**Supplementary material (simulation study)**

**Table SI.** Parameter values for simulation under three-level mixed-effects location scale model

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters (n = 15) | True value | | | | | | | |
| Variance scale 1  (small) | |  | Variance scale 2  (medium) | |  | Variance scale 3  (large) | |
| Design  (a1, b1)b | Design  (a2, b2)b |  | Design  (a3, b3)b | Design  (a4, b4)b |  | Design  (a5, b5)b | Design  (a6, b6)b |
| : (Intercept) | 6.9 | 6.9 |  | 6.9 | 6.9 |  | 6.9 | 6.9 |
| : (X1a) | -0.4 | -0.4 |  | -0.4 | -0.4 |  | -0.4 | -0.4 |
| : (X2a) | 0.2 | 0.2 |  | 0.2 | 0.2 |  | 0.2 | 0.2 |
| : (X3a) | 0.6 | 0.6 |  | 0.6 | 0.6 |  | 0.6 | 0.6 |
| : (Intercept) | 0.2 | 0.2 |  | 0.2 | 0.2 |  | 0.2 | 0.2 |
| : (X3a) | -0.1 | -0.1 |  | -0.1 | -0.1 |  | -0.1 | -0.1 |
| : (Intercept) | -1.2 | -1.2 |  | -1.2 | -1.2 |  | -1.2 | -1.2 |
| : (X2a) | -0.1 | -0.1 |  | -0.1 | -0.1 |  | -0.1 | -0.1 |
| : (X3a) | -0.4 | -0.4 |  | -0.4 | -0.4 |  | -0.4 | -0.4 |
| : (Intercept) | 0.4 | 0.4 |  | 0.4 | 0.4 |  | 0.4 | 0.4 |
| : (X1a) | 0.1 | 0.1 |  | 0.1 | 0.1 |  | 0.1 | 0.1 |
| : (X2a) | -0.1 | -0.1 |  | -0.1 | -0.1 |  | -0.1 | -0.1 |
| : (X3a) | -0.2 | -0.2 |  | -0.2 | -0.2 |  | -0.2 | -0.2 |
| scale | 0.30 | 0.30 |  | 0.60 | 0.60 |  | 1.2 | 1.2 |
| Covariance | 0.15 | -0.15 |  | 0.35 | -0.35 |  | 0.5 | -0.5 |

a X1: occasion-level (level-1) covariate; X2: day-level (level-2) covariate; X3: subject-level (level-3) covariate

b Design a1-a6: X1, X2, X3 are all continuous covariates; Design b1-b6: X1, X2 are binary covariates, and X3 is continuous covariate.

**Table SII**. Results from 1000 simulations under the three-level mixed-effects location scale model (***design a2 in Table SI***)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | True Value | Three-level random intercept model | | | | | | |  |  | Three-level mixed-effects location scale model | | | | | | |
| EST | SE | Bias | SB | RMSE | 95% COV | AW |  | EST | SE | Bias | SB | RMSE | 95% COV | AW |
| : (Intercept) | 6.90 | 6.899 | 0.06 | -0.0013 | -2.19 | 0.06 | 95.9 | 0.23 |  |  | 6.899 | 0.06 | -0.0014 | -2.44 | 0.06 | 95.7 | 0.23 |
| : (X1) | -0.40 | -0.400 | 0.03 | 0.0003 | 0.92 | 0.03 | 95.4 | 0.11 |  |  | -0.400 | 0.02 | 0.0003 | 1.11 | 0.02 | 95.3 | 0.10 |
| : (X2) | 0.20 | 0.200 | 0.01 | 0.0001 | 0.46 | 0.01 | 95.5 | 0.06 |  |  | 0.200 | 0.01 | 0.0001 | 0.66 | 0.01 | 95.6 | 0.06 |
| : (X3) | 0.60 | 0.603 | 0.08 | 0.0032 | 3.76 | 0.08 | 94.6 | 0.32 |  |  | 0.604 | 0.08 | 0.0038 | 4.54 | 0.08 | 94.1 | 0.32 |
| : (Intercept) | 0.20 | 0.195 | 0.08 | -0.0055 | -7.20 | 0.08 | 96.3 | 0.30 |  |  | 0.186 | 0.08 | -0.0140 | -18.26 | 0.08 | 95.6 | 0.30 |
| : (X3) | -0.10 |  |  |  |  |  |  |  |  |  | -0.099 | 0.11 | 0.0006 | 0.60 | 0.11 | 94.5 | 0.42 |
| : (Intercept) | -1.20 | -1.136 | 0.08 | 0.0640 | 77.15 | 0.10 | 82.3 | 0.29 |  |  | -1.199 | 0.07 | 0.0015 | 2.11 | 0.07 | 95.5 | 0.28 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.102 | 0.06 | -0.0016 | -2.62 | 0.06 | 94.3 | 0.24 |
| : (X3) | -0.40 |  |  |  |  |  |  |  |  |  | -0.402 | 0.10 | -0.0021 | -2.10 | 0.10 | 95.1 | 0.38 |
| : (Intercept) | 0.40 | 0.635 | 0.04 | 0.2350 | 639.72 | 0.24 | 0.0 | 0.06 |  |  | 0.399 | 0.04 | -0.0006 | -1.63 | 0.04 | 95.1 | 0.14 |
| : (X1) | 0.10 |  |  |  |  |  |  |  |  |  | 0.099 | 0.03 | -0.0013 | -4.37 | 0.03 | 96.6 | 0.13 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.100 | 0.01 | -0.0002 | -1.10 | 0.01 | 94.2 | 0.05 |
| : (X3) | -0.20 |  |  |  |  |  |  |  |  |  | -0.201 | 0.05 | -0.0013 | -2.91 | 0.05 | 94.6 | 0.17 |
|  | 0.30 |  |  |  |  |  |  |  |  |  | 0.288 | 0.03 | -0.0119 | -42.24 | 0.03 | 89.1 | 0.11 |
|  | -0.15 |  |  |  |  |  |  |  |  |  | -0.147 | 0.04 | 0.0030 | 7.72 | 0.04 | 93.2 | 0.14 |
| -2LogL |  | 41337.3 | | | | | | |  |  | 40332.6 | | | | | | |
| # of converged solutions | | 1000 | | | | | | |  |  | 987 | | | | | | |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

**Table SIII**. Results from 1000 simulations under the three-level mixed-effects location scale model (***design a3 in Table SI***)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | True Value | Three-level random intercept model | | | | | | |  |  | Three-level mixed-effects location scale model | | | | | | |
| EST | SE | Bias | SB | RMSE | 95% COV | AW |  | EST | SE | Bias | SB | RMSE | 95% COV | AW |
| : (Intercept) | 6.90 | 6.899 | 0.06 | -0.0012 | -2.01 | 0.06 | 95.8 | 0.24 |  |  | 6.900 | 0.06 | -0.0001 | -0.25 | 0.06 | 96.0 | 0.23 |
| : (X1) | -0.40 | -0.400 | 0.03 | 0.0001 | 0.32 | 0.03 | 95.7 | 0.12 |  |  | -0.400 | 0.02 | 0.0004 | 1.90 | 0.02 | 94.5 | 0.09 |
| : (X2) | 0.20 | 0.200 | 0.02 | 0.0001 | 0.59 | 0.02 | 95.2 | 0.06 |  |  | 0.200 | 0.01 | -0.0001 | -0.41 | 0.01 | 95.6 | 0.06 |
| : (X3) | 0.60 | 0.603 | 0.08 | 0.0030 | 3.52 | 0.08 | 94.7 | 0.33 |  |  | 0.602 | 0.08 | 0.0024 | 2.80 | 0.08 | 94.0 | 0.32 |
| : (Intercept) | 0.20 | 0.194 | 0.08 | -0.0057 | -7.38 | 0.08 | 96.0 | 0.31 |  |  | 0.185 | 0.08 | -0.0147 | -19.28 | 0.08 | 96.0 | 0.31 |
| : (X3) | -0.10 |  |  |  |  |  |  |  |  |  | -0.101 | 0.10 | -0.0011 | -1.07 | 0.10 | 94.1 | 0.38 |
| : (Intercept) | -1.20 | -1.137 | 0.10 | 0.0627 | 63.93 | 0.12 | 80.1 | 0.32 |  |  | -1.199 | 0.07 | 0.0007 | 1.04 | 0.07 | 95.1 | 0.27 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.102 | 0.06 | -0.0022 | -3.66 | 0.06 | 94.0 | 0.23 |
| : (X3) | -0.40 |  |  |  |  |  |  |  |  |  | -0.404 | 0.10 | -0.0038 | -3.97 | 0.10 | 94.0 | 0.37 |
| : (Intercept) | 0.40 | 0.775 | 0.05 | 0.3753 | 743.96 | 0.38 | 0.0 | 0.06 |  |  | 0.399 | 0.04 | -0.0014 | -3.28 | 0.04 | 94.5 | 0.17 |
| : (X1) | 0.10 |  |  |  |  |  |  |  |  |  | 0.099 | 0.03 | -0.0009 | -3.02 | 0.03 | 96.5 | 0.13 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.100 | 0.01 | -0.0001 | -0.53 | 0.01 | 94.2 | 0.05 |
| : (X3) | -0.20 |  |  |  |  |  |  |  |  |  | -0.200 | 0.06 | -0.0002 | -0.28 | 0.06 | 95.8 | 0.23 |
|  | 0.60 |  |  |  |  |  |  |  |  |  | 0.570 | 0.05 | -0.0295 | -60.43 | 0.06 | 86.8 | 0.18 |
|  | 0.35 |  |  |  |  |  |  |  |  |  | 0.350 | 0.05 | 0.0000 | 0.08 | 0.05 | 93.7 | 0.20 |
| -2LogL |  | 42724.7 | | | | | | |  |  | 40586.9 | | | | | | |
| # of converged solutions | | 998 | | | | | | |  |  | 904 | | | | | | |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

**Table SIV**. Results from 1000 simulations under the three-level mixed-effects location scale model (***design a4 in Table SI***)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | True Value | Three-level random intercept model | | | | | | |  |  | Three-level mixed-effects location scale model | | | | | | |
| EST | SE | Bias | SB | RMSE | 95% COV | AW |  | EST | SE | Bias | SB | RMSE | 95% COV | AW |
| : (Intercept) | 6.90 | 6.899 | 0.06 | -0.0012 | -2.07 | 0.06 | 96.1 | 0.24 |  |  | 6.898 | 0.06 | -0.0019 | -3.30 | 0.06 | 95.9 | 0.23 |
| : (X1) | -0.40 | -0.400 | 0.03 | 0.0002 | 0.55 | 0.03 | 95.2 | 0.12 |  |  | -0.400 | 0.02 | -0.0001 | -0.36 | 0.02 | 95.4 | 0.09 |
| : (X2) | 0.20 | 0.200 | 0.02 | 0.0001 | 0.42 | 0.02 | 95.1 | 0.06 |  |  | 0.200 | 0.01 | 0.0002 | 1.73 | 0.01 | 95.5 | 0.06 |
| : (X3) | 0.60 | 0.603 | 0.08 | 0.0032 | 3.83 | 0.08 | 94.7 | 0.33 |  |  | 0.602 | 0.08 | 0.0023 | 2.76 | 0.08 | 93.7 | 0.32 |
| : (Intercept) | 0.20 | 0.195 | 0.08 | -0.0055 | -7.12 | 0.08 | 96.4 | 0.31 |  |  | 0.185 | 0.08 | -0.0155 | -20.17 | 0.08 | 95.5 | 0.31 |
| : (X3) | -0.10 |  |  |  |  |  |  |  |  |  | -0.099 | 0.10 | 0.0012 | 1.24 | 0.10 | 94.8 | 0.38 |
| : (Intercept) | -1.20 | -1.137 | 0.10 | 0.0625 | 64.17 | 0.12 | 81.8 | 0.32 |  |  | -1.198 | 0.07 | 0.0017 | 2.44 | 0.07 | 95.6 | 0.27 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.102 | 0.06 | -0.0022 | -3.72 | 0.06 | 93.6 | 0.23 |
| : (X3) | -0.40 |  |  |  |  |  |  |  |  |  | -0.402 | 0.09 | -0.0023 | -2.42 | 0.09 | 95.2 | 0.37 |
| : (Intercept) | 0.40 | 0.775 | 0.05 | 0.3749 | 731.31 | 0.38 | 0.0 | 0.06 |  |  | 0.399 | 0.04 | -0.0006 | -1.36 | 0.04 | 95.2 | 0.17 |
| : (X1) | 0.10 |  |  |  |  |  |  |  |  |  | 0.098 | 0.03 | -0.0018 | -5.98 | 0.03 | 96.1 | 0.13 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.100 | 0.01 | -0.0001 | -0.36 | 0.01 | 94.4 | 0.05 |
| : (X3) | -0.20 |  |  |  |  |  |  |  |  |  | -0.203 | 0.06 | -0.0030 | -5.08 | 0.06 | 93.9 | 0.23 |
|  | 0.60 |  |  |  |  |  |  |  |  |  | 0.566 | 0.05 | -0.0338 | -69.51 | 0.06 | 84.1 | 0.18 |
|  | -0.35 |  |  |  |  |  |  |  |  |  | -0.344 | 0.05 | 0.0057 | 10.89 | 0.05 | 93.1 | 0.20 |
| -2LogL |  | 42720.5 | | | | | | |  |  | 40590.1 | | | | | | |
| # of converged solutions | | 1000 | | | | | | |  |  | 940 | | | | | | |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

**Table SV**. Results from 1000 simulations under the three-level mixed-effects location scale model (***design a5 in Table SI***)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | True Value | Three-level random intercept model | | | | | | |  |  | Three-level mixed-effects location scale model | | | | | | |
| EST | SE | Bias | SB | RMSE | 95% COV | AW |  | EST | SE | Bias | SB | RMSE | 95% COV | AW |
| : (Intercept) | 6.90 | 6.899 | 0.06 | -0.0009 | -1.56 | 0.06 | 95.9 | 0.24 |  |  | 6.900 | 0.06 | -0.0001 | -0.17 | 0.06 | 95.2 | 0.23 |
| : (X1) | -0.40 | -0.400 | 0.03 | -0.0002 | -0.57 | 0.03 | 95.6 | 0.13 |  |  | -0.400 | 0.02 | -0.0005 | -2.36 | 0.02 | 95.5 | 0.08 |
| : (X2) | 0.20 | 0.200 | 0.02 | 0.0001 | 0.79 | 0.02 | 94.7 | 0.07 |  |  | 0.201 | 0.01 | 0.0005 | 3.83 | 0.01 | 95.5 | 0.06 |
| : (X3) | 0.60 | 0.603 | 0.09 | 0.0029 | 3.38 | 0.09 | 94.6 | 0.33 |  |  | 0.605 | 0.08 | 0.0052 | 6.19 | 0.08 | 94.7 | 0.33 |
| : (Intercept) | 0.20 | 0.194 | 0.08 | -0.0058 | -7.27 | 0.08 | 95.3 | 0.31 |  |  | 0.184 | 0.08 | -0.0161 | -20.44 | 0.08 | 94.7 | 0.31 |
| : (X3) | -0.10 |  |  |  |  |  |  |  |  |  | -0.097 | 0.10 | 0.0032 | 3.31 | 0.10 | 94.8 | 0.38 |
| : (Intercept) | -1.20 | -1.144 | 0.15 | 0.0561 | 37.00 | 0.16 | 77.9 | 0.40 |  |  | -1.199 | 0.06 | 0.0011 | 1.78 | 0.06 | 96.1 | 0.25 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.100 | 0.06 | 0.0001 | 0.19 | 0.06 | 94.7 | 0.21 |
| : (X3) | -0.40 |  |  |  |  |  |  |  |  |  | -0.402 | 0.09 | -0.0025 | -2.79 | 0.09 | 95.4 | 0.35 |
| : (Intercept) | 0.40 | 1.062 | 0.08 | 0.6621 | 825.62 | 0.67 | 0.0 | 0.06 |  |  | 0.399 | 0.06 | -0.0014 | -2.50 | 0.06 | 95.6 | 0.23 |
| : (X1) | 0.10 |  |  |  |  |  |  |  |  |  | 0.099 | 0.03 | -0.0008 | -2.46 | 0.03 | 96.5 | 0.13 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.100 | 0.01 | 0.0003 | 2.02 | 0.01 | 94.4 | 0.05 |
| : (X3) | -0.20 |  |  |  |  |  |  |  |  |  | -0.199 | 0.08 | 0.0014 | 1.90 | 0.08 | 96.1 | 0.31 |
|  | 1.20 |  |  |  |  |  |  |  |  |  | 1.142 | 0.09 | -0.0577 | -64.29 | 0.11 | 86.0 | 0.34 |
|  | 0.50 |  |  |  |  |  |  |  |  |  | 0.499 | 0.07 | -0.0013 | -1.79 | 0.07 | 94.0 | 0.28 |
| -2LogL |  | 45596.5 | | | | | | |  |  | 40981.7 | | | | | | |
| # of converged solutions | | 999 | | | | | | |  |  | 735 | | | | | | |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

**Table SVI**. Results from 1000 simulations under the three-level mixed-effects location scale model (***design a6 in Table SI***)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | True Value | Three-level random intercept model | | | | | | |  |  | Three-level mixed-effects location scale model | | | | | | |
| EST | SE | Bias | SB | RMSE | 95% COV | AW |  | EST | SE | Bias | SB | RMSE | 95% COV | AW |
| : (Intercept) | 6.90 | 6.899 | 0.06 | -0.0011 | -1.85 | 0.06 | 96.1 | 0.24 |  |  | 6.896 | 0.06 | -0.0036 | -6.26 | 0.06 | 95.8 | 0.23 |
| : (X1) | -0.40 | -0.400 | 0.03 | 0.0000 | -0.02 | 0.03 | 94.9 | 0.13 |  |  | -0.400 | 0.02 | 0.0003 | 1.63 | 0.02 | 95.8 | 0.08 |
| : (X2) | 0.20 | 0.200 | 0.02 | 0.0001 | 0.34 | 0.02 | 95.4 | 0.07 |  |  | 0.200 | 0.01 | -0.0001 | -0.87 | 0.01 | 95.3 | 0.06 |
| : (X3) | 0.60 | 0.603 | 0.09 | 0.0033 | 3.86 | 0.09 | 94.4 | 0.33 |  |  | 0.603 | 0.08 | 0.0035 | 4.12 | 0.08 | 93.9 | 0.33 |
| : (Intercept) | 0.20 | 0.195 | 0.08 | -0.0055 | -6.84 | 0.08 | 95.8 | 0.31 |  |  | 0.183 | 0.08 | -0.0174 | -22.14 | 0.08 | 95.0 | 0.31 |
| : (X3) | -0.10 |  |  |  |  |  |  |  |  |  | -0.098 | 0.10 | 0.0017 | 1.75 | 0.10 | 95.6 | 0.38 |
| : (Intercept) | -1.20 | -1.144 | 0.15 | 0.0557 | 37.18 | 0.16 | 78.4 | 0.40 |  |  | -1.200 | 0.06 | 0.0002 | 0.33 | 0.06 | 95.1 | 0.25 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.101 | 0.06 | -0.0012 | -2.07 | 0.06 | 93.4 | 0.21 |
| : (X3) | -0.40 |  |  |  |  |  |  |  |  |  | -0.404 | 0.09 | -0.0039 | -4.43 | 0.09 | 95.2 | 0.35 |
| : (Intercept) | 0.40 | 1.061 | 0.08 | 0.6611 | 812.81 | 0.67 | 0.0 | 0.06 |  |  | 0.400 | 0.06 | 0.0003 | 0.57 | 0.06 | 94.7 | 0.23 |
| : (X1) | 0.10 |  |  |  |  |  |  |  |  |  | 0.099 | 0.03 | -0.0013 | -4.07 | 0.03 | 96.2 | 0.13 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.100 | 0.01 | -0.0001 | -1.06 | 0.01 | 95.0 | 0.05 |
| : (X3) | -0.20 |  |  |  |  |  |  |  |  |  | -0.203 | 0.08 | -0.0027 | -3.31 | 0.08 | 93.9 | 0.31 |
|  | 1.20 |  |  |  |  |  |  |  |  |  | 1.139 | 0.09 | -0.0605 | -67.16 | 0.11 | 85.2 | 0.34 |
|  | -0.50 |  |  |  |  |  |  |  |  |  | -0.492 | 0.07 | 0.0079 | 10.99 | 0.07 | 93.5 | 0.28 |
| -2LogL |  | 45586.0 | | | | | | |  |  | 40999.6 | | | | | | |
| # of converged solutions | | 1000 | | | | | | |  |  | 837 | | | | | | |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

**Table SVII**. Results from 1000 simulations under the three-level mixed-effects location scale model (***design b1 in Table SI***)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | True Value | Three-level random intercept model | | | | | | |  |  | Three-level mixed-effects location scale model | | | | | | |
| EST | SE | Bias | SB | RMSE | 95% COV | AW |  | EST | SE | Bias | SB | RMSE | 95% COV | AW |
| : (Intercept) | 6.90 | 6.901 | 0.06 | 0.0011 | 1.84 | 0.06 | 94.7 | 0.24 |  |  | 6.902 | 0.06 | 0.0016 | 2.72 | 0.06 | 95.4 | 0.24 |
| : (X1) | -0.40 | -0.401 | 0.03 | -0.0008 | -3.13 | 0.03 | 95.5 | 0.11 |  |  | -0.401 | 0.02 | -0.0012 | -5.08 | 0.02 | 96.2 | 0.09 |
| : (X2) | 0.20 | 0.200 | 0.04 | -0.0001 | -0.20 | 0.04 | 95.2 | 0.15 |  |  | 0.201 | 0.03 | 0.0005 | 1.49 | 0.03 | 95.6 | 0.14 |
| : (X3) | 0.60 | 0.600 | 0.08 | -0.0001 | -0.13 | 0.08 | 94.5 | 0.33 |  |  | 0.600 | 0.09 | -0.0002 | -0.28 | 0.09 | 95.1 | 0.32 |
| : (Intercept) | 0.20 | 0.196 | 0.08 | -0.0035 | -4.44 | 0.08 | 94.2 | 0.30 |  |  | 0.188 | 0.08 | -0.0119 | -15.17 | 0.08 | 94.5 | 0.30 |
| : (X3) | -0.10 |  |  |  |  |  |  |  |  |  | -0.098 | 0.11 | 0.0022 | 2.01 | 0.11 | 94.0 | 0.42 |
| : (Intercept) | -1.20 | -1.195 | 0.08 | 0.0046 | 5.50 | 0.08 | 92.6 | 0.30 |  |  | -1.202 | 0.08 | -0.0016 | -1.88 | 0.08 | 94.8 | 0.33 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.104 | 0.16 | -0.0039 | -2.43 | 0.16 | 94.7 | 0.63 |
| : (X3) | -0.40 |  |  |  |  |  |  |  |  |  | -0.398 | 0.10 | 0.0017 | 1.74 | 0.10 | 96.0 | 0.39 |
| : (Intercept) | 0.40 | 0.579 | 0.04 | 0.1791 | 494.51 | 0.18 | 0.0 | 0.06 |  |  | 0.398 | 0.04 | -0.0016 | -4.27 | 0.04 | 94.8 | 0.14 |
| : (X1) | 0.10 |  |  |  |  |  |  |  |  |  | 0.100 | 0.03 | 0.0000 | -0.11 | 0.03 | 95.8 | 0.13 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.099 | 0.04 | 0.0010 | 2.66 | 0.04 | 94.9 | 0.14 |
| : (X3) | -0.20 |  |  |  |  |  |  |  |  |  | -0.200 | 0.05 | 0.0003 | 0.65 | 0.05 | 94.5 | 0.18 |
|  | 0.30 |  |  |  |  |  |  |  |  |  | 0.290 | 0.03 | -0.0104 | -38.28 | 0.03 | 90.8 | 0.11 |
|  | 0.15 |  |  |  |  |  |  |  |  |  | 0.150 | 0.04 | -0.0004 | -0.93 | 0.04 | 93.3 | 0.14 |
| -2LogL |  | 40729.1 | | | | | | |  |  | 39785.1 | | | | | | |
| # of converged solutions | | 1000 | | | | | | |  |  | 973 | | | | | | |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

**Table SVIII**. Results from 1000 simulations under the three-level mixed-effects location scale model (***design b2 in Table SI***)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | True Value | Three-level random intercept model | | | | | | |  |  | Three-level mixed-effects location scale model | | | | | | |
| EST | SE | Bias | SB | RMSE | 95% COV | AW |  | EST | SE | Bias | SB | RMSE | 95% COV | AW |
| : (Intercept) | 6.90 | 6.901 | 0.06 | 0.0012 | 1.96 | 0.06 | 94.9 | 0.24 |  |  | 6.901 | 0.06 | 0.0013 | 2.17 | 0.06 | 95.5 | 0.24 |
| : (X1) | -0.40 | -0.401 | 0.03 | -0.0010 | -3.60 | 0.03 | 95.4 | 0.11 |  |  | -0.401 | 0.02 | -0.0007 | -3.05 | 0.02 | 96.5 | 0.09 |
| : (X2) | 0.20 | 0.200 | 0.04 | 0.0000 | -0.01 | 0.04 | 95.2 | 0.15 |  |  | 0.200 | 0.04 | 0.0005 | 1.38 | 0.04 | 96.1 | 0.14 |
| : (X3) | 0.60 | 0.600 | 0.08 | -0.0001 | -0.17 | 0.08 | 94.6 | 0.33 |  |  | 0.600 | 0.08 | -0.0001 | -0.17 | 0.08 | 95.1 | 0.32 |
| : (Intercept) | 0.20 | 0.196 | 0.08 | -0.0037 | -4.61 | 0.08 | 94.3 | 0.30 |  |  | 0.188 | 0.08 | -0.0118 | -14.96 | 0.08 | 94.3 | 0.30 |
| : (X3) | -0.10 |  |  |  |  |  |  |  |  |  | -0.099 | 0.11 | 0.0006 | 0.59 | 0.11 | 94.7 | 0.42 |
| : (Intercept) | -1.20 | -1.195 | 0.08 | 0.0045 | 5.42 | 0.08 | 92.7 | 0.30 |  |  | -1.202 | 0.08 | -0.0019 | -2.23 | 0.08 | 95.1 | 0.33 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.105 | 0.16 | -0.0045 | -2.81 | 0.16 | 95.6 | 0.63 |
| : (X3) | -0.40 |  |  |  |  |  |  |  |  |  | -0.398 | 0.10 | 0.0020 | 2.11 | 0.10 | 96.0 | 0.39 |
| : (Intercept) | 0.40 | 0.579 | 0.04 | 0.1791 | 489.91 | 0.18 | 0.0 | 0.06 |  |  | 0.398 | 0.04 | -0.0016 | -4.30 | 0.04 | 95.5 | 0.14 |
| : (X1) | 0.10 |  |  |  |  |  |  |  |  |  | 0.100 | 0.03 | 0.0001 | 0.29 | 0.03 | 96.1 | 0.13 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.099 | 0.04 | 0.0006 | 1.79 | 0.04 | 94.9 | 0.14 |
| : (X3) | -0.20 |  |  |  |  |  |  |  |  |  | -0.199 | 0.05 | 0.0006 | 1.21 | 0.05 | 93.6 | 0.18 |
|  | 0.30 |  |  |  |  |  |  |  |  |  | 0.289 | 0.03 | -0.0106 | -39.66 | 0.03 | 91.9 | 0.11 |
|  | -0.15 |  |  |  |  |  |  |  |  |  | -0.149 | 0.04 | 0.0012 | 3.16 | 0.04 | 94.5 | 0.14 |
| -2LogL |  | 40729.0 | | | | | | |  |  | 39784.7 | | | | | | |
| # of converged solutions | | 1000 | | | | | | |  |  | 981 | | | | | | |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

**Table SIX**. Results from 1000 simulations under the three-level mixed-effects location scale model (***design b3 in Table SI***)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | True Value | Three-level random intercept model | | | | | | |  |  | Three-level mixed-effects location scale model | | | | | | |
| EST | SE | Bias | SB | RMSE | 95% COV | AW |  | EST | SE | Bias | SB | RMSE | 95% COV | AW |
| : (Intercept) | 6.90 | 6.901 | 0.06 | 0.0011 | 1.79 | 0.06 | 94.7 | 0.24 |  |  | 6.902 | 0.06 | 0.0023 | 3.74 | 0.06 | 95.4 | 0.24 |
| : (X1) | -0.40 | -0.401 | 0.03 | -0.0007 | -2.52 | 0.03 | 95.6 | 0.11 |  |  | -0.401 | 0.02 | -0.0008 | -3.85 | 0.02 | 96.0 | 0.09 |
| : (X2) | 0.20 | 0.200 | 0.04 | -0.0002 | -0.55 | 0.04 | 95.2 | 0.16 |  |  | 0.200 | 0.03 | 0.0001 | 0.37 | 0.03 | 95.4 | 0.14 |
| : (X3) | 0.60 | 0.600 | 0.08 | 0.0000 | -0.03 | 0.08 | 94.7 | 0.33 |  |  | 0.600 | 0.08 | -0.0003 | -0.36 | 0.08 | 95.1 | 0.32 |
| : (Intercept) | 0.20 | 0.197 | 0.08 | -0.0034 | -4.25 | 0.08 | 94.0 | 0.30 |  |  | 0.187 | 0.08 | -0.0125 | -15.61 | 0.08 | 93.9 | 0.31 |
| : (X3) | -0.10 |  |  |  |  |  |  |  |  |  | -0.095 | 0.10 | 0.0045 | 4.46 | 0.10 | 93.9 | 0.38 |
| : (Intercept) | -1.20 | -1.196 | 0.10 | 0.0036 | 3.61 | 0.10 | 89.9 | 0.32 |  |  | -1.201 | 0.08 | -0.0014 | -1.73 | 0.08 | 94.9 | 0.32 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.103 | 0.15 | -0.0032 | -2.10 | 0.15 | 95.1 | 0.60 |
| : (X3) | -0.40 |  |  |  |  |  |  |  |  |  | -0.398 | 0.09 | 0.0021 | 2.32 | 0.09 | 96.4 | 0.37 |
| : (Intercept) | 0.40 | 0.719 | 0.05 | 0.3193 | 628.47 | 0.32 | 0.0 | 0.06 |  |  | 0.398 | 0.05 | -0.0017 | -3.79 | 0.05 | 94.7 | 0.18 |
| : (X1) | 0.10 |  |  |  |  |  |  |  |  |  | 0.100 | 0.03 | 0.0005 | 1.56 | 0.03 | 95.9 | 0.13 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.099 | 0.04 | 0.0008 | 2.22 | 0.04 | 94.8 | 0.14 |
| : (X3) | -0.20 |  |  |  |  |  |  |  |  |  | -0.200 | 0.06 | 0.0005 | 0.79 | 0.06 | 94.3 | 0.23 |
|  | 0.60 |  |  |  |  |  |  |  |  |  | 0.569 | 0.05 | -0.0305 | -63.91 | 0.06 | 86.8 | 0.18 |
|  | 0.35 |  |  |  |  |  |  |  |  |  | 0.348 | 0.05 | -0.0015 | -2.99 | 0.05 | 94.6 | 0.20 |
| -2LogL |  | 42116.2 | | | | | | |  |  | 40049.6 | | | | | | |
| # of converged solutions | | 1000 | | | | | | |  |  | 900 | | | | | | |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

**Table SX**. Results from 1000 simulations under the three-level mixed-effects location scale model (***design b4 in Table SI***)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | True Value | Three-level random intercept model | | | | | | |  |  | Three-level mixed-effects location scale model | | | | | | |
| EST | SE | Bias | SB | RMSE | 95% COV | AW |  | EST | SE | Bias | SB | RMSE | 95% COV | AW |
| : (Intercept) | 6.90 | 6.901 | 0.06 | 0.0013 | 2.03 | 0.06 | 95.1 | 0.24 |  |  | 6.901 | 0.06 | 0.0009 | 1.51 | 0.06 | 95.5 | 0.24 |
| : (X1) | -0.40 | -0.401 | 0.03 | -0.0010 | -3.54 | 0.03 | 95.1 | 0.11 |  |  | -0.401 | 0.02 | -0.0007 | -3.25 | 0.02 | 96.3 | 0.09 |
| : (X2) | 0.20 | 0.200 | 0.04 | -0.0001 | -0.16 | 0.04 | 95.3 | 0.16 |  |  | 0.200 | 0.03 | 0.0004 | 1.28 | 0.03 | 96.4 | 0.14 |
| : (X3) | 0.60 | 0.600 | 0.08 | -0.0001 | -0.09 | 0.08 | 94.6 | 0.33 |  |  | 0.600 | 0.08 | -0.0005 | -0.53 | 0.08 | 95.1 | 0.32 |
| : (Intercept) | 0.20 | 0.196 | 0.08 | -0.0038 | -4.74 | 0.08 | 94.3 | 0.31 |  |  | 0.187 | 0.08 | -0.0134 | -16.73 | 0.08 | 93.9 | 0.31 |
| : (X3) | -0.10 |  |  |  |  |  |  |  |  |  | -0.098 | 0.10 | 0.0024 | 2.46 | 0.10 | 94.8 | 0.38 |
| : (Intercept) | -1.20 | -1.196 | 0.10 | 0.0035 | 3.59 | 0.10 | 91.0 | 0.32 |  |  | -1.202 | 0.08 | -0.0017 | -2.12 | 0.08 | 95.4 | 0.32 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.103 | 0.15 | -0.0030 | -1.98 | 0.15 | 95.4 | 0.60 |
| : (X3) | -0.40 |  |  |  |  |  |  |  |  |  | -0.398 | 0.09 | 0.0018 | 2.00 | 0.09 | 96.0 | 0.37 |
| : (Intercept) | 0.40 | 0.719 | 0.05 | 0.3195 | 622.82 | 0.32 | 0.0 | 0.06 |  |  | 0.398 | 0.05 | -0.0018 | -3.80 | 0.05 | 95.3 | 0.18 |
| : (X1) | 0.10 |  |  |  |  |  |  |  |  |  | 0.100 | 0.03 | 0.0001 | 0.22 | 0.03 | 96.0 | 0.13 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.099 | 0.04 | 0.0005 | 1.53 | 0.04 | 95.0 | 0.14 |
| : (X3) | -0.20 |  |  |  |  |  |  |  |  |  | -0.199 | 0.06 | 0.0009 | 1.58 | 0.06 | 94.4 | 0.23 |
|  | 0.60 |  |  |  |  |  |  |  |  |  | 0.569 | 0.05 | -0.0306 | -65.37 | 0.06 | 86.6 | 0.18 |
|  | -0.35 |  |  |  |  |  |  |  |  |  | -0.348 | 0.05 | 0.0023 | 4.48 | 0.05 | 93.7 | 0.20 |
| -2LogL |  | 42117.3 | | | | | | |  |  | 40043.7 | | | | | | |
| # of converged solutions | | 1000 | | | | | | |  |  | 942 | | | | | | |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

**Table SXI**. Results from 1000 simulations under the three-level mixed-effects location scale model (***design b5 in Table SI***)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | True Value | Three-level random intercept model | | | | | | |  |  | Three-level mixed-effects location scale model | | | | | | |
| EST | SE | Bias | SB | RMSE | 95% COV | AW |  | EST | SE | Bias | SB | RMSE | 95% COV | AW |
| : (Intercept) | 6.90 | 6.901 | 0.06 | 0.0011 | 1.74 | 0.06 | 95.0 | 0.24 |  |  | 6.901 | 0.06 | 0.0010 | 1.60 | 0.06 | 94.6 | 0.24 |
| : (X1) | -0.40 | -0.401 | 0.03 | -0.0005 | -1.64 | 0.03 | 95.0 | 0.13 |  |  | -0.402 | 0.02 | -0.0015 | -7.94 | 0.02 | 96.0 | 0.08 |
| : (X2) | 0.20 | 0.200 | 0.04 | -0.0005 | -1.04 | 0.04 | 94.9 | 0.17 |  |  | 0.200 | 0.03 | 0.0002 | 0.68 | 0.03 | 95.6 | 0.14 |
| : (X3) | 0.60 | 0.600 | 0.09 | 0.0001 | 0.06 | 0.09 | 94.7 | 0.33 |  |  | 0.598 | 0.09 | -0.0017 | -1.99 | 0.09 | 94.8 | 0.33 |
| : (Intercept) | 0.20 | 0.197 | 0.08 | -0.0032 | -3.89 | 0.08 | 94.4 | 0.31 |  |  | 0.188 | 0.08 | -0.0118 | -14.79 | 0.08 | 95.1 | 0.31 |
| : (X3) | -0.10 |  |  |  |  |  |  |  |  |  | -0.094 | 0.10 | 0.0059 | 5.90 | 0.10 | 94.2 | 0.38 |
| : (Intercept) | -1.20 | -1.203 | 0.15 | -0.0027 | -1.79 | 0.15 | 82.4 | 0.40 |  |  | -1.202 | 0.08 | -0.0020 | -2.63 | 0.08 | 95.3 | 0.30 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.103 | 0.14 | -0.0029 | -2.11 | 0.14 | 96.0 | 0.56 |
| : (X3) | -0.40 |  |  |  |  |  |  |  |  |  | -0.399 | 0.09 | 0.0009 | 1.05 | 0.09 | 96.6 | 0.35 |
| : (Intercept) | 0.40 | 1.006 | 0.08 | 0.6057 | 747.40 | 0.61 | 0.0 | 0.06 |  |  | 0.398 | 0.06 | -0.0019 | -3.13 | 0.06 | 94.4 | 0.23 |
| : (X1) | 0.10 |  |  |  |  |  |  |  |  |  | 0.100 | 0.03 | 0.0000 | 0.01 | 0.03 | 95.3 | 0.13 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.101 | 0.04 | -0.0006 | -1.54 | 0.04 | 95.7 | 0.14 |
| : (X3) | -0.20 |  |  |  |  |  |  |  |  |  | -0.201 | 0.08 | -0.0009 | -1.02 | 0.08 | 94.3 | 0.31 |
|  | 1.20 |  |  |  |  |  |  |  |  |  | 1.142 | 0.09 | -0.0575 | -65.69 | 0.10 | 87.4 | 0.34 |
|  | 0.50 |  |  |  |  |  |  |  |  |  | 0.497 | 0.07 | -0.0034 | -4.89 | 0.07 | 93.9 | 0.28 |
| -2LogL |  | 44983.7 | | | | | | |  |  | 40437.9 | | | | | | |
| # of converged solutions | | 999 | | | | | | |  |  | 792 | | | | | | |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

**Table SXII**. Results from 1000 simulations under the three-level mixed-effects location scale model (***design b6 in Table SI***)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | True Value | Three-level random intercept model | | | | | | |  |  | Three-level mixed-effects location scale model | | | | | | |
| EST | SE | Bias | SB | RMSE | 95% COV | AW |  | EST | SE | Bias | SB | RMSE | 95% COV | AW |
| : (Intercept) | 6.90 | 6.901 | 0.06 | 0.0013 | 2.07 | 0.06 | 95.2 | 0.24 |  |  | 6.901 | 0.06 | 0.0007 | 1.18 | 0.06 | 95.4 | 0.24 |
| : (X1) | -0.40 | -0.401 | 0.03 | -0.0010 | -3.13 | 0.03 | 94.9 | 0.13 |  |  | -0.401 | 0.02 | -0.0009 | -4.65 | 0.02 | 96.3 | 0.08 |
| : (X2) | 0.20 | 0.200 | 0.04 | -0.0003 | -0.70 | 0.04 | 95.0 | 0.17 |  |  | 0.201 | 0.03 | 0.0009 | 2.48 | 0.03 | 95.9 | 0.14 |
| : (X3) | 0.60 | 0.600 | 0.09 | 0.0001 | 0.11 | 0.09 | 94.5 | 0.33 |  |  | 0.600 | 0.09 | -0.0001 | -0.17 | 0.09 | 94.9 | 0.33 |
| : (Intercept) | 0.20 | 0.196 | 0.08 | -0.0043 | -5.18 | 0.08 | 94.0 | 0.31 |  |  | 0.185 | 0.08 | -0.0148 | -18.06 | 0.08 | 93.6 | 0.31 |
| : (X3) | -0.10 |  |  |  |  |  |  |  |  |  | -0.096 | 0.10 | 0.0038 | 3.79 | 0.10 | 94.2 | 0.38 |
| : (Intercept) | -1.20 | -1.202 | 0.15 | -0.0018 | -1.20 | 0.15 | 83.1 | 0.40 |  |  | -1.202 | 0.08 | -0.0022 | -2.95 | 0.08 | 94.8 | 0.30 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.100 | 0.14 | 0.0002 | 0.15 | 0.14 | 95.7 | 0.56 |
| : (X3) | -0.40 |  |  |  |  |  |  |  |  |  | -0.399 | 0.08 | 0.0008 | 0.99 | 0.08 | 96.0 | 0.35 |
| : (Intercept) | 0.40 | 1.006 | 0.08 | 0.6063 | 747.64 | 0.61 | 0.0 | 0.06 |  |  | 0.398 | 0.06 | -0.0018 | -2.88 | 0.06 | 94.9 | 0.23 |
| : (X1) | 0.10 |  |  |  |  |  |  |  |  |  | 0.100 | 0.03 | -0.0003 | -0.91 | 0.03 | 95.7 | 0.13 |
| : (X2) | -0.10 |  |  |  |  |  |  |  |  |  | -0.099 | 0.04 | 0.0008 | 2.10 | 0.04 | 94.9 | 0.14 |
| : (X3) | -0.20 |  |  |  |  |  |  |  |  |  | -0.198 | 0.08 | 0.0018 | 2.19 | 0.08 | 94.3 | 0.31 |
|  | 1.20 |  |  |  |  |  |  |  |  |  | 1.143 | 0.09 | -0.0566 | -66.63 | 0.10 | 86.9 | 0.34 |
|  | -0.50 |  |  |  |  |  |  |  |  |  | -0.496 | 0.07 | 0.0039 | 5.41 | 0.07 | 93.8 | 0.28 |
| -2LogL |  | 44990.1 | | | | | | |  |  | 40439.5 | | | | | | |
| # of converged solutions | | 1000 | | | | | | |  |  | 910 | | | | | | |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |