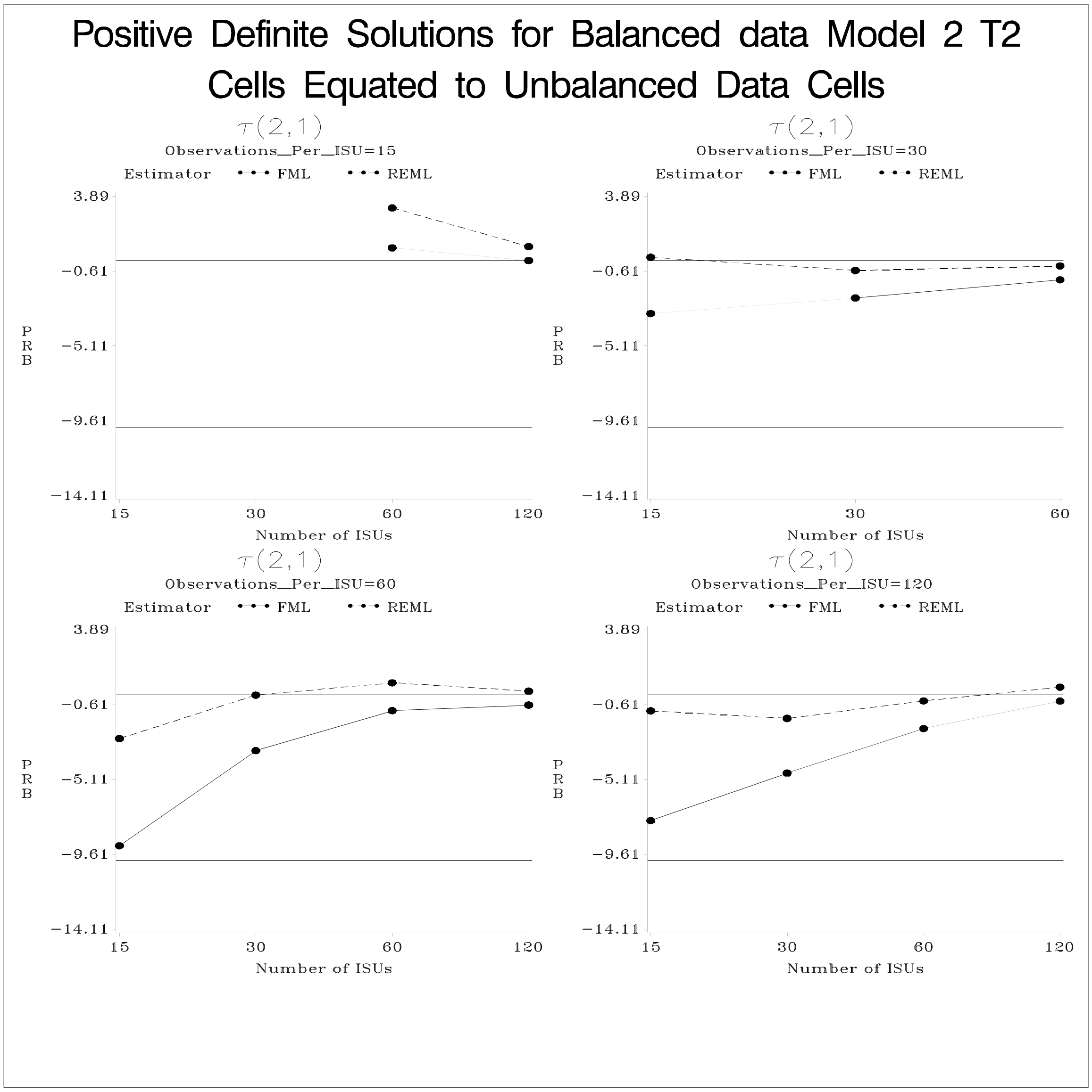

Figure 5.30: τ_{21} PRB Balance Data Cells Restricted PRB Model 2 T2 REML & FML

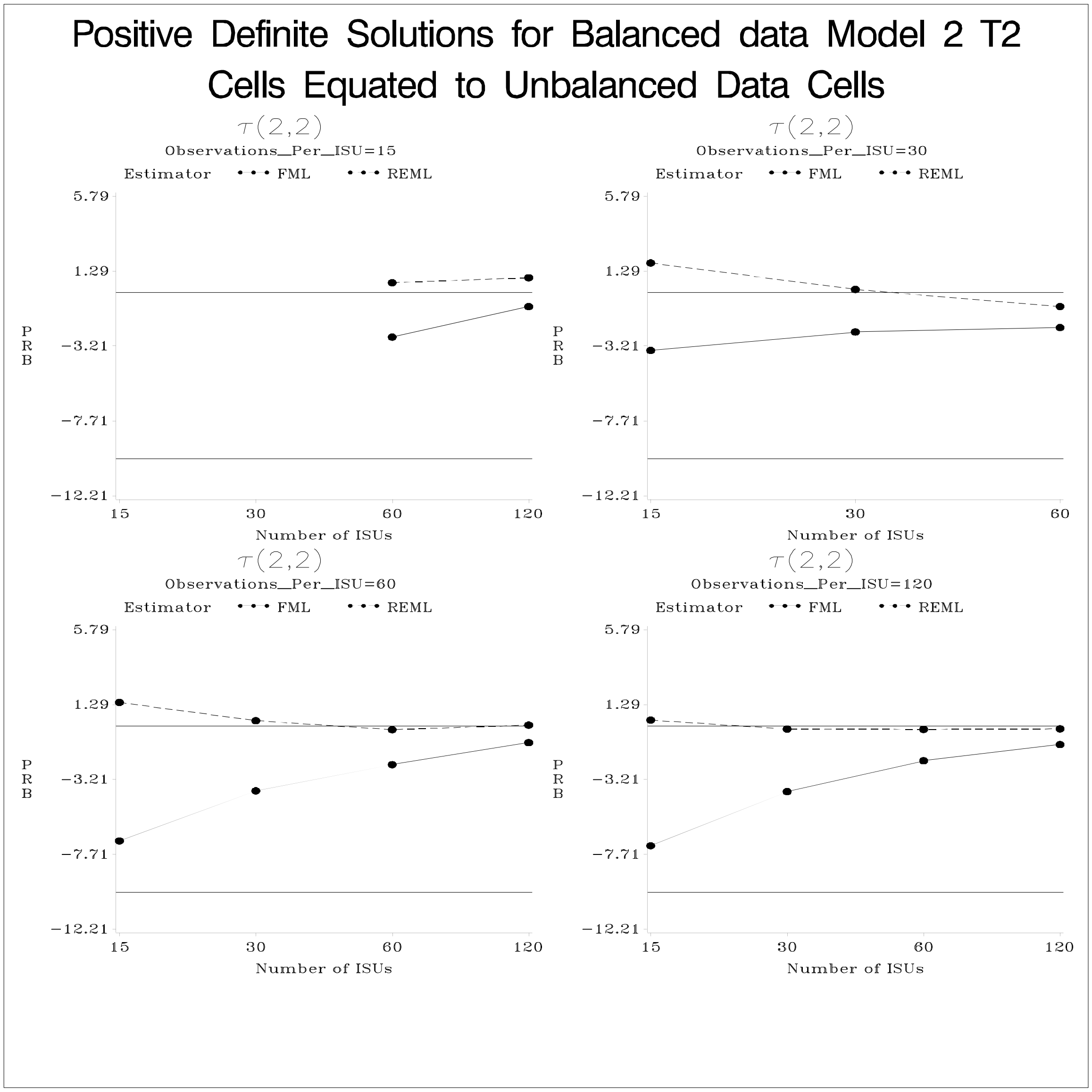

Figure 5.31: τ_{22} PRB Balance Data Cells Restricted PRB Model 2 T2 REML & FML

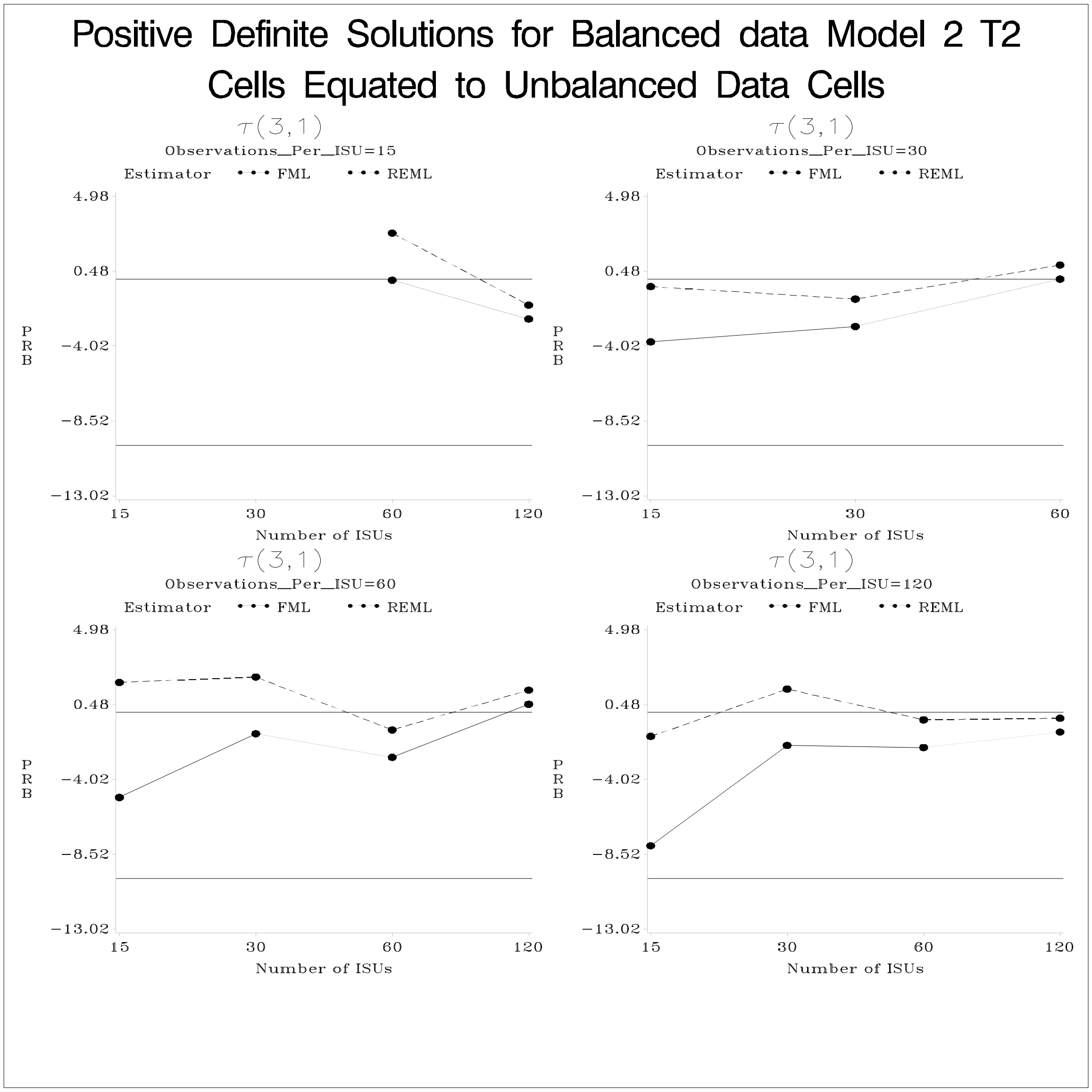

Figure 5.32: τ_{31} PRB Balance Data Cells Restricted PRB Model 2 T2 REML & FML

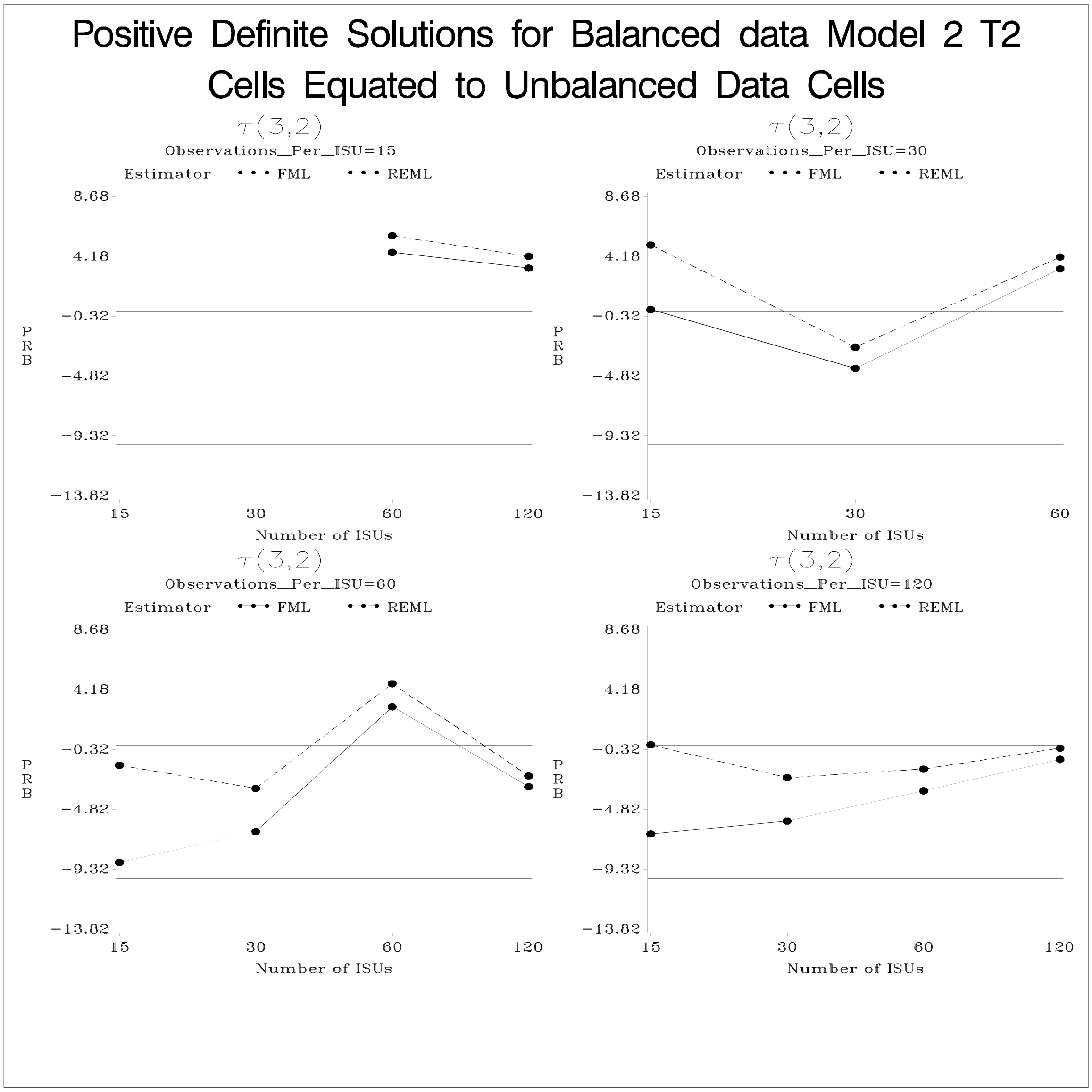

Figure 5.33: τ_{32} PRB Balance Data Cells Restricted Model 2 T2 REML & FML

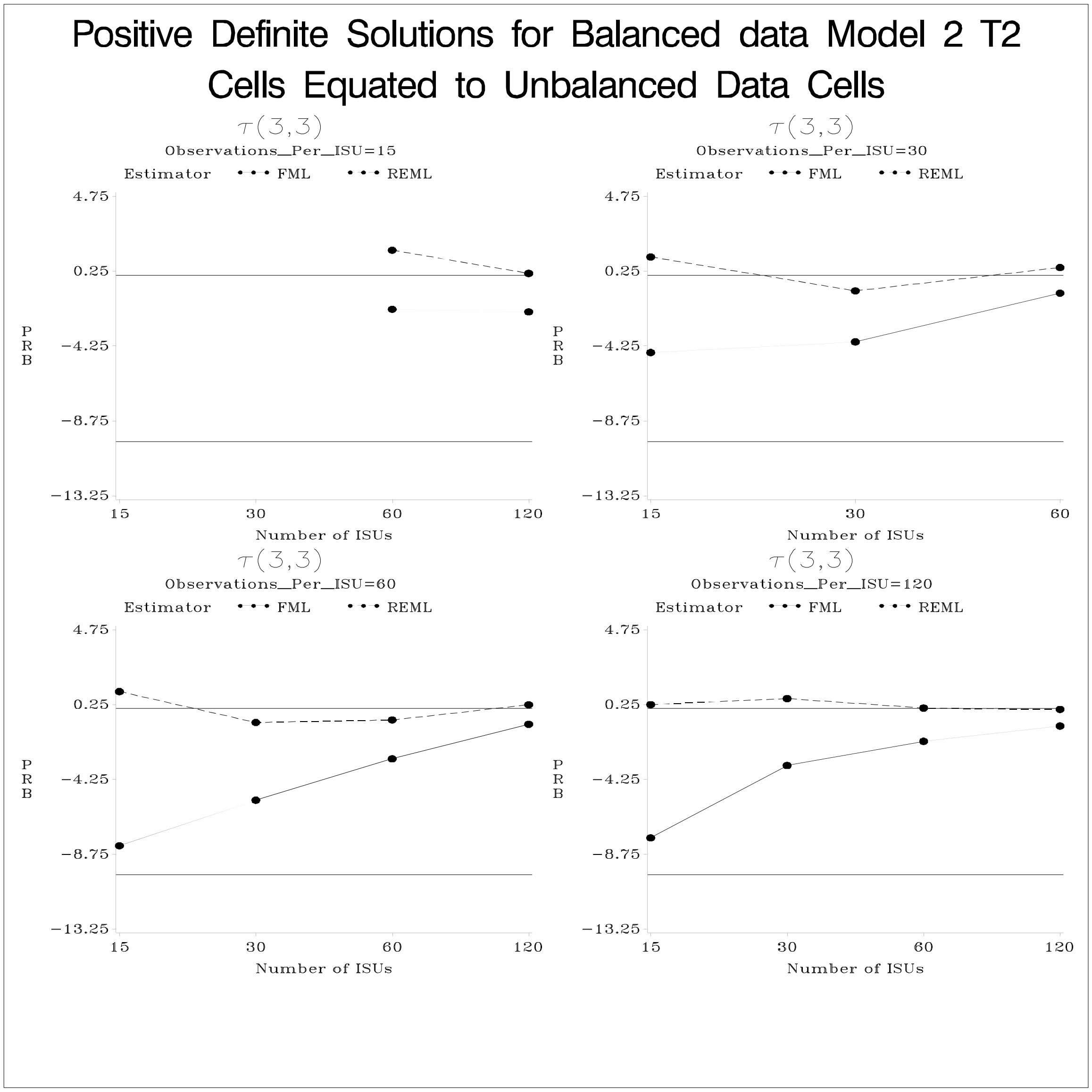

Figure 5.34: τ_{33} PRB Balance Data Cells Restricted Model 2 T2 REML & FML

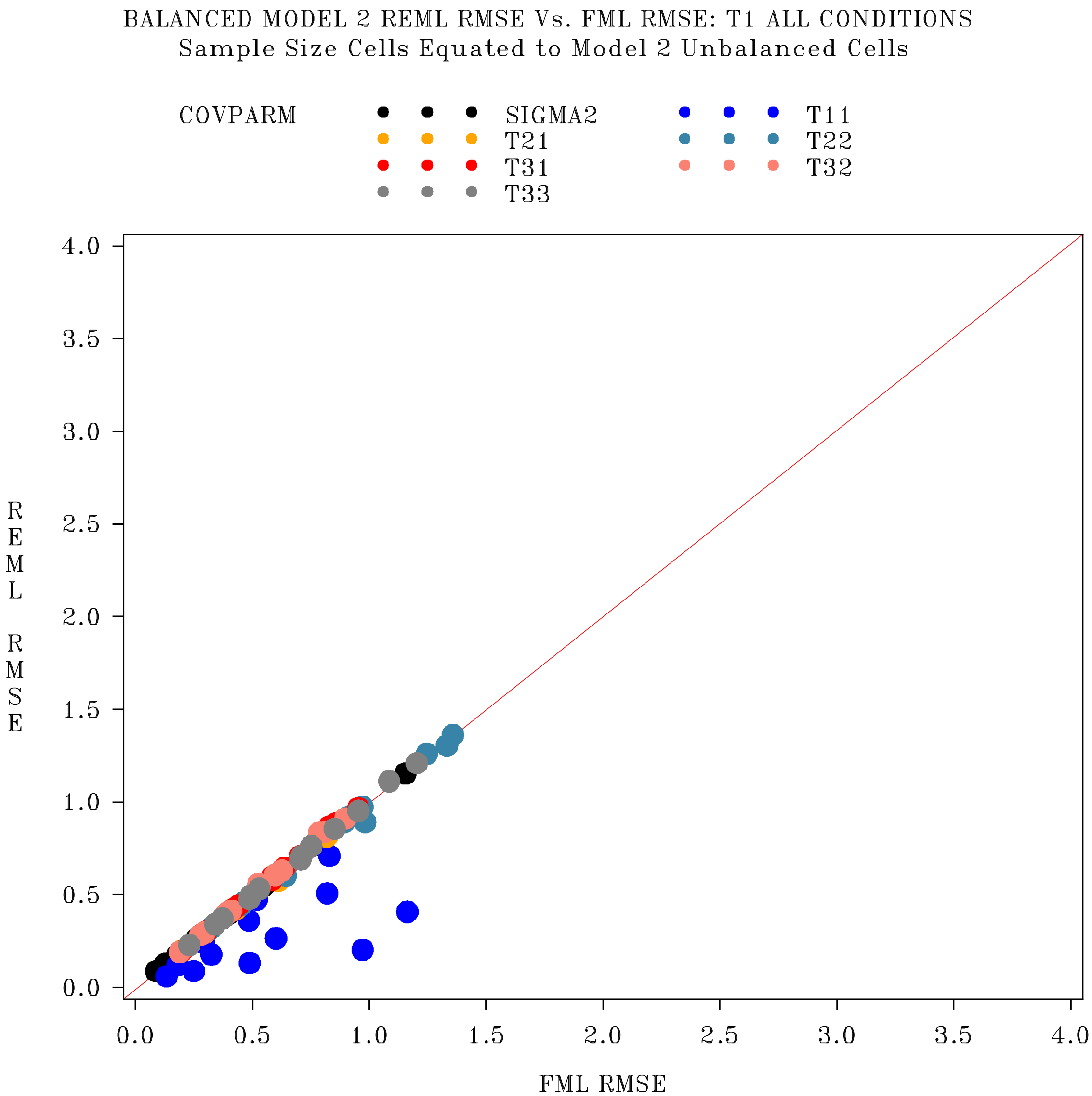

Figure 5.35: Random Effect RMSE Balanced Data Cells Restricted Model 2 T1 REML & FML

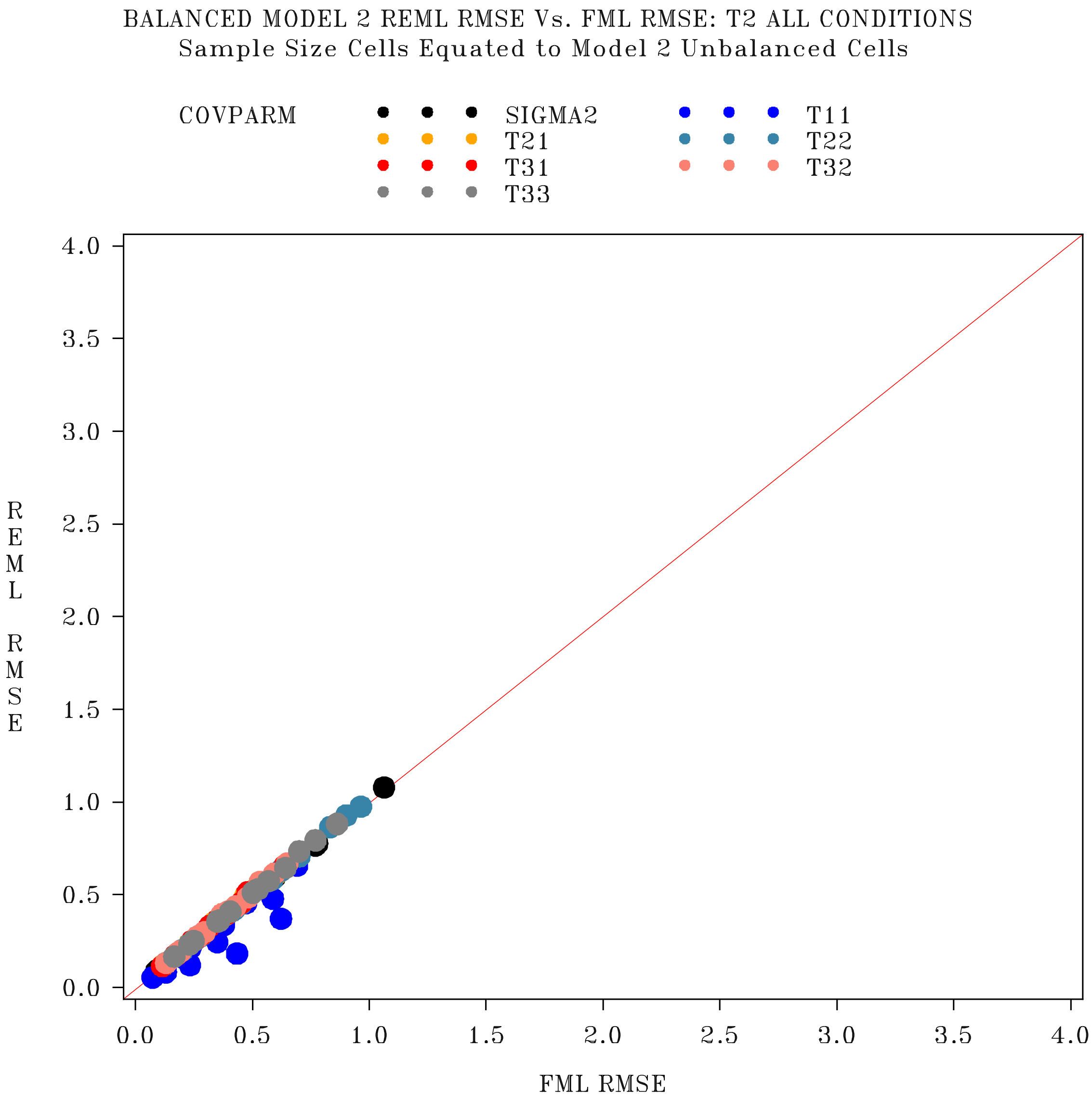

Figure 5.36: Random Effect RMSE Balanced Data Cells Restricted Model 2 T2 REML & FML

5.4 Appendix 2: Covariance Component RMSE Tables

5.4.1 Model 1

Table 5.5: Positive Definite Solutions for Model 1 Comparing Root Mean Squared Error (RMSE) for REML and FML Estimates of Covariance Parameters Across T1 and T2

					T1		**T2**	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
σ^2	1	1	48.86	48.86	3.82	3.83	3.71	3.65
σ^2	2	1	48.86	48.86	2.65	2.65	2.53	2.53
σ^2	3	1	48.86	48.86	1.79	1.79	1.89	1.89
σ^2	4	1	48.86	48.86	1.26	1.26	1.28	1.28
σ^2	1	2	48.86	48.86	2.41	2.41	2.38	2.39
σ^2	2	2	48.86	48.86	1.69	1.69	1.70	1.70
σ^2	3	2	48.86	48.86	1.21	1.21	1.14	1.14
σ^2	4	2	48.86	48.86	0.84	0.84	0.81	0.81
σ^2	1	3	48.86	48.86	1.64	1.64	1.62	1.62
σ^2	2	3	48.86	48.86	1.14	1.14	1.09	1.09
σ^2	3	3	48.86	48.86	0.81	0.81	0.82	0.82
σ^2	4	3	48.86	48.86	0.58	0.58	0.59	0.59
σ^2	1	4	48.86	48.86	1.13	1.13	1.20	1.20
σ^2	2	4	48.86	48.86	0.78	0.78	0.75	0.75
σ^2	3	4	48.86	48.86	0.55	0.55	0.58	0.58
σ^2	4	4	48.86	48.86	0.39	0.39	0.39	0.39
τ_{11}	1	1	12	4	3.50	3.76	2.07	2.12
τ_{11}	2	1	12	4	2.32	2.44	1.63	1.67
τ_{11}	3	1	12	4	1.56	1.60	1.15	1.17
τ_{11}	4	1	12	4	1.17	1.18	0.81	0.81

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Table 5.5 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{11}	1	2	12	4	2.30	2.57	1.41	1.51
τ_{11}	2	2	12	4	1.55	1.68	0.99	1.04
τ_{11}	3	2	12	4	1.02	1.06	0.69	0.71
τ_{11}	4	2	12	4	0.78	0.79	0.49	0.49
τ_{11}	1	3	12	4	1.50	1.79	0.95	1.07
τ_{11}	2	3	12	4	1.09	1.20	0.67	0.72
τ_{11}	3	3	12	4	0.74	0.79	0.46	0.48
τ_{11}	4	3	12	4	0.53	0.55	0.32	0.32
τ_{11}	1	4	12	4	1.03	1.37	0.68	0.76
τ_{11}	2	4	12	4	0.75	0.88	0.44	0.48
τ_{11}	3	4	12	4	0.53	0.57	0.30	0.32
τ_{11}	4	4	12	4	0.37	0.39	0.21	0.22

5.4.2 Model 2

Table 5.6: Positive Definite Solutions for Model 2 Comparing Root Mean Squared Error (RMSE) for REML and FML Estimates of Covariance Parameters Across T1 and T2

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
σ^2	15	$\bar{4}0$	46.58	.	1.81	1.82	.	.
σ^2	15	$\bar{8}0$	46.58	.	1.15	1.05	.	.
σ^2	30	$\bar{2}0$	46.58	46.58	1.75	1.76	2.03	2.08

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Table 5.6 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
σ^2	30	$\bar{4}0$	46.58	.	1.21	1.21	.	.
σ^2	30	$\bar{8}0$	46.58	46.58	0.82	0.82	0.84	0.84
σ^2	60	$\bar{1}0$	46.58	.	2.20	2.27	.	.
σ^2	60	$\bar{2}0$	46.58	46.58	1.34	1.34	1.32	1.32
σ^2	60	$\bar{4}0$	46.58	46.58	0.86	0.86	0.86	0.86
σ^2	60	$\bar{8}0$	46.58	46.58	0.57	0.57	0.56	0.56
σ^2	120	$\bar{1}0$	46.58	46.58	1.54	1.54	1.55	1.55
σ^2	120	$\bar{2}0$	46.58	46.58	1.00	1.00	0.91	0.91
σ^2	120	$\bar{4}0$	46.58	46.58	0.61	0.61	0.59	0.59
σ^2	120	$\bar{8}0$	46.58	46.58	0.42	0.42	0.39	0.39
τ_{11}	15	$\bar{4}0$	12	.	3.65	3.57	.	.
τ_{11}	15	$\bar{8}0$	12	.	3.34	3.41	.	.
τ_{11}	30	$\bar{2}0$	12	4	3.23	3.22	1.42	1.44
τ_{11}	30	$\bar{4}0$	12	.	2.63	2.58	.	.
τ_{11}	30	$\bar{8}0$	12	4	2.05	2.03	0.92	0.91
τ_{11}	60	$\bar{1}0$	12	.	2.76	2.80	.	.
τ_{11}	60	$\bar{2}0$	12	4	2.11	2.10	1.00	1.00
τ_{11}	60	$\bar{4}0$	12	4	1.59	1.60	0.77	0.77
τ_{11}	60	$\bar{8}0$	12	4	1.37	1.38	0.62	0.62
τ_{11}	120	$\bar{1}0$	12	4	1.83	1.82	1.04	1.04
τ_{11}	120	$\bar{2}0$	12	4	1.42	1.43	0.73	0.73
τ_{11}	120	$\bar{4}0$	12	4	1.16	1.17	0.54	0.53
τ_{11}	120	$\bar{8}0$	12	4	1.01	1.01	0.42	0.42

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Table 5.6 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{21}	15	$\bar{4}0$	4	.	2.52	2.37	.	.
τ_{21}	15	$\bar{8}0$	4	.	2.34	2.25	.	.
τ_{21}	30	$\bar{2}0$	4	1	2.22	2.15	1.15	1.10
τ_{21}	30	$\bar{4}0$	4	.	1.81	1.74	.	.
τ_{21}	30	$\bar{8}0$	4	1	1.43	1.39	0.66	0.64
τ_{21}	60	$\bar{1}0$	4	.	2.05	2.08	.	.
τ_{21}	60	$\bar{2}0$	4	1	1.54	1.51	0.74	0.73
τ_{21}	60	$\bar{4}0$	4	1	1.19	1.18	0.60	0.59
τ_{21}	60	$\bar{8}0$	4	1	0.97	0.96	0.47	0.46
τ_{21}	120	$\bar{1}0$	4	1	1.41	1.40	0.78	0.77
τ_{21}	120	$\bar{2}0$	4	1	1.04	1.03	0.57	0.56
τ_{21}	120	$\bar{4}0$	4	1	0.87	0.86	0.42	0.42
τ_{21}	120	$\bar{8}0$	4	1	0.68	0.68	0.31	0.31
τ_{22}	15	$\bar{4}0$	7	.	2.85	2.71	.	.
τ_{22}	15	$\bar{8}0$	7	.	2.40	2.29	.	.
τ_{22}	30	$\bar{2}0$	7	3	2.46	2.41	1.66	1.61
τ_{22}	30	$\bar{4}0$	7	.	1.94	1.88	.	.
τ_{22}	30	$\bar{8}0$	7	3	1.52	1.49	0.89	0.86
τ_{22}	60	$\bar{1}0$	7	.	2.44	2.50	.	.
τ_{22}	60	$\bar{2}0$	7	3	1.79	1.78	1.10	1.08
τ_{22}	60	$\bar{4}0$	7	3	1.36	1.35	0.77	0.76
τ_{22}	60	$\bar{8}0$	7	3	1.06	1.06	0.59	0.58
τ_{22}	120	$\bar{1}0$	7	3	1.73	1.72	1.15	1.14

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Table 5.6 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{22}	120	$\bar{20}$	7	3	1.25	1.24	0.75	0.75
τ_{22}	120	$\bar{40}$	7	3	0.98	0.98	0.54	0.54
τ_{22}	120	$\bar{80}$	7	3	0.72	0.72	0.42	0.42
τ_{31}	15	$\bar{40}$	3	.	1.83	1.73	.	.
τ_{31}	15	$\bar{80}$	3	.	1.36	1.34	.	.
τ_{31}	30	$\bar{20}$	3	0.9	1.49	1.44	0.95	0.93
τ_{31}	30	$\bar{40}$	3	.	1.14	1.11	.	.
τ_{31}	30	$\bar{80}$	3	0.9	0.87	0.85	0.49	0.47
τ_{31}	60	$\bar{10}$	3	.	1.56	1.54	.	.
τ_{31}	60	$\bar{20}$	3	0.9	1.09	1.07	0.64	0.63
τ_{31}	60	$\bar{40}$	3	0.9	0.76	0.75	0.46	0.46
τ_{31}	60	$\bar{80}$	3	0.9	0.59	0.59	0.34	0.34
τ_{31}	120	$\bar{10}$	3	0.9	1.09	1.08	0.71	0.71
τ_{31}	120	$\bar{20}$	3	0.9	0.73	0.72	0.46	0.46
τ_{31}	120	$\bar{40}$	3	0.9	0.56	0.55	0.33	0.32
τ_{31}	120	$\bar{80}$	3	0.9	0.42	0.41	0.23	0.23
τ_{32}	15	$\bar{40}$	1	.	1.58	1.45	.	.
τ_{32}	15	$\bar{80}$	1	.	1.14	1.10	.	.
τ_{32}	30	$\bar{20}$	1	0.3	1.37	1.32	0.81	0.74
τ_{32}	30	$\bar{40}$	1	.	1.02	0.99	.	.
τ_{32}	30	$\bar{80}$	1	0.3	0.78	0.75	0.49	0.47
τ_{32}	60	$\bar{10}$	1	.	1.40	1.35	.	.
τ_{32}	60	$\bar{20}$	1	0.3	0.96	0.94	0.65	0.64

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Table 5.6 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{32}	60	$\bar{4}0$	1	0.3	0.70	0.69	0.45	0.44
τ_{32}	60	$\bar{8}0$	1	0.3	0.48	0.47	0.33	0.32
τ_{32}	120	$\bar{1}0$	1	0.3	1.01	1.00	0.70	0.69
τ_{32}	120	$\bar{2}0$	1	0.3	0.69	0.69	0.46	0.45
τ_{32}	120	$\bar{4}0$	1	0.3	0.49	0.49	0.32	0.32
τ_{32}	120	$\bar{8}0$	1	0.3	0.37	0.37	0.23	0.22
τ_{33}	15	$\bar{4}0$	4	.	1.32	1.26	.	.
τ_{33}	15	$\bar{8}0$	4	.	0.94	0.93	.	.
τ_{33}	30	$\bar{2}0$	4	2	1.40	1.34	0.92	0.85
τ_{33}	30	$\bar{4}0$	4	.	0.96	0.95	.	.
τ_{33}	30	$\bar{8}0$	4	2	0.65	0.65	0.48	0.48
τ_{33}	60	$\bar{1}0$	4	.	1.58	1.54	.	.
τ_{33}	60	$\bar{2}0$	4	2	1.04	1.03	0.74	0.72
τ_{33}	60	$\bar{4}0$	4	2	0.66	0.65	0.51	0.50
τ_{33}	60	$\bar{8}0$	4	2	0.45	0.45	0.33	0.33
τ_{33}	120	$\bar{1}0$	4	2	1.14	1.12	0.84	0.83
τ_{33}	120	$\bar{2}0$	4	2	0.69	0.69	0.54	0.54
τ_{33}	120	$\bar{4}0$	4	2	0.47	0.46	0.35	0.34
τ_{33}	120	$\bar{8}0$	4	2	0.32	0.33	0.24	0.24

5.4.3 Balanced Model 2

Table 5.7: Balanced Positive Definite Solutions for Model 2 Comparing Root Mean Squared Error (RMSE) for REML and FML Estimates of Covariance Parameters Across T1 and T2

					T1 RMSE		**T2 RMSE**	
Parm	**OBS**	**ISU**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
σ^2	2	1	46.58	46.58	1.67	1.66	1.54	1.53
σ^2	3	1	46.58	46.58	1.15	1.16	1.08	1.06
σ^2	4	1	46.58	46.58	0.77	0.77	0.78	0.78
σ^2	1	2	46.58	46.58	1.22	1.22	1.16	1.19
σ^2	2	2	46.58	46.58	0.78	0.78	0.77	0.77
σ^2	3	2	46.58	46.58	0.55	0.55	0.53	0.53
σ^2	4	2	46.58	46.58	0.37	0.37	0.37	0.37
σ^2	1	3	46.58	46.58	0.63	0.63	0.59	0.6
σ^2	2	3	46.58	46.58	0.4	0.4	0.39	0.39
σ^2	3	3	46.58	46.58	0.26	0.26	0.26	0.26
σ^2	4	3	46.58	46.58	0.18	0.18	0.18	0.18
σ^2	1	4	46.58	46.58	0.29	0.29	0.3	0.3
σ^2	2	4	46.58	46.58	0.19	0.19	0.19	0.19
σ^2	3	4	46.58	46.58	0.13	0.13	0.13	0.13
σ^2	4	4	46.58	46.58	0.09	0.09	0.09	0.09
τ_{11}	2	1	12	4	1.08	1.37	0.99	1.07
τ_{11}	3	1	12	4	0.71	0.83	0.66	0.69
τ_{11}	4	1	12	4	0.48	0.52	0.45	0.47
τ_{11}	1	2	12	4	0.81	1.52	0.74	1.04
τ_{11}	2	2	12	4	0.51	0.82	0.48	0.59
τ_{11}	3	2	12	4	0.36	0.49	0.34	0.38

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Table 5.7 – continued from previous page

					T1 RMSE		T2 RMSE	
Parm	**OBS**	**ISU**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{11}	4	2	12	4	0.24	0.29	0.22	0.24
τ_{11}	1	3	12	4	0.41	1.16	0.37	0.62
τ_{11}	2	3	12	4	0.27	0.6	0.25	0.35
τ_{11}	3	3	12	4	0.18	0.33	0.16	0.2
τ_{11}	4	3	12	4	0.12	0.18	0.11	0.13
τ_{11}	1	4	12	4	0.2	0.97	0.18	0.44
τ_{11}	2	4	12	4	0.13	0.49	0.12	0.23
τ_{11}	3	4	12	4	0.09	0.25	0.08	0.13
τ_{11}	4	4	12	4	0.06	0.13	0.05	0.07
τ_{21}	2	1	4	1	1.3	1.26	0.89	0.84
τ_{21}	3	1	4	1	0.91	0.89	0.61	0.6
τ_{21}	4	1	4	1	0.63	0.63	0.43	0.43
τ_{21}	1	2	4	1	1.26	1.21	0.69	0.64
τ_{21}	2	2	4	1	0.85	0.84	0.53	0.51
τ_{21}	3	2	4	1	0.61	0.6	0.39	0.39
τ_{21}	4	2	4	1	0.42	0.42	0.28	0.27
τ_{21}	1	3	4	1	0.81	0.82	0.5	0.47
τ_{21}	2	3	4	1	0.61	0.6	0.37	0.35
τ_{21}	3	3	4	1	0.42	0.41	0.25	0.25
τ_{21}	4	3	4	1	0.3	0.3	0.17	0.17
τ_{21}	1	4	4	1	0.57	0.61	0.36	0.34
τ_{21}	2	4	4	1	0.42	0.43	0.23	0.23
τ_{21}	3	4	4	1	0.3	0.3	0.17	0.17
τ_{21}	4	4	4	1	0.2	0.2	0.12	0.12

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Table 5.7 – continued from previous page

					T1 RMSE		T2 RMSE	
Parm	**OBS**	**ISU**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{22}	2	1	7	3	2	1.93	1.42	1.31
τ_{22}	3	1	7	3	1.36	1.36	0.98	0.97
τ_{22}	4	1	7	3	0.97	0.97	0.71	0.7
τ_{22}	1	2	7	3	1.89	1.86	1.27	1.11
τ_{22}	2	2	7	3	1.26	1.25	0.93	0.9
τ_{22}	3	2	7	3	0.92	0.91	0.63	0.62
τ_{22}	4	2	7	3	0.65	0.64	0.45	0.45
τ_{22}	1	3	7	3	1.31	1.33	0.87	0.83
τ_{22}	2	3	7	3	0.89	0.89	0.63	0.62
τ_{22}	3	3	7	3	0.63	0.63	0.42	0.42
τ_{22}	4	3	7	3	0.46	0.46	0.3	0.3
τ_{22}	1	4	7	3	0.89	0.98	0.58	0.59
τ_{22}	2	4	7	3	0.6	0.64	0.42	0.42
τ_{22}	3	4	7	3	0.45	0.45	0.28	0.28
τ_{22}	4	4	7	3	0.32	0.32	0.2	0.2
τ_{31}	2	1	3	0.9	1.34	1.29	0.88	0.85
τ_{31}	3	1	3	0.9	0.97	0.95	0.65	0.64
τ_{31}	4	1	3	0.9	0.71	0.71	0.46	0.45
τ_{31}	1	2	3	0.9	1.25	1.18	0.75	0.72
τ_{31}	2	2	3	0.9	0.89	0.86	0.55	0.53
τ_{31}	3	2	3	0.9	0.65	0.64	0.4	0.4
τ_{31}	4	2	3	0.9	0.44	0.44	0.28	0.28
τ_{31}	1	3	3	0.9	0.87	0.83	0.51	0.48
τ_{31}	2	3	3	0.9	0.6	0.59	0.37	0.35

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Table 5.7 – continued from previous page

					T1 RMSE		T2 RMSE	
Parm	**OBS**	**ISU**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{31}	3	3	3	0.9	0.42	0.42	0.26	0.26
τ_{31}	4	3	3	0.9	0.3	0.3	0.18	0.18
τ_{31}	1	4	3	0.9	0.58	0.58	0.33	0.32
τ_{31}	2	4	3	0.9	0.43	0.42	0.25	0.24
τ_{31}	3	4	3	0.9	0.29	0.29	0.17	0.17
τ_{31}	4	4	3	0.9	0.2	0.2	0.12	0.12
τ_{32}	2	1	1	0.3	1.34	1.28	0.91	0.79
τ_{32}	3	1	1	0.3	0.91	0.9	0.67	0.65
τ_{32}	4	1	1	0.3	0.63	0.63	0.49	0.48
τ_{32}	1	2	1	0.3	1.24	1.16	0.9	0.84
τ_{32}	2	2	1	0.3	0.84	0.81	0.62	0.6
τ_{32}	3	2	1	0.3	0.61	0.6	0.44	0.43
τ_{32}	4	2	1	0.3	0.41	0.41	0.3	0.3
τ_{32}	1	3	1	0.3	0.84	0.79	0.57	0.53
τ_{32}	2	3	1	0.3	0.55	0.53	0.41	0.4
τ_{32}	3	3	1	0.3	0.39	0.38	0.27	0.27
τ_{32}	4	3	1	0.3	0.3	0.3	0.2	0.2
τ_{32}	1	4	1	0.3	0.56	0.53	0.4	0.37
τ_{32}	2	4	1	0.3	0.4	0.39	0.28	0.27
τ_{32}	3	4	1	0.3	0.28	0.28	0.19	0.18
τ_{32}	4	4	1	0.3	0.19	0.19	0.13	0.13
τ_{33}	2	1	4	2	1.65	1.59	1.21	1.13
τ_{33}	3	1	4	2	1.21	1.2	0.88	0.86
τ_{33}	4	1	4	2	0.86	0.85	0.65	0.64

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Table 5.7 – continued from previous page

					T1 RMSE		T2 RMSE	
Parm	**OBS**	**ISU**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{33}	1	2	4	2	1.47	1.41	1.17	1.1
τ_{33}	2	2	4	2	1.11	1.09	0.79	0.77
τ_{33}	3	2	4	2	0.76	0.75	0.57	0.57
τ_{33}	4	2	4	2	0.53	0.53	0.41	0.41
τ_{33}	1	3	4	2	0.95	0.95	0.74	0.7
τ_{33}	2	3	4	2	0.71	0.71	0.53	0.52
τ_{33}	3	3	4	2	0.5	0.5	0.36	0.36
τ_{33}	4	3	4	2	0.37	0.37	0.25	0.25
τ_{33}	1	4	4	2	0.69	0.71	0.51	0.5
τ_{33}	2	4	4	2	0.48	0.49	0.36	0.35
τ_{33}	3	4	4	2	0.34	0.34	0.23	0.23
τ_{33}	4	4	4	2	0.23	0.23	0.17	0.17

5.4.4 Model 3

Table 5.8: Positive Definite Solutions for Model 3 Comparing Root Mean Squared Error (RMSE) for REML and FML Estimates of Covariance Parameters Across T1 and T2

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
σ^2	15	$\bar{8}0$	46.58	.	1.17	1.19	.	.
σ^2	30	$\bar{2}0$	46.58	.	1.98	1.82	.	.
σ^2	30	$\bar{4}0$	46.58	46.58	1.25	1.25	1.25	1.25

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Table 5.8 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
σ^2	30	$\bar{80}$	46.58	46.58	0.82	0.82	0.80	0.80
σ^2	60	$\bar{10}$	46.58	46.58	2.33	2.32	2.01	1.93
σ^2	60	$\bar{20}$	46.58	46.58	1.35	1.34	1.36	1.36
σ^2	60	$\bar{40}$	46.58	46.58	0.83	0.83	0.84	0.83
σ^2	60	$\bar{80}$	46.58	46.58	0.59	0.59	0.58	0.58
σ^2	120	$\bar{10}$	46.58	46.58	1.59	1.58	1.54	1.52
σ^2	120	$\bar{20}$	46.58	46.58	0.92	0.92	0.97	0.96
σ^2	120	$\bar{40}$	46.58	46.58	0.59	0.59	0.57	0.57
σ^2	120	$\bar{80}$	46.58	46.58	0.41	0.41	0.42	0.42
τ_{11}	15	$\bar{80}$	12	.	3.63	3.88	.	.
τ_{11}	30	$\bar{20}$	12	.	3.31	3.21	.	.
τ_{11}	30	$\bar{40}$	12	4	2.75	2.79	1.23	1.25
τ_{11}	30	$\bar{80}$	12	4	2.25	2.25	1.02	1.01
τ_{11}	60	$\bar{10}$	12	4	2.96	3.03	1.49	1.47
τ_{11}	60	$\bar{20}$	12	4	2.33	2.38	1.12	1.16
τ_{11}	60	$\bar{40}$	12	4	1.71	1.75	0.84	0.86
τ_{11}	60	$\bar{80}$	12	4	1.49	1.47	0.67	0.69
τ_{11}	120	$\bar{10}$	12	4	2.03	2.07	1.08	1.10
τ_{11}	120	$\bar{20}$	12	4	1.46	1.48	0.76	0.78
τ_{11}	120	$\bar{40}$	12	4	1.18	1.20	0.55	0.56
τ_{11}	120	$\bar{80}$	12	4	0.99	1.00	0.45	0.46
τ_{21}	15	$\bar{80}$	4	.	2.43	2.28	.	.
τ_{21}	30	$\bar{20}$	4	.	2.29	2.23	.	.

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Table 5.8 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{21}	30	$\bar{40}$	4	1	1.96	1.90	0.89	0.85
τ_{21}	30	$\bar{80}$	4	1	1.58	1.52	0.73	0.69
τ_{21}	60	$\bar{10}$	4	1	2.07	2.06	1.24	1.07
τ_{21}	60	$\bar{20}$	4	1	1.68	1.66	0.82	0.81
τ_{21}	60	$\bar{40}$	4	1	1.28	1.27	0.62	0.61
τ_{21}	60	$\bar{80}$	4	1	1.03	1.01	0.48	0.47
τ_{21}	120	$\bar{10}$	4	1	1.45	1.45	0.77	0.76
τ_{21}	120	$\bar{20}$	4	1	1.05	1.05	0.58	0.58
τ_{21}	120	$\bar{40}$	4	1	0.86	0.86	0.42	0.42
τ_{21}	120	$\bar{80}$	4	1	0.71	0.71	0.33	0.33
τ_{22}	15	$\bar{80}$	7	.	2.57	2.29	.	.
τ_{22}	30	$\bar{20}$	7	.	2.64	2.69	.	.
τ_{22}	30	$\bar{40}$	7	3	2.11	2.05	1.16	1.13
τ_{22}	30	$\bar{80}$	7	3	1.69	1.63	0.93	0.90
τ_{22}	60	$\bar{10}$	7	3	2.29	2.30	1.73	1.62
τ_{22}	60	$\bar{20}$	7	3	1.84	1.83	1.17	1.15
τ_{22}	60	$\bar{40}$	7	3	1.40	1.41	0.82	0.81
τ_{22}	60	$\bar{80}$	7	3	1.05	1.04	0.61	0.60
τ_{22}	120	$\bar{10}$	7	3	1.72	1.72	1.14	1.12
τ_{22}	120	$\bar{20}$	7	3	1.21	1.21	0.80	0.79
τ_{22}	120	$\bar{40}$	7	3	0.93	0.93	0.55	0.55
τ_{22}	120	$\bar{80}$	7	3	0.73	0.73	0.42	0.42
τ_{31}	15	$\bar{80}$	3	.	1.59	1.35	.	.

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Table 5.8 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{31}	30	$\bar{20}$	3	.	1.67	1.42	.	.
τ_{31}	30	$\bar{40}$	3	0.9	1.25	1.17	0.71	0.66
τ_{31}	30	$\bar{80}$	3	0.9	0.91	0.85	0.52	0.49
τ_{31}	60	$\bar{10}$	3	0.9	1.43	1.40	1.05	1.04
τ_{31}	60	$\bar{20}$	3	0.9	1.15	1.12	0.69	0.67
τ_{31}	60	$\bar{40}$	3	0.9	0.82	0.79	0.48	0.47
τ_{31}	60	$\bar{80}$	3	0.9	0.61	0.59	0.35	0.34
τ_{31}	120	$\bar{10}$	3	0.9	1.15	1.13	0.69	0.68
τ_{31}	120	$\bar{20}$	3	0.9	0.75	0.74	0.48	0.47
τ_{31}	120	$\bar{40}$	3	0.9	0.58	0.58	0.32	0.31
τ_{31}	120	$\bar{80}$	3	0.9	0.42	0.41	0.24	0.24
τ_{32}	15	$\bar{80}$	1	.	1.34	1.14	.	.
τ_{32}	30	$\bar{20}$	1	.	1.53	1.37	.	.
τ_{32}	30	$\bar{40}$	1	0.3	1.06	0.99	0.66	0.61
τ_{32}	30	$\bar{80}$	1	0.3	0.78	0.72	0.51	0.47
τ_{32}	60	$\bar{10}$	1	0.3	1.28	1.24	1.14	1.13
τ_{32}	60	$\bar{20}$	1	0.3	1.05	1.01	0.66	0.63
τ_{32}	60	$\bar{40}$	1	0.3	0.72	0.70	0.47	0.45
τ_{32}	60	$\bar{80}$	1	0.3	0.53	0.51	0.33	0.32
τ_{32}	120	$\bar{10}$	1	0.3	1.00	0.98	0.73	0.71
τ_{32}	120	$\bar{20}$	1	0.3	0.70	0.68	0.47	0.46
τ_{32}	120	$\bar{40}$	1	0.3	0.50	0.49	0.32	0.32
τ_{32}	120	$\bar{80}$	1	0.3	0.37	0.37	0.23	0.23

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Table 5.8 – continued from previous page

					T1		T2	
Covparm	**ISU**	**OBS**	$\boldsymbol{\theta}_{T1}$	$\boldsymbol{\theta}_{T2}$	**RML**	**FML**	**RML**	**FML**
τ_{33}	15	$\bar{8}0$	4	.	1.13	0.98	.	.
τ_{33}	30	$\bar{2}0$	4	.	1.51	1.38	.	.
τ_{33}	30	$\bar{4}0$	4	2	1.00	0.97	0.75	0.71
τ_{33}	30	$\bar{8}0$	4	2	0.66	0.64	0.47	0.46
τ_{33}	60	$\bar{1}0$	4	2	1.72	1.62	1.00	0.91
τ_{33}	60	$\bar{2}0$	4	2	1.06	1.02	0.74	0.72
τ_{33}	60	$\bar{4}0$	4	2	0.71	0.69	0.49	0.47
τ_{33}	60	$\bar{8}0$	4	2	0.47	0.46	0.36	0.35
τ_{33}	120	$\bar{1}0$	4	2	1.17	1.17	0.83	0.81
τ_{33}	120	$\bar{2}0$	4	2	0.73	0.73	0.54	0.53
τ_{33}	120	$\bar{4}0$	4	2	0.48	0.48	0.35	0.34
τ_{33}	120	$\bar{8}0$	4	2	0.32	0.32	0.23	0.23

5.5 Appendix 3: Fixed Effect PRB Tables

5.5.1 Model 1

Table 5.9: Positive Definite Solutions for Model 1 Comparing Percent Relative Bias for REML and FML Estimates of Fixed Effects Across T1 and T2

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{00}	1	1	5	-0.17	-0.16	0.08	0.12

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Table 5.9 – continued from previous page

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{00}	2	1	5	0.27	0.27	0.06	0.06
γ_{00}	3	1	5	-0.01	-0.00	-0.05	-0.05
γ_{00}	4	1	5	-0.03	-0.03	-0.01	-0.01
γ_{00}	1	2	5	0.12	0.12	-0.01	0.01
γ_{00}	2	2	5	0.16	0.16	-0.06	-0.06
γ_{00}	3	2	5	-0.05	-0.05	0.08	0.08
γ_{00}	4	2	5	-0.08	-0.08	0.00	0.00
γ_{00}	1	3	5	0.08	0.08	0.01	0.01
γ_{00}	2	3	5	0.05	0.05	-0.01	-0.01
γ_{00}	3	3	5	-0.05	-0.05	0.01	0.01
γ_{00}	4	3	5	0.05	0.05	0.00	-0.00
γ_{00}	1	4	5	-0.06	-0.06	-0.04	-0.03
γ_{00}	2	4	5	-0.09	-0.09	-0.05	-0.05
γ_{00}	3	4	5	-0.03	-0.03	0.00	0.00
γ_{00}	4	4	5	-0.06	-0.06	0.03	0.03

5.5.2 Model 2

Table 5.10: Positive Definite Solutions for Model 2 Comparing Percent Relative Bias for REML and FML Estimates of Fixed Effects Across T1 and T2

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{00}	15	$\bar{4}0$	5	-0.93	-1.17	.	.

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Table 5.10 – continued from previous page

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{00}	15	$\bar{8}0$	5	0.00	0.03	.	.
γ_{00}	30	$\bar{2}0$	5	0.55	0.52	0.85	0.70
γ_{00}	30	$\bar{4}0$	5	0.39	0.38	.	.
γ_{00}	30	$\bar{8}0$	5	-0.10	-0.10	0.18	0.18
γ_{00}	60	$\bar{1}0$	5	0.18	0.20	.	.
γ_{00}	60	$\bar{2}0$	5	0.26	0.25	-0.05	-0.08
γ_{00}	60	$\bar{4}0$	5	0.02	0.02	0.03	0.03
γ_{00}	60	$\bar{8}0$	5	-0.10	-0.10	0.11	0.11
γ_{00}	120	$\bar{1}0$	5	0.20	0.20	0.06	0.07
γ_{00}	120	$\bar{2}0$	5	0.17	0.17	-0.00	-0.00
γ_{00}	120	$\bar{4}0$	5	0.17	0.17	0.02	0.02
γ_{00}	120	$\bar{8}0$	5	0.02	0.02	-0.02	-0.02
γ_{10}	15	$\bar{4}0$	0.98	-5.56	-6.84	.	.
γ_{10}	15	$\bar{8}0$	0.98	0.61	0.43	.	.
γ_{10}	30	$\bar{2}0$	0.98	2.90	2.80	2.37	1.04
γ_{10}	30	$\bar{4}0$	0.98	1.74	1.72	.	.
γ_{10}	30	$\bar{8}0$	0.98	-0.18	-0.19	0.90	0.92
γ_{10}	60	$\bar{1}0$	0.98	0.62	-0.10	.	.
γ_{10}	60	$\bar{2}0$	0.98	1.79	1.76	0.43	0.28
γ_{10}	60	$\bar{4}0$	0.98	0.36	0.36	0.35	0.36
γ_{10}	60	$\bar{8}0$	0.98	-0.60	-0.61	0.35	0.34
γ_{10}	120	$\bar{1}0$	0.98	0.86	0.85	0.13	0.22
γ_{10}	120	$\bar{2}0$	0.98	0.63	0.63	0.20	0.19
γ_{10}	120	$\bar{4}0$	0.98	0.72	0.72	0.07	0.07

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Table 5.10 – continued from previous page

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{10}	120	$\bar{8}0$	0.98	0.15	0.16	-0.07	-0.07
γ_{20}	15	$\bar{4}0$	2.3	-0.93	-0.87	.	.
γ_{20}	15	$\bar{8}0$	2.3	0.04	-0.58	.	.
γ_{20}	30	$\bar{2}0$	2.3	-1.84	-1.80	-1.67	-1.71
γ_{20}	30	$\bar{4}0$	2.3	-0.25	-0.25	.	.
γ_{20}	30	$\bar{8}0$	2.3	-0.18	-0.18	-0.01	-0.01
γ_{20}	60	$\bar{1}0$	2.3	0.24	0.68	.	.
γ_{20}	60	$\bar{2}0$	2.3	0.02	0.02	-0.25	-0.20
γ_{20}	60	$\bar{4}0$	2.3	-0.01	-0.01	0.14	0.14
γ_{20}	60	$\bar{8}0$	2.3	0.03	0.03	0.01	0.01
γ_{20}	120	$\bar{1}0$	2.3	0.01	0.01	0.43	0.37
γ_{20}	120	$\bar{2}0$	2.3	0.14	0.14	-0.37	-0.37
γ_{20}	120	$\bar{4}0$	2.3	0.03	0.03	0.14	0.14
γ_{20}	120	$\bar{8}0$	2.3	-0.03	-0.03	0.05	0.05

5.5.3 Model 3

Table 5.11: Positive Definite Solutions for Model 3 Comparing Percent Relative Bias for REML and FML Estimates of Fixed Effects Across T1 and T2

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{00}	15	$\bar{8}0$	5	0.48	1.69	.	.
γ_{00}	30	$\bar{2}0$	5	-1.23	0.60	.	.

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Table 5.11 – continued from previous page

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{00}	30	$\bar{4}0$	5	0.07	0.08	0.17	0.10
γ_{00}	30	$\bar{8}0$	5	-0.16	-0.17	0.23	0.25
γ_{00}	60	$\bar{1}0$	5	6.58	6.69	-1.32	-0.96
γ_{00}	60	$\bar{2}0$	5	1.25	1.26	-0.18	-0.22
γ_{00}	60	$\bar{4}0$	5	0.19	0.20	-0.03	-0.03
γ_{00}	60	$\bar{8}0$	5	-0.54	-0.54	0.05	0.05
γ_{00}	120	$\bar{1}0$	5	0.30	0.37	-0.19	-0.14
γ_{00}	120	$\bar{2}0$	5	0.05	0.05	-0.10	-0.08
γ_{00}	120	$\bar{4}0$	5	0.11	0.11	0.21	0.21
γ_{00}	120	$\bar{8}0$	5	-0.28	-0.29	0.03	0.03
γ_{01}	15	$\bar{8}0$	1.9	-2.67	-6.44	.	.
γ_{01}	30	$\bar{2}0$	1.9	7.17	-0.39	.	.
γ_{01}	30	$\bar{4}0$	1.9	-0.68	-0.71	-1.53	-1.30
γ_{01}	30	$\bar{8}0$	1.9	0.41	0.43	-0.53	-0.58
γ_{01}	60	$\bar{1}0$	1.9	-22.19	-22.53	3.66	2.26
γ_{01}	60	$\bar{2}0$	1.9	-4.39	-4.41	0.31	0.37
γ_{01}	60	$\bar{4}0$	1.9	0.03	0.01	0.24	0.23
γ_{01}	60	$\bar{8}0$	1.9	1.83	1.84	-0.61	-0.63
γ_{01}	120	$\bar{1}0$	1.9	-1.29	-1.54	0.32	0.18
γ_{01}	120	$\bar{2}0$	1.9	-0.82	-0.82	0.38	0.31
γ_{01}	120	$\bar{4}0$	1.9	-0.15	-0.15	-0.37	-0.37
γ_{01}	120	$\bar{8}0$	1.9	0.93	0.94	0.03	0.02
γ_{10}	15	$\bar{8}0$	0.98	1.72	7.63	.	.
γ_{10}	30	$\bar{2}0$	0.98	-4.38	5.16	.	.

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Table 5.11 – continued from previous page

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{10}	30	$\bar{4}0$	0.98	0.29	0.31	0.57	0.29
γ_{10}	30	$\bar{8}0$	0.98	-0.59	-0.63	0.94	1.03
γ_{10}	60	$\bar{1}0$	0.98	30.29	30.81	-6.07	-4.91
γ_{10}	60	$\bar{2}0$	0.98	5.49	5.53	-0.59	-0.84
γ_{10}	60	$\bar{4}0$	0.98	0.84	0.86	-0.25	-0.23
γ_{10}	60	$\bar{8}0$	0.98	-2.13	-2.15	0.25	0.27
γ_{10}	120	$\bar{1}0$	0.98	1.37	1.68	-0.76	-0.58
γ_{10}	120	$\bar{2}0$	0.98	0.29	0.29	-0.28	-0.21
γ_{10}	120	$\bar{4}0$	0.98	0.53	0.52	1.12	1.12
γ_{10}	120	$\bar{8}0$	0.98	-1.09	-1.10	0.25	0.25
γ_{11}	15	$\bar{8}0$	1.3	-2.16	-6.42	.	.
γ_{11}	30	$\bar{2}0$	1.3	9.41	-1.40	.	.
γ_{11}	30	$\bar{4}0$	1.3	-0.56	-0.60	-1.37	-1.09
γ_{11}	30	$\bar{8}0$	1.3	0.40	0.42	-0.75	-0.81
γ_{11}	60	$\bar{1}0$	1.3	-27.91	-28.31	3.98	2.26
γ_{11}	60	$\bar{2}0$	1.3	-6.01	-6.04	-0.32	-0.18
γ_{11}	60	$\bar{4}0$	1.3	0.48	0.45	0.53	0.52
γ_{11}	60	$\bar{8}0$	1.3	2.43	2.45	-0.97	-1.00
γ_{11}	120	$\bar{1}0$	1.3	-1.31	-1.63	-0.33	-0.45
γ_{11}	120	$\bar{2}0$	1.3	-0.55	-0.55	0.23	0.13
γ_{11}	120	$\bar{4}0$	1.3	0.20	0.21	-0.63	-0.63
γ_{11}	120	$\bar{8}0$	1.3	0.87	0.88	0.23	0.23
γ_{20}	15	$\bar{8}0$	2.3	-0.24	-0.24	.	.
γ_{20}	30	$\bar{2}0$	2.3	0.41	0.61	.	.

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Table 5.11 – continued from previous page

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{20}	30	$\bar{4}0$	2.3	-0.39	-0.39	0.13	0.09
γ_{20}	30	$\bar{8}0$	2.3	-0.10	-0.10	-0.04	-0.04
γ_{20}	60	$\bar{1}0$	2.3	0.22	0.18	1.46	1.24
γ_{20}	60	$\bar{2}0$	2.3	0.17	0.17	0.32	0.33
γ_{20}	60	$\bar{4}0$	2.3	-0.25	-0.25	0.26	0.26
γ_{20}	60	$\bar{8}0$	2.3	-0.01	-0.01	0.15	0.16
γ_{20}	120	$\bar{1}0$	2.3	-0.38	-0.41	0.04	0.03
γ_{20}	120	$\bar{2}0$	2.3	-0.46	-0.46	0.07	0.06
γ_{20}	120	$\bar{4}0$	2.3	-0.13	-0.13	0.13	0.13
γ_{20}	120	$\bar{8}0$	2.3	0.05	0.05	-0.12	-0.12
γ_{21}	15	$\bar{8}0$	0.85	2.02	0.79	.	.
γ_{21}	30	$\bar{2}0$	0.85	1.30	0.39	.	.
γ_{21}	30	$\bar{4}0$	0.85	0.96	0.97	-2.28	-2.05
γ_{21}	30	$\bar{8}0$	0.85	1.13	1.13	-0.20	-0.19
γ_{21}	60	$\bar{1}0$	0.85	-13.11	-13.20	-4.31	-4.34
γ_{21}	60	$\bar{2}0$	0.85	-1.50	-1.52	-0.64	-0.70
γ_{21}	60	$\bar{4}0$	0.85	0.42	0.42	-0.18	-0.17
γ_{21}	60	$\bar{8}0$	0.85	-0.11	-0.11	0.26	0.25
γ_{21}	120	$\bar{1}0$	0.85	2.55	2.56	-0.24	0.05
γ_{21}	120	$\bar{2}0$	0.85	0.65	0.66	-0.05	-0.03
γ_{21}	120	$\bar{4}0$	0.85	0.29	0.29	-0.54	-0.54
γ_{21}	120	$\bar{8}0$	0.85	0.11	0.11	0.08	0.08

5.6 Appendix 4: Fixed Effect RMSE Tables

5.6.1 Model 1

Table 5.12: Positive Definite Solutions for Model 1 Comparing Root Mean Squared Error (RMSE) for REML and FML Estimates of Fixed Effects Across T1 and T2

				T1		T2	
Effect	**ISU**	**OBS**	θ	**RML**	**FML**	**RML**	**FML**
γ_{00}	1	1	5	0.31	0.32	0.29	0.29
γ_{00}	2	1	5	0.23	0.23	0.20	0.20
γ_{00}	3	1	5	0.15	0.15	0.14	0.14
γ_{00}	4	1	5	0.10	0.10	0.10	0.10
γ_{00}	1	2	5	0.23	0.23	0.21	0.21
γ_{00}	2	2	5	0.15	0.15	0.15	0.15
γ_{00}	3	2	5	0.11	0.11	0.11	0.11
γ_{00}	4	2	5	0.08	0.08	0.07	0.07
γ_{00}	1	3	5	0.16	0.16	0.15	0.16
γ_{00}	2	3	5	0.11	0.11	0.11	0.11
γ_{00}	3	3	5	0.08	0.08	0.08	0.08
γ_{00}	4	3	5	0.06	0.06	0.05	0.05
γ_{00}	1	4	5	0.11	0.11	0.11	0.11
γ_{00}	2	4	5	0.08	0.08	0.08	0.08
γ_{00}	3	4	5	0.06	0.06	0.05	0.05
γ_{00}	4	4	5	0.04	0.04	0.04	0.04

5.6.2 Model 2

Table 5.13: Positive Definite Solutions for Model 2 Comparing Root Mean Squared Error (RMSE) for REML and FML Estimates of Fixed Effects Across T1 and T2

				T1		**T2**	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{00}	15	$\bar{40}$	5	0.56	0.56	.	.
γ_{00}	15	$\bar{80}$	5	0.48	0.47	.	.
γ_{00}	30	$\bar{20}$	5	0.43	0.43	0.45	0.46
γ_{00}	30	$\bar{40}$	5	0.36	0.36	.	.
γ_{00}	30	$\bar{80}$	5	0.31	0.31	0.24	0.24
γ_{00}	60	$\bar{10}$	5	0.36	0.37	.	.
γ_{00}	60	$\bar{20}$	5	0.30	0.30	0.23	0.23
γ_{00}	60	$\bar{40}$	5	0.26	0.26	0.19	0.19
γ_{00}	60	$\bar{80}$	5	0.21	0.21	0.16	0.16
γ_{00}	120	$\bar{10}$	5	0.25	0.25	0.18	0.18
γ_{00}	120	$\bar{20}$	5	0.20	0.20	0.16	0.16
γ_{00}	120	$\bar{40}$	5	0.18	0.18	0.14	0.14
γ_{00}	120	$\bar{80}$	5	0.15	0.15	0.11	0.11
γ_{10}	15	$\bar{40}$	0.98	0.50	0.51	.	.
γ_{10}	15	$\bar{80}$	0.98	0.41	0.40	.	.
γ_{10}	30	$\bar{20}$	0.98	0.39	0.40	0.41	0.42
γ_{10}	30	$\bar{40}$	0.98	0.32	0.32	.	.
γ_{10}	30	$\bar{80}$	0.98	0.27	0.27	0.22	0.22
γ_{10}	60	$\bar{10}$	0.98	0.35	0.35	.	.
γ_{10}	60	$\bar{20}$	0.98	0.28	0.28	0.22	0.22
γ_{10}	60	$\bar{40}$	0.98	0.23	0.23	0.17	0.17
γ_{10}	60	$\bar{80}$	0.98	0.18	0.18	0.15	0.15
γ_{10}	120	$\bar{10}$	0.98	0.24	0.24	0.18	0.18

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Table 5.13 – continued from previous page

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{10}	120	$\bar{2}0$	0.98	0.19	0.19	0.15	0.15
γ_{10}	120	$\bar{4}0$	0.98	0.16	0.16	0.13	0.13
γ_{10}	120	$\bar{8}0$	0.98	0.13	0.13	0.10	0.10
γ_{20}	15	$\bar{4}0$	2.3	0.19	0.19	.	.
γ_{20}	15	$\bar{8}0$	2.3	0.15	0.15	.	.
γ_{20}	30	$\bar{2}0$	2.3	0.22	0.22	0.22	0.23
γ_{20}	30	$\bar{4}0$	2.3	0.16	0.16	.	.
γ_{20}	30	$\bar{8}0$	2.3	0.11	0.11	0.10	0.10
γ_{20}	60	$\bar{1}0$	2.3	0.22	0.22	.	.
γ_{20}	60	$\bar{2}0$	2.3	0.16	0.16	0.15	0.14
γ_{20}	60	$\bar{4}0$	2.3	0.11	0.11	0.10	0.10
γ_{20}	60	$\bar{8}0$	2.3	0.07	0.07	0.08	0.08
γ_{20}	120	$\bar{1}0$	2.3	0.16	0.16	0.14	0.14
γ_{20}	120	$\bar{2}0$	2.3	0.10	0.10	0.10	0.10
γ_{20}	120	$\bar{4}0$	2.3	0.08	0.08	0.07	0.07
γ_{20}	120	$\bar{8}0$	2.3	0.05	0.05	0.05	0.05

5.6.3 Model 3

Table 5.14: Positive Definite Solutions for Model 3 Comparing Root Mean Squared Error (RMSE) for REML and FML Estimates of Fixed Effects Across T1 and T2

				T1		**T2**	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{00}	15	$\bar{8}0$	5	0.67	0.72	.	.
γ_{00}	30	$\bar{2}0$	5	0.96	1.00	.	.
γ_{00}	30	$\bar{4}0$	5	0.67	0.69	0.63	0.65
γ_{00}	30	$\bar{8}0$	5	0.48	0.49	0.47	0.48
γ_{00}	60	$\bar{1}0$	5	0.83	0.84	0.86	0.82
γ_{00}	60	$\bar{2}0$	5	0.71	0.72	0.63	0.64
γ_{00}	60	$\bar{4}0$	5	0.49	0.50	0.47	0.47
γ_{00}	60	$\bar{8}0$	5	0.32	0.32	0.34	0.34
γ_{00}	120	$\bar{1}0$	5	0.73	0.73	0.64	0.64
γ_{00}	120	$\bar{2}0$	5	0.49	0.50	0.47	0.48
γ_{00}	120	$\bar{4}0$	5	0.35	0.35	0.34	0.34
γ_{00}	120	$\bar{8}0$	5	0.24	0.24	0.24	0.25
γ_{01}	15	$\bar{8}0$	1.9	0.77	0.82	.	.
γ_{01}	30	$\bar{2}0$	1.9	1.21	1.28	.	.
γ_{01}	30	$\bar{4}0$	1.9	0.84	0.86	0.79	0.81
γ_{01}	30	$\bar{8}0$	1.9	0.62	0.63	0.59	0.60
γ_{01}	60	$\bar{1}0$	1.9	1.15	1.16	1.11	1.06
γ_{01}	60	$\bar{2}0$	1.9	0.94	0.95	0.82	0.83
γ_{01}	60	$\bar{4}0$	1.9	0.66	0.66	0.61	0.62
γ_{01}	60	$\bar{8}0$	1.9	0.43	0.44	0.45	0.46
γ_{01}	120	$\bar{1}0$	1.9	0.98	0.98	0.84	0.85
γ_{01}	120	$\bar{2}0$	1.9	0.69	0.69	0.62	0.63
γ_{01}	120	$\bar{4}0$	1.9	0.49	0.49	0.47	0.47

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Table 5.14 – continued from previous page

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{01}	120	$\bar{8}0$	1.9	0.33	0.33	0.34	0.34
γ_{10}	15	$\bar{8}0$	0.98	0.56	0.60	.	.
γ_{10}	30	$\bar{2}0$	0.98	0.83	0.86	.	.
γ_{10}	30	$\bar{4}0$	0.98	0.58	0.59	0.55	0.56
γ_{10}	30	$\bar{8}0$	0.98	0.41	0.42	0.40	0.41
γ_{10}	60	$\bar{1}0$	0.98	0.71	0.72	0.75	0.71
γ_{10}	60	$\bar{2}0$	0.98	0.61	0.62	0.55	0.55
γ_{10}	60	$\bar{4}0$	0.98	0.42	0.42	0.40	0.40
γ_{10}	60	$\bar{8}0$	0.98	0.27	0.27	0.29	0.29
γ_{10}	120	$\bar{1}0$	0.98	0.63	0.63	0.56	0.56
γ_{10}	120	$\bar{2}0$	0.98	0.43	0.43	0.41	0.41
γ_{10}	120	$\bar{4}0$	0.98	0.29	0.30	0.29	0.29
γ_{10}	120	$\bar{8}0$	0.98	0.20	0.20	0.21	0.21
γ_{11}	15	$\bar{8}0$	1.3	0.65	0.67	.	.
γ_{11}	30	$\bar{2}0$	1.3	1.02	1.09	.	.
γ_{11}	30	$\bar{4}0$	1.3	0.72	0.74	0.68	0.69
γ_{11}	30	$\bar{8}0$	1.3	0.53	0.54	0.49	0.50
γ_{11}	60	$\bar{1}0$	1.3	0.99	0.99	0.89	0.87
γ_{11}	60	$\bar{2}0$	1.3	0.79	0.80	0.70	0.70
γ_{11}	60	$\bar{4}0$	1.3	0.55	0.56	0.51	0.52
γ_{11}	60	$\bar{8}0$	1.3	0.37	0.37	0.38	0.38
γ_{11}	120	$\bar{1}0$	1.3	0.82	0.82	0.71	0.71
γ_{11}	120	$\bar{2}0$	1.3	0.57	0.58	0.53	0.53
γ_{11}	120	$\bar{4}0$	1.3	0.41	0.41	0.39	0.39

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Table 5.14 – continued from previous page

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{11}	120	$\bar{8}0$	1.3	0.28	0.28	0.28	0.29
γ_{20}	15	$\bar{8}0$	2.3	0.17	0.17	.	.
γ_{20}	30	$\bar{2}0$	2.3	0.25	0.25	.	.
γ_{20}	30	$\bar{4}0$	2.3	0.17	0.17	0.17	0.17
γ_{20}	30	$\bar{8}0$	2.3	0.12	0.12	0.11	0.11
γ_{20}	60	$\bar{1}0$	2.3	0.26	0.26	0.27	0.27
γ_{20}	60	$\bar{2}0$	2.3	0.17	0.17	0.16	0.16
γ_{20}	60	$\bar{4}0$	2.3	0.12	0.12	0.12	0.12
γ_{20}	60	$\bar{8}0$	2.3	0.08	0.08	0.08	0.08
γ_{20}	120	$\bar{1}0$	2.3	0.18	0.18	0.16	0.17
γ_{20}	120	$\bar{2}0$	2.3	0.12	0.12	0.12	0.12
γ_{20}	120	$\bar{4}0$	2.3	0.09	0.09	0.08	0.08
γ_{20}	120	$\bar{8}0$	2.3	0.05	0.05	0.06	0.06
γ_{21}	15	$\bar{8}0$	0.85	0.26	0.27	.	.
γ_{21}	30	$\bar{2}0$	0.85	0.39	0.39	.	.
γ_{21}	30	$\bar{4}0$	0.85	0.28	0.28	0.26	0.27
γ_{21}	30	$\bar{8}0$	0.85	0.18	0.18	0.18	0.18
γ_{21}	60	$\bar{1}0$	0.85	0.44	0.44	0.37	0.39
γ_{21}	60	$\bar{2}0$	0.85	0.27	0.27	0.26	0.26
γ_{21}	60	$\bar{4}0$	0.85	0.19	0.19	0.18	0.18
γ_{21}	60	$\bar{8}0$	0.85	0.13	0.13	0.13	0.13
γ_{21}	120	$\bar{1}0$	0.85	0.29	0.29	0.26	0.26
γ_{21}	120	$\bar{2}0$	0.85	0.20	0.20	0.19	0.19
γ_{21}	120	$\bar{4}0$	0.85	0.14	0.14	0.13	0.13

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Table 5.14 – continued from previous page

				T1		T2	
Effect	**ISU**	**OBS**	$\boldsymbol{\theta}$	**RML**	**FML**	**RML**	**FML**
γ_{21}	120	$\bar{8}0$	0.85	0.09	0.09	0.09	0.09

References

Ahrens, H. (1976). Multivariate variance-covariance components (mvcc) and generalized intraclass correlation coefficient (gicc). *Biometrische Zeitschrift*, *18*, 527-534.

Bassiri, D. (1988). *Large and small sample properties of maximum likelihood estimates for the hierarchical linear model.* Unpublished doctoral dissertation, Michigan State University, East Lansing, MI.

Box, G. E. P. (1979). Some problems in statistics and everyday life. *Journal of the American Statistical Association*, *74*, 1-4.

Cohen, J. (1988). *Statistical power analysis for the behavioral sciences.* New York: LEA.

Corbeil, R. R., & Searle, S. R. (1976). A comparison of variance component estimators. *Biometrics*, *32*, 779-791.

Cudeck, R., & Browne, M. W. (1992). Constructing a covariance matrix that yields a specified minimizer and a specified minimum discrepancy function value. *Journal of Statistical Computing and Simulation*, *57*, 357-369.

Demidenko, E. (2004). *Mixed models: Theory and applications.* New York: Wiley.

Fai, A. H. T., & Cornelius, P. L. (1996). Approximate f-tests of multiple degree of freedom hypotheses in generalized least squares analyses of unbalanced split-plot experiments. *Journal of Statistical Computing and Simulation*, *54*, 363-378.

Goldstein, H. (1986). Multilevel mixed linear model analysis using Iterative Generalized Least Squares. *Biometrika*, *73*, 43-56.

Hartley, H. O., & Rao, J. (1967). Maximum likelihood estimation for the mixed analysis of variance model. *Biometrika*, *54*, 93-108.

Harville, D. A. (1974). Optimal procedures for some constrained selection problems. *Journal of the American Statistical Association*, *69*, 446-452.

Harville, D. A., & Jeske, D. R. (1992). Mean squared error of estimation or prediction under a general linear model. *Journal of the American Statistical Association*, *87*, 724-731.

Henderson, C. R. (1953). Estimation of variance and covariance components. *Biometrics*, *9*, 226-252.

Hoel, P. G., Port, S. C., & Stone, C. J. (1971). *Introduction to statistical theory.* Boston: Houghton Mifflin.

Hox, J., & Maas, C. (2002). *Social science methodology in the new millennium. proceedings of the fifth international conference on logic and methodology. second expanded edition.*

Huttonlocher, J. E., Haight, W., Bryk, A. S., & Sletzer, M. (1991). Early vocabulary growth: Relation to language input and gender. *Developmental Psychology*, *27*, 236-249.

Kackar, R. N., & Harville, D. A. (1984). Approximations for standard errors of estimators of fixed and random effects in mixed linear models. *Journal of the American Statistical Association*, *79*, 853-861.

Kaplan, D. (1988). The impact of specification error on the estimation, testing, and improvement of structural equation models. *Multivariate Behavioral Research*, *23*, 69-86.

Kellam, S. G., Ling, X., Merisca, R., Brown, C. H., & Ialongo, N. (1998). The effect of the level of aggression in the first grade classroom on the course and malleability of aggressive behavior into middle school. *Development and Psychopathology*, *10*, 165-185.

Kenward, M. G., & Roger, J. H. (1997). Small sample inference for fixed effects from restricted maximum likelihood. *Biometrics*, *53*, 983-997.

Keselman, H. J., Algina, J., Kowalchuck, R. K., & Wolfinger, R. D. (1998). A comparison of two approaches for selecting covariance structures in the analysis of repeated measuarements. *Communications in Statistics: Simulation and Computation*, *27*, 591-604.

Kovacevic, M. S., & Rai, S. N. (2003). A pseudo maximum likelihood approach to multilevel modelling of survey data. *Communications in Statistics: Theory and Methods*, *32*, 103-121.

Longford, N. T. (1995). *Random coefficient models*. New York: Oxford University Press.

Mok, M. (1995). Sample size requirements for 2-level designs in educational research. *Multilevel Modeling Newsletter*, *7*, 11-15.

Morrell, C. H. (1998). Likelihood ratio testing of variance components in the linear mixed-effects model using restricted maximum likelihood. *Biometrics*, *54*, 1560-1568.

Muller, K. E., & Stewart, P. W. (2006). *Linear model theory: Univariate, multivariate, and mixed models*. New Jersey: Wiley.

Patterson, H. D., & Thompson, R. (1971). Recovery of inter-block information when block sizes are unequal. *Biometrika*, *58*, 545-554.

Pfefferman, D., Skinner, C. J., Holmes, D. J., Goldstein, H., & Rasbash, J. (1998). Weighting for unequal selection probabilities in multilevel models. *Journal of the Royal Statistical Society, Series B, Statistical Methodology*, *60*, 23-40.

Prasad, N. G. N., & Rao, J. N. K. (1990). The estimation of the mean squared error of small-area-estimators. *Journal of the American Statistical Association*, *85*, 163-171.

Rabe-Hesketh, S., & Skrondal, A. (2005). Multilevel modeling of complex survey data. *Journal of the Royal Statistical Society, Series A, Statistics in Society*, *169*, 805-827.

Rao, J. N. K. (1977). Maximum likelihood approaches to variance component estimation and to related problems: Comment. *Journal of the American Statistical Association*, *72*, 338-339.

Raudenbush, S. W., & Bryk, A. S. (2002). *Hierarchical linear models: Applications and data analysis methods (2nd ed.).* Thousand Oaks, CA: Sage.

Schalje, M. J. B., B. G., & Fellingham, G. W. (2001). Approximations to distributions of test statistics in complex mixed linear models using sas proc mixed. *Proceedings of the Twenty Sixth Annual SAS Users Group International Conference*, *26*, 1-5.

Scott, A. J., & Holt, D. (1982). The effect of two-stage sampling on ordinary least squares methods. *Journal of the American Statistical Association*, *77*, 848-854.

Searle, S. R., Casella, G., & McCulloch, C. E. (1992). *Variance components*. New York: Wiley.

Swallow, W. H., & Monahan, J. F. (1984). Monte Carlo comparison of ANOVA, MIVQUE, REML, and ML estimators of variance components. *Technometrics*, *28*, 47-57.

Swallow, W. H., & Searle, S. R. (1978). Minimum variance quadratic unbiased estimation (mivque) of variance components. *Technometrics*, *20*, 265-272.

Wolfinger, R. D. (1993). Covariance structure selection in general mixed models. *Communications in Statistics: Simulation and Computation*, *22*, 1079-1106.

Wolfinger, R. D. (1996). Heterogeneous variance-covariance structures for repeated measures. *Journal of Agricultural, Biological, and Environmental Statistics*, *1*, 205-230.

Wolfinger, R. D., Tobias, S., & Sall, J. (1994). Computing gaussian likelihoods and their derivatives for general linear mixed models. *SIAM Journal of Scientific Computing*, *15*, 1294-1310.