Multi-level Modelling and Spatial Inference for Large-Scale Neuroimaging Data

Supplementary Material A

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Submitted in support of the thesis "Multi-level Modelling and Spatial Inference for Large-Scale Neuroimaging Data".

S1 Baseline Truth for Parameter Estimation Simulations

Parameter	Simulation Setting 1	Simulation Setting 2	Simulation Setting 3
β (Fixed effects parameters)	$\begin{bmatrix}5 & 4 & 3 & 2 & 1 & 0\end{bmatrix}'$	$\begin{bmatrix}5 & 4 & 3 & 2 & 1 & 0\end{bmatrix}'$	$\begin{bmatrix}5 & 4 & 3 & 2 & 1 & 0\end{bmatrix}'$
σ^2 (Fixed effects variance)	1	1	1
D_1 (Random effects covariance matrix for the 1^{st} random factor):	$\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$	$\begin{bmatrix}1 & 0.7 & 0.5\\ 0.7 & 0.9 & 0.6\\ 0.5 & 0.6 & 0.8\end{bmatrix}$	$\begin{bmatrix}1 & 0.75 & 0.5 & 0.25\\ 0.75 & 1 & 0.75 & 0.5\\ 0.5 & 0.75 & 1 & 0.75\\ 0.25 & 0.5 & 0.75 & 1\end{bmatrix}$
D_2 (Random effects covariance matrix for the 2^{nd} random factor):	–	$\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$	$\begin{bmatrix}1 & 0.7 & 0.5\\ 0.7 & 0.9 & 0.6\\ 0.5 & 0.6 & 0.8\end{bmatrix}$
D_3 (Random effects covariance matrix for the 3^{rd} random factor):	–	–	$\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$

Table S1: Parameters chosen as baseline truth for the parameter estimation simulations. Entries marked as '–' indicate that the design for the corresponding simulation setting did not include the specified parameter.

S2 MAE and MRD Definition

Here, we formally define the Mean Absolute Error (*MAE*) and Mean Relative Difference (*MRD*) which were used in Chapter 3 as performance metrics for between-method comparison. For a model parameter γ, these were defined as:

$$MAE(\gamma) = \frac{1}{n_{sim}} \sum_i \|\hat{\gamma}_i - \bar{\gamma}_i\|_\infty,$$

$$MRD(\gamma) = \frac{1}{n_{sim}} \sum_i \left\| \frac{\hat{\gamma}_i - \bar{\gamma}_i}{\frac{1}{2}(\hat{\gamma}_i + \bar{\gamma}_i)} \right\|_\infty,$$

where n_{sim} is the total number of simulations run, $\hat{\gamma}_i$ is an estimate of the parameter vector γ obtained during the i^{th} simulation using the parameter estimation method of interest, and $\bar{\gamma}_i$ is a baseline truth to which $\hat{\gamma}_i$ is to be compared.

S3 MAE Results for ML Estimation

Method (m_1)	FS	FFS	SFS	FSFS	CSFS	lmer
Simulation 1						
$MAE_l(\beta)$	7.12×10^{-6}	7.12×10^{-6}	3.41×10^{-6}	3.41×10^{-6}	1.95×10^{-5}	-
	(1.08×10^{-5})	(1.08×10^{-5})	(8.01×10^{-6})	(8.01×10^{-6})	(1.74×10^{-5})	-
$MAE_t(\beta)$	1.28×10^{-1}	1.28×10^{-1}	1.28×10^{-1}	1.28×10^{-1}	1.28×10^{-1}	1.28×10^{-1}
	(8.39×10^{-2})	(8.39×10^{-2})	(8.39×10^{-2})	(8.39×10^{-2})	(8.39×10^{-2})	(8.39×10^{-2})
$MAE_l(\sigma^2D)$	2.12×10^{-5}	2.12×10^{-5}	1.96×10^{-5}	1.96×10^{-5}	9.07×10^{-5}	-
	(3.72×10^{-5})	(3.72×10^{-5})	(3.72×10^{-5})	(3.72×10^{-5})	(3.48×10^{-5})	-
$MAE_t(\sigma^2D)$	2.58×10^{-1}	2.58×10^{-1}	2.58×10^{-1}	2.58×10^{-1}	2.58×10^{-1}	2.58×10^{-1}
	(1.21×10^{-1})	(1.21×10^{-1})	(1.21×10^{-1})	(1.21×10^{-1})	(1.21×10^{-1})	(1.21×10^{-1})
Simulation 2						
$MAE_l(\beta)$	9.75×10^{-6}	9.75×10^{-6}	5.40×10^{-6}	5.40×10^{-6}	1.30×10^{-5}	-
	(1.38×10^{-5})	(1.38×10^{-5})	(1.25×10^{-5})	(1.25×10^{-5})	(1.69×10^{-5})	-
$MAE_t(\beta)$	9.77×10^{-2}	9.77×10^{-2}	9.77×10^{-2}	9.77×10^{-2}	9.77×10^{-2}	9.77×10^{-2}
	(5.92×10^{-2})	(5.92×10^{-2})	(5.92×10^{-2})	(5.92×10^{-2})	(5.92×10^{-2})	(5.92×10^{-2})
$MAE_l(\sigma^2D)$	1.05×10^{-4}	1.05×10^{-4}	1.04×10^{-4}	1.04×10^{-4}	1.08×10^{-4}	-
	(1.96×10^{-4})	(1.96×10^{-4})	(1.96×10^{-4})	(1.96×10^{-4})	(1.95×10^{-4})	-
$MAE_t(\sigma^2D)$	3.93×10^{-1}	3.93×10^{-1}	3.93×10^{-1}	3.93×10^{-1}	3.93×10^{-1}	3.93×10^{-1}
	(1.52×10^{-1})	(1.52×10^{-1})	(1.52×10^{-1})	(1.52×10^{-1})	(1.52×10^{-1})	(1.52×10^{-1})
Simulation 3						
$MAE_l(\beta)$	7.50×10^{-6}	7.50×10^{-6}	5.30×10^{-6}	5.30×10^{-6}	1.54×10^{-4}	-
	(9.08×10^{-6})	(9.08×10^{-6})	(8.06×10^{-6})	(8.06×10^{-6})	(5.61×10^{-4})	-
$MAE_t(\beta)$	8.34×10^{-2}	8.34×10^{-2}	8.34×10^{-2}	8.34×10^{-2}	8.34×10^{-2}	8.34×10^{-2}
	(3.99×10^{-2})	(3.99×10^{-2})	(3.99×10^{-2})	(3.99×10^{-2})	(3.99×10^{-2})	(3.99×10^{-2})
$MAE_l(\sigma^2D)$	4.08×10^{-4}	4.08×10^{-4}	4.08×10^{-4}	4.08×10^{-4}	2.96×10^{-3}	-
	(6.23×10^{-4})	(6.23×10^{-4})	(6.23×10^{-4})	(6.23×10^{-4})	(7.97×10^{-3})	-
$MAE_t(\sigma^2D)$	5.76×10^{-1}	5.76×10^{-1}	5.76×10^{-1}	5.76×10^{-1}	5.76×10^{-1}	5.76×10^{-1}
	(2.54×10^{-1})	(2.54×10^{-1})	(2.54×10^{-1})	(2.54×10^{-1})	(2.54×10^{-1})	(2.54×10^{-1})

Table S2: Average MAE values for the β and σ^2D parameter estimates, taken relative to the baseline truth used for simulation (t) and the parameter estimates produced by lmer (l). All reported results were obtained through averages taken from 1000 simulations performed for each simulation setting, with parameter estimation performed using the ML likelihood criteria. Empirical standard errors are also given in brackets underneath each entry in the table.

S4 MAE Results for ReML Estimation

Method ($\mathbf{m_1}$)	FS	FFS	SFS	FSFS	CSFS	lmer
Simulation 1						
$MAE_l(\beta)$	7.47×10^{-6}	7.47×10^{-6}	3.39×10^{-6}	3.39×10^{-6}	2.00×10^{-5}	-
	(1.14×10^{-5})	(1.14×10^{-5})	(8.18×10^{-6})	(8.18×10^{-6})	(1.66×10^{-5})	-
$MAE_t(\beta)$	1.21×10^{-1}	1.21×10^{-1}	1.21×10^{-1}	1.21×10^{-1}	1.21×10^{-1}	1.21×10^{-1}
	(8.10×10^{-2})	(8.10×10^{-2})	(8.10×10^{-2})	(8.10×10^{-2})	(8.10×10^{-2})	(8.10×10^{-2})
$MAE_l(\sigma^2 D)$	2.08×10^{-5}	2.08×10^{-5}	1.87×10^{-5}	1.87×10^{-5}	9.30×10^{-5}	-
	(4.12×10^{-5})	(4.12×10^{-5})	(4.13×10^{-5})	(4.13×10^{-5})	(4.13×10^{-5})	-
$MAE_t(\sigma^2 D)$	2.59×10^{-1}	2.59×10^{-1}	2.59×10^{-1}	2.59×10^{-1}	2.59×10^{-1}	2.59×10^{-1}
	(1.17×10^{-1})	(1.17×10^{-1})	(1.17×10^{-1})	(1.17×10^{-1})	(1.17×10^{-1})	(1.17×10^{-1})
Simulation 2						
$MAE_l(\beta)$	1.02×10^{-5}	1.02×10^{-5}	5.57×10^{-6}	5.57×10^{-6}	1.29×10^{-5}	-
	(1.18×10^{-5})	(1.18×10^{-5})	(9.62×10^{-6})	(9.62×10^{-6})	(1.43×10^{-5})	-
$MAE_t(\beta)$	9.37×10^{-2}	9.37×10^{-2}	9.37×10^{-2}	9.37×10^{-2}	9.37×10^{-2}	9.37×10^{-2}
	(5.25×10^{-2})	(5.25×10^{-2})	(5.25×10^{-2})	(5.25×10^{-2})	(5.25×10^{-2})	(5.25×10^{-2})
$MAE_l(\sigma^2 D)$	1.14×10^{-4}	1.14×10^{-4}	1.14×10^{-4}	1.14×10^{-4}	1.17×10^{-4}	-
	(2.24×10^{-4})	(2.24×10^{-4})	(2.24×10^{-4})	(2.24×10^{-4})	(2.23×10^{-4})	-
$MAE_t(\sigma^2 D)$	3.87×10^{-1}	3.87×10^{-1}	3.87×10^{-1}	3.87×10^{-1}	3.87×10^{-1}	3.87×10^{-1}
	(1.51×10^{-1})	(1.51×10^{-1})	(1.51×10^{-1})	(1.51×10^{-1})	(1.51×10^{-1})	(1.51×10^{-1})
Simulation 3						
$MAE_l(\beta)$	8.01×10^{-6}	8.01×10^{-6}	5.57×10^{-6}	5.57×10^{-6}	2.38×10^{-4}	-
	(1.21×10^{-5})	(1.21×10^{-5})	(1.10×10^{-5})	(1.10×10^{-5})	(1.18×10^{-3})	-
$MAE_t(\beta)$	8.61×10^{-2}	8.61×10^{-2}	8.61×10^{-2}	8.61×10^{-2}	8.61×10^{-2}	8.61×10^{-2}
	(4.15×10^{-2})	(4.15×10^{-2})	(4.15×10^{-2})	(4.15×10^{-2})	(4.15×10^{-2})	(4.15×10^{-2})
$MAE_l(\sigma^2 D)$	4.30×10^{-4}	4.30×10^{-4}	4.30×10^{-4}	4.30×10^{-4}	4.01×10^{-3}	-
	(8.40×10^{-4})	(8.40×10^{-4})	(8.40×10^{-4})	(8.40×10^{-4})	(1.42×10^{-2})	-
$MAE_t(\sigma^2 D)$	5.88×10^{-1}	5.88×10^{-1}	5.88×10^{-1}	5.88×10^{-1}	5.88×10^{-1}	5.88×10^{-1}
	(2.57×10^{-1})	(2.57×10^{-1})	(2.57×10^{-1})	(2.57×10^{-1})	(2.57×10^{-1})	(2.57×10^{-1})

Table S3: Average MAE values for the β and $\sigma^2 D$ parameter estimates, taken relative to the baseline truth used for simulation (t) and the parameter estimates produced by lmer (l). All reported results were obtained through averages taken from 1000 simulations performed for each simulation setting, with parameter estimation performed using the ReML likelihood criteria. Empirical standard errors are also given in brackets underneath each entry in the table.

S5 MRD Results for ML Estimation

Method ($\mathbf{m_1}$)	FS	FFS	SFS	FSFS	CSFS	lmer
Simulation 1						
$MRD_l(\beta)$	1.63×10^{-5}	1.63×10^{-5}	1.09×10^{-5}	1.09×10^{-5}	4.17×10^{-5}	-
	(1.79×10^{-4})	(1.79×10^{-4})	(1.13×10^{-4})	(1.13×10^{-4})	(3.75×10^{-4})	-
$MRD_t(\beta)$	4.17×10^{-2}	4.17×10^{-2}	4.17×10^{-2}	4.17×10^{-2}	4.17×10^{-2}	4.17×10^{-2}
	(2.09×10^{-2})	(2.09×10^{-2})	(2.09×10^{-2})	(2.09×10^{-2})	(2.09×10^{-2})	(2.09×10^{-2})
$MRD_l(\sigma^2 D)$	5.18×10^{-4}	5.18×10^{-4}	4.63×10^{-4}	4.63×10^{-4}	2.81×10^{-3}	-
	(8.58×10^{-3})	(8.58×10^{-3})	(9.52×10^{-3})	(9.52×10^{-3})	(2.53×10^{-2})	-
$MRD_t(\sigma^2 D)$	2.42×10^{-1}	2.42×10^{-1}	2.42×10^{-1}	2.42×10^{-1}	2.42×10^{-1}	2.42×10^{-1}
	(1.35×10^{-1})	(1.35×10^{-1})	(1.35×10^{-1})	(1.35×10^{-1})	(1.35×10^{-1})	(1.35×10^{-1})
Simulation 2						
$MRD_l(\beta)$	3.92×10^{-5}	3.92×10^{-5}	4.51×10^{-5}	4.51×10^{-5}	7.20×10^{-5}	-
	(3.15×10^{-4})	(3.15×10^{-4})	(4.46×10^{-4})	(4.46×10^{-4})	(6.62×10^{-4})	-
$MRD_t(\beta)$	3.73×10^{-2}	3.73×10^{-2}	3.73×10^{-2}	3.73×10^{-2}	3.73×10^{-2}	3.73×10^{-2}
	(1.85×10^{-2})	(1.85×10^{-2})	(1.85×10^{-2})	(1.85×10^{-2})	(1.85×10^{-2})	(1.85×10^{-2})
$MRD_l(\sigma^2 D)$	5.35×10^{-4}	5.35×10^{-4}	5.34×10^{-4}	5.34×10^{-4}	5.65×10^{-4}	-
	(2.30×10^{-3})	(2.30×10^{-3})	(2.31×10^{-3})	(2.31×10^{-3})	(2.35×10^{-3})	-
$MRD_t(\sigma^2 D)$	3.25×10^{-1}	3.25×10^{-1}	3.25×10^{-1}	3.25×10^{-1}	3.25×10^{-1}	3.25×10^{-1}
	(1.96×10^{-1})	(1.96×10^{-1})	(1.96×10^{-1})	(1.96×10^{-1})	(1.96×10^{-1})	(1.96×10^{-1})
Simulation 3						
$MRD_l(\beta)$	7.03×10^{-4}	7.03×10^{-4}	1.03×10^{-3}	1.03×10^{-3}	2.89×10^{-3}	-
	(1.25×10^{-2})	(1.25×10^{-2})	(2.47×10^{-2})	(2.47×10^{-2})	(3.90×10^{-2})	-
$MRD_t(\beta)$	3.96×10^{-2}	3.96×10^{-2}	3.96×10^{-2}	3.96×10^{-2}	3.95×10^{-2}	3.96×10^{-2}
	(2.09×10^{-2})	(2.09×10^{-2})	(2.09×10^{-2})	(2.09×10^{-2})	(2.09×10^{-2})	(2.09×10^{-2})
$MRD_l(\sigma^2 D)$	2.12×10^{-3}	2.12×10^{-3}	2.12×10^{-3}	2.12×10^{-3}	4.99×10^{-3}	-
	(1.92×10^{-2})	(1.92×10^{-2})	(1.91×10^{-2})	(1.91×10^{-2})	(2.10×10^{-2})	-
$MRD_t(\sigma^2 D)$	2.44×10^{-1}	2.44×10^{-1}	2.44×10^{-1}	2.44×10^{-1}	2.44×10^{-1}	2.44×10^{-1}
	(1.43×10^{-1})	(1.43×10^{-1})	(1.43×10^{-1})	(1.43×10^{-1})	(1.43×10^{-1})	(1.43×10^{-1})

Table S4: Average MRD values for the β and $\sigma^2 D$ parameter estimates, taken relative to the baseline truth used for simulation (t) and the parameter estimates produced by lmer (l). All reported results were obtained through averages taken from 1000 simulations performed for each simulation setting, with parameter estimation performed using the ML likelihood criteria. Empirical standard errors are also given in brackets underneath each entry in the table.

S6 MRD Results for ReML Estimation

Method ($\mathbf{m_1}$)	FS	FFS	SFS	FSFS	CSFS	lmer
Simulation 1						
$MRD_l(\beta)$	2.55×10^{-5}	2.55×10^{-5}	1.93×10^{-5}	1.93×10^{-5}	4.32×10^{-5}	-
	(2.81×10^{-4})	(2.81×10^{-4})	(2.39×10^{-4})	(2.39×10^{-4})	(3.24×10^{-4})	-
$MRD_t(\beta)$	4.05×10^{-2}	4.05×10^{-2}	4.05×10^{-2}	4.05×10^{-2}	4.05×10^{-2}	4.05×10^{-2}
	(1.99×10^{-2})	(1.99×10^{-2})	(1.99×10^{-2})	(1.99×10^{-2})	(1.99×10^{-2})	(1.99×10^{-2})
$MRD_l(\sigma^2 D)$	2.42×10^{-4}	2.42×10^{-4}	2.05×10^{-4}	2.05×10^{-4}	3.99×10^{-3}	-
	(1.89×10^{-3})	(1.89×10^{-3})	(1.78×10^{-3})	(1.78×10^{-3})	(8.35×10^{-2})	-
$MRD_t(\sigma^2 D)$	2.42×10^{-1}	2.42×10^{-1}	2.42×10^{-1}	2.42×10^{-1}	2.42×10^{-1}	2.42×10^{-1}
	(1.27×10^{-1})	(1.27×10^{-1})	(1.27×10^{-1})	(1.27×10^{-1})	(1.27×10^{-1})	(1.27×10^{-1})
Simulation 2						
$MRD_l(\beta)$	1.08×10^{-4}	1.08×10^{-4}	7.74×10^{-5}	7.74×10^{-5}	7.45×10^{-5}	-
	(2.16×10^{-3})	(2.16×10^{-3})	(1.45×10^{-3})	(1.45×10^{-3})	(5.37×10^{-4})	-
$MRD_t(\beta)$	3.61×10^{-2}	3.61×10^{-2}	3.61×10^{-2}	3.61×10^{-2}	3.61×10^{-2}	3.61×10^{-2}
	(1.75×10^{-2})	(1.75×10^{-2})	(1.75×10^{-2})	(1.75×10^{-2})	(1.75×10^{-2})	(1.75×10^{-2})
$MRD_l(\sigma^2 D)$	5.02×10^{-4}	5.02×10^{-4}	5.01×10^{-4}	5.01×10^{-4}	5.16×10^{-4}	-
	(2.35×10^{-3})	(2.35×10^{-3})	(2.35×10^{-3})	(2.35×10^{-3})	(2.30×10^{-3})	-
$MRD_t(\sigma^2 D)$	3.27×10^{-1}	3.27×10^{-1}	3.27×10^{-1}	3.27×10^{-1}	3.27×10^{-1}	3.27×10^{-1}
	(1.86×10^{-1})	(1.86×10^{-1})	(1.86×10^{-1})	(1.86×10^{-1})	(1.86×10^{-1})	(1.86×10^{-1})
Simulation 3						
$MRD_l(\beta)$	1.22×10^{-4}	1.22×10^{-4}	1.22×10^{-4}	1.22×10^{-4}	5.45×10^{-3}	-
	(7.38×10^{-4})	(7.38×10^{-4})	(8.57×10^{-4})	(8.57×10^{-4})	(6.22×10^{-2})	-
$MRD_t(\beta)$	3.86×10^{-2}	3.86×10^{-2}	3.86×10^{-2}	3.86×10^{-2}	3.86×10^{-2}	3.86×10^{-2}
	(1.93×10^{-2})	(1.93×10^{-2})	(1.93×10^{-2})	(1.93×10^{-2})	(1.92×10^{-2})	(1.93×10^{-2})
$MRD_l(\sigma^2 D)$	1.82×10^{-3}	1.82×10^{-3}	1.82×10^{-3}	1.82×10^{-3}	5.56×10^{-3}	-
	(1.14×10^{-2})	(1.14×10^{-2})	(1.14×10^{-2})	(1.14×10^{-2})	(1.65×10^{-2})	-
$MRD_t(\sigma^2 D)$	2.54×10^{-1}	2.54×10^{-1}	2.54×10^{-1}	2.54×10^{-1}	2.54×10^{-1}	2.54×10^{-1}
	(1.53×10^{-1})	(1.53×10^{-1})	(1.53×10^{-1})	(1.53×10^{-1})	(1.53×10^{-1})	(1.53×10^{-1})

Table S5: Average MRD values for the β and $\sigma^2 D$ parameter estimates, taken relative to the baseline truth used for simulation (t) and the parameter estimates produced by lmer (l). All reported results were obtained through averages taken from 1000 simulations performed for each simulation setting, with parameter estimation performed using the ReML likelihood criteria. Empirical standard errors are also given in brackets underneath each entry in the table.

S7 ML Likelihood Criteria

Method	FS	FFS	SFS	FSFS	CSFS	lmer
Simulation 1						
$\hat{l}$ (Mean log-likelihood)	−1564.860	−1564.860	−1564.860	−1564.860	−1564.860	−1564.860
	(22.203)	(22.203)	(22.203)	(22.203)	(22.203)	(22.203)
$\hat{l} - \hat{l}_{lmer}$ (Mean difference from	0.030	0.030	0.031	0.031	−0.166	-
`lmer` log-likelihood, $\times 10^6$)	(0.306)	(0.306)	(0.306)	(0.306)	(0.318)	-
Simulation 2						
$\hat{l}$ (Mean log-likelihood)	−1683.238	−1683.238	−1683.238	−1683.238	−1683.238	−1683.238
	(22.598)	(22.598)	(22.598)	(22.598)	(22.598)	(22.598)
$\hat{l} - \hat{l}_{lmer}$ (Mean difference from	0.756	0.756	0.749	0.749	0.562	-
`lmer` log-likelihood, $\times 10^6$)	(12.977)	(12.977)	(12.977)	(12.977)	(12.975)	-
Simulation 3						
$\hat{l}$ (Mean log-likelihood)	−1918.952	−1918.952	−1918.952	−1918.952	−1918.974	−1918.952
	(22.925)	(22.925)	(22.925)	(22.925)	(22.916)	(22.925)
$\hat{l} - \hat{l}_{lmer}$ (Mean difference from	5.696	5.696	5.543	5.543	−2000.163	-
`lmer` log-likelihood, $\times 10^6$)	(50.795)	(50.795)	(50.793)	(50.793)	(22942.480)	-

Table S6: Maximized ML log-likelihood criteria averaged across the 1000 simulations performed for each simulation setting. Mean differences observed between each of the Fisher Scoring methods and lmer are reported on a scale of 10^{-6}. Underneath each entry in the table, empirical standard errors are displayed in brackets. All reported likelihoods can be seen to be indistinguishable from one another, apart from the CSFS method, which experienced convergence failure in a small number of instances.

S8 ReML Likelihood Criteria

Method	FS	FFS	SFS	FSFS	CSFS	lmer
Simulation 1						
$\hat{l}_R$ (Mean log-likelihood)	-1574.069	-1574.069	-1574.069	-1574.069	-1574.069	-1574.069
	(22.602)	(22.602)	(22.602)	(22.602)	(22.602)	(22.602)
$\hat{l}_R - \hat{l}_{R,lmer}$ (Mean difference from	0.024	0.024	0.024	0.024	-0.174	-
`lmer` log-likelihood, $\times 10^6$)	(0.327)	(0.327)	(0.326)	(0.326)	(0.336)	-
Simulation 2						
$\hat{l}_R$ (Mean log-likelihood)	-1694.464	-1694.464	-1694.464	-1694.464	-1694.464	-1694.464
	(22.721)	(22.721)	(22.721)	(22.721)	(22.721)	(22.721)
$\hat{l}_R - \hat{l}_{R,lmer}$ (Mean difference from	0.990	0.990	0.985	0.985	0.801	-
`lmer` log-likelihood, $\times 10^6$)	(9.905)	(9.905)	(9.903)	(9.903)	(9.909)	-
Simulation 3						
$\hat{l}_R$ (Mean log-likelihood)	-1930.486	-1930.486	-1930.486	-1930.486	-1930.530	-1930.486
	(22.460)	(22.460)	(22.460)	(22.460)	(22.468)	(22.460)
$\hat{l}_R - \hat{l}_{R,lmer}$ (Mean difference from	6.022	6.022	5.865	5.865	-43966.471	-
`lmer` log-likelihood, $\times 10^6$)	(43.037)	(43.037)	(43.037)	(43.037)	(345579.800)	-

Table S7: Maximized ReML log-likelihood criteria averaged across the 1000 simulations performed for each simulation setting. Mean differences observed between each of the Fisher Scoring methods and lmer are reported on a scale of 10^{-6}. Underneath each entry in the table, empirical standard errors are displayed in brackets. All reported likelihoods can be seen to be indistinguishable from one another, apart from the CSFS method, which experienced convergence failure in a small number of instances.

S9 The SAT Score Results

Estimation Method	FS	FFS	SFS	FSFS	CSFS	lmer
Fixed effects parameters						
β_0 (Intercept)	597.715	597.715	597.714	597.714	597.714	597.714
(Standard Error)	(7.534)	(7.534)	(7.535)	(7.535)	(7.535)	(7.535)
β_1 (Year)	28.556	28.556	28.557	28.557	28.557	28.557
(Standard Error)	(8.638)	(8.638)	(8.639)	(8.639)	(8.639)	(8.639)
Covariance parameters						
σ_i^2 (Student)	340.712	340.712	340.684	340.684	340.688	340.690
σ_j^2 (Teacher)	604.877	604.877	604.954	604.954	604.956	604.973
σ^2 (Residual)	237.943	237.973	237.972	237.972	237.966	237.962
Performance						
$\lvert l - l_{lmer} \rvert$ (Log-likelihood $\times 10^{-7}$)	0.313	0.313	3.321	3.321	1.933	–
t (Time in seconds)	0.216	0.176	0.200	0.175	0.282	0.178
n_{it} (Number of Iterations)	7	7	16	16	14	–

Table S8: Parameter estimates and performance metrics for the SAT score model. Provided are the results for the FS, FFS, SFS, FSFS and CSFS methods, as well as the results produced on the same dataset using lmer. All values in this table were obtained using ML, including the results of lmer which usually by default employs ReML. Log-likelihood values are given as absolute differences from lmer and reported on a scale of 10^{-7}.