Supplementary Materials

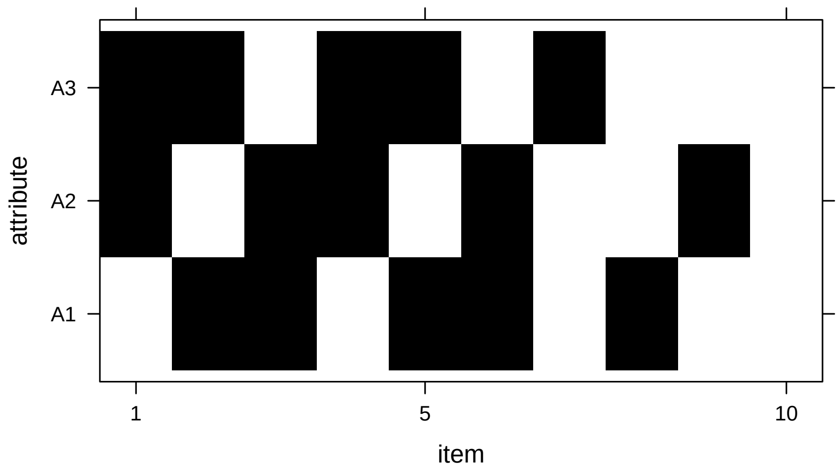
Supplementary Material A

The following are the true Q-matrices for the simulation study. Regarding the small-scale conditions, the three-attribute Q-matrix with 10 items comprises two sets of the identity matrix and all possible q-vectors that require two and three attributes. We then concatenated two of the three-attribute Q-matrix for the Q-matrix with 20 items. Specifically, the four-attribute Q-matrix with 10 items contains one set of the identity matrix, all possible q-vectors that require two attributes, and two q-vectors that measure three attributes. Meanwhile, the four-attribute Q-matrix with 20 items includes two sets of the identity matrix, two sets of all possible q-vectors that require two attributes, and four q-vectors that measure three attributes.

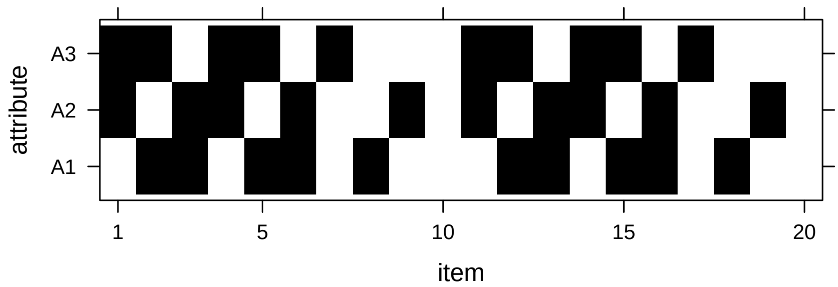
Regarding the large-scale conditions, the seven-attribute Q-matrix with 40 items comprises two sets of the identity matrix and 26 randomly selected items from the set of possible q-vectors that require two and three attributes. The 26 items were randomly selected in such a manner that half of those q-vectors measure two attributes, and the other half measure three attributes. In addition, the number of items that measure each attribute was set to be approximately equal across attributes. The seven-attribute Q-matrix with 80 items is the double stacking of the seven-attribute Q-matrix with 40 items. The eight-attribute Q-matrix contains two sets of the identity matrix and 24 randomly selected items from the set of possible q-vectors that require two and three attributes. The 24 items were randomly selected in the same manner as the seven-attribute Q-matrix with 40 items. Additionally, the eight-attribute Q-matrix with 80 items is the double stacking of the eight-attribute Q-matrix with 40 items.

In the following figures for the specifications of the true Q-matrices, a white box denotes an entry of a Q-matrix that takes the value of 1, and a black box denotes the one that takes the value of 0. The files for these true Q-matrices can be obtained from the data repository in the Open Science Framework: https://osf.io/jev9q/?view_only=85edc4684e0b46dc9e05e14a761d0650.

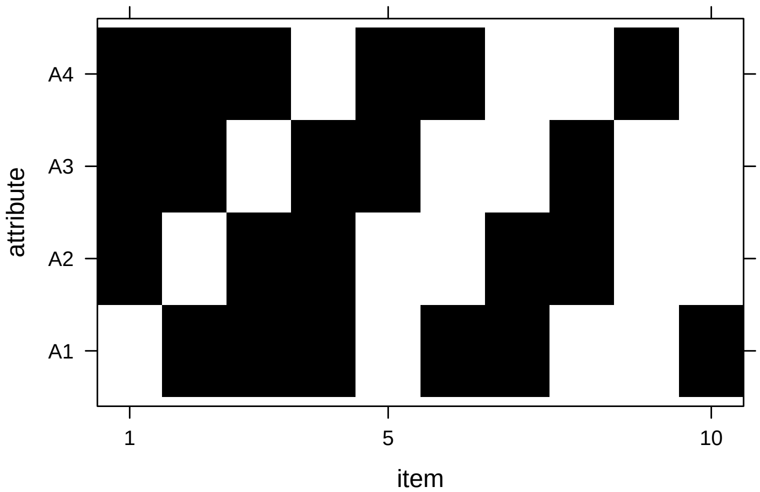
True Q−matrix (K=3, J=10)



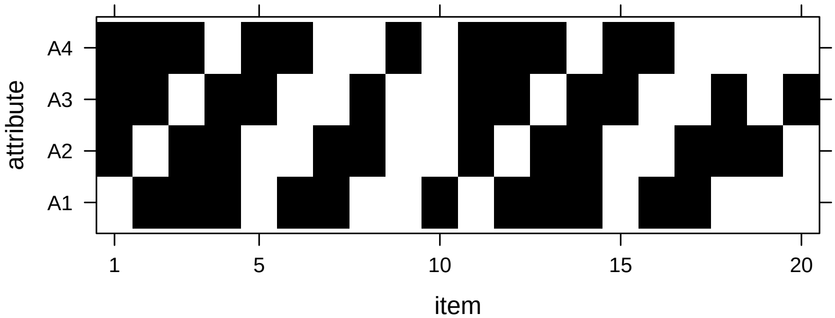
True Q−matrix (K=3, J=20)

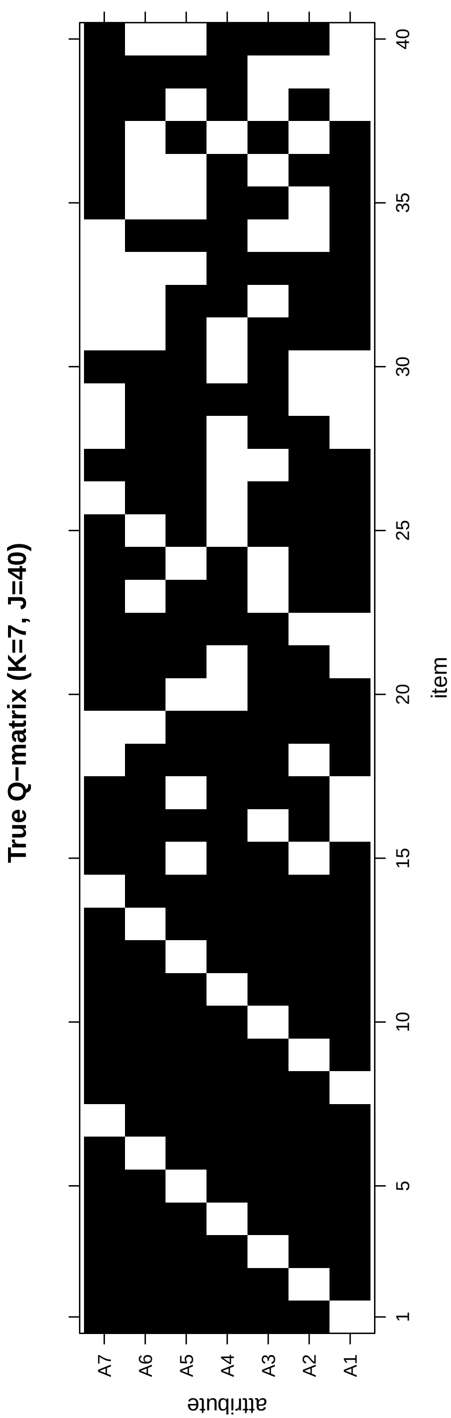


True Q−matrix (K=4, J=10)

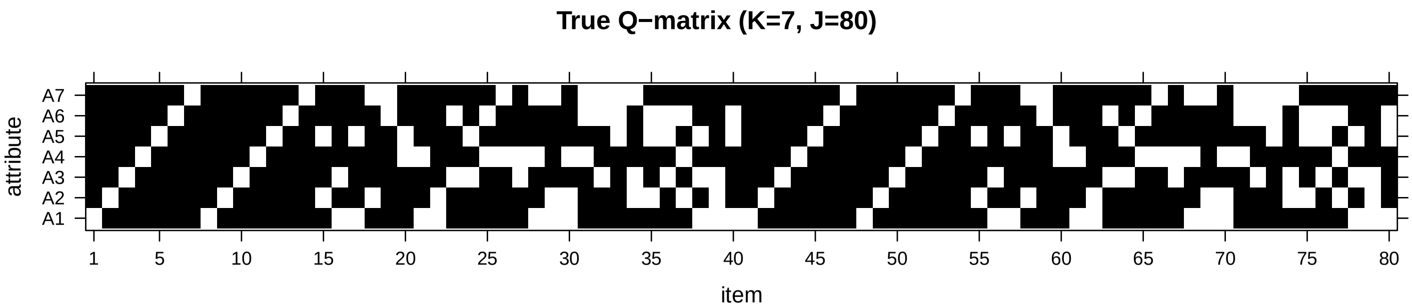


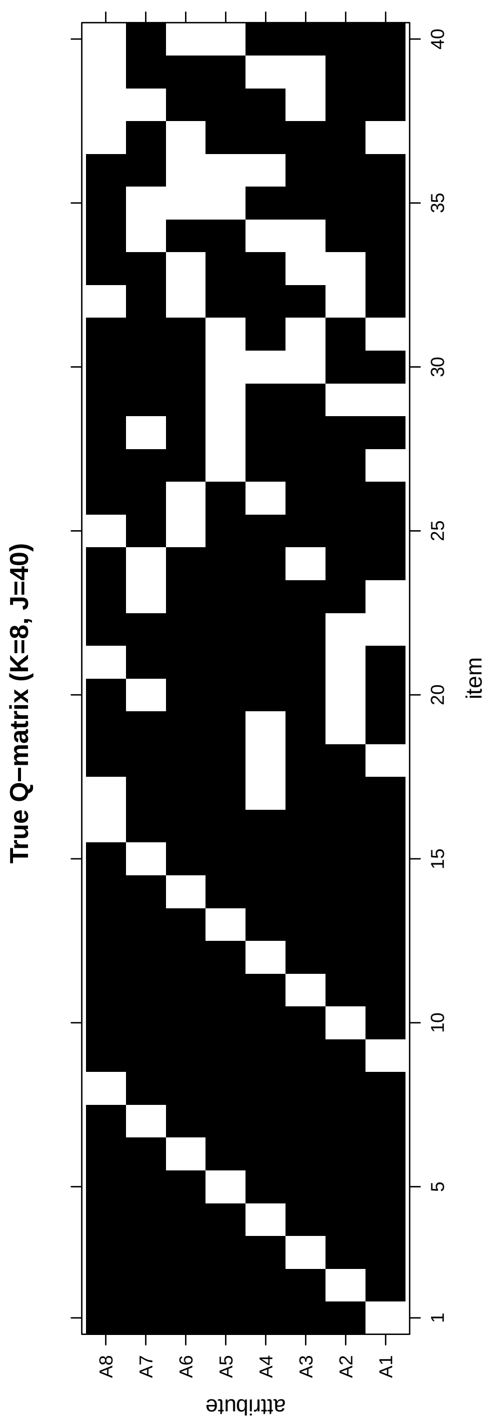
True Q−matrix (K=4, J=20)



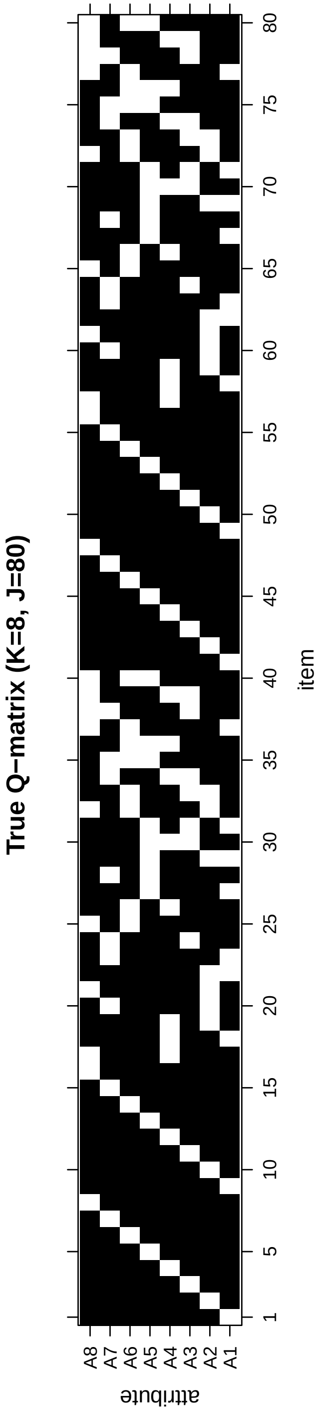


True Q−matrix (K=7, J=40)
item
attribute
A7
A6
A5
A4
A3
A2
A1
1
5
10
15
20
25
30
35
40


True Q−matrix (K=7, J=80)
attribute
A7
A6
A5
A4
A3
A2
A1
item
1
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80



True Q−matrix (K=8, J=40)
attribute
A8
A7
A6
A5
A4
A3
A2
A1
item
1
5
10
15
20
25
30
35
40


True Q−matrix (K=8, J=80)
attribute
A8
A7
A6
A5
A4
A3
A2
A1
item
1
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80

Supplementary Material B

Table B1: Q-matrices for the comparison in the fraction subtraction dataset

Proposed method					Gibbs sampler (Chung, 2019)					EM-based algorithm (Chen et al., 2015)				
Item	Attributes				Item	Attributes				Item	Attributes			
	A1	A2	A3	A4		A1	A2	A3	A4		A1	A2	A3	A4
1	1	0	0	0	1	1	0	0	0	1	1	0	0	0
2	1	0	0	0	2	1	0	0	0	2	1	0	0	0
3	1	0	0	0	3	1	0	0	0	3	1	0	0	0
4	0	1	0	0	4	0	1	1	0	4	0	1	1	0
5	0	0	1	0	5	0	0	1	0	5	0	0	1	0
6	0	0	1	0	6	0	0	1	0	6	0	0	1	0
7	0	0	1	0	7	0	0	1	0	7	0	0	1	0
8	1	0	1	0	8	1	0	1	0	8	1	0	1	0
9	0	0	0	1	9	0	0	1	1	9	0	0	1	1
10	0	0	1	1	10	0	0	1	1	10	0	0	1	1
11	0	1	0	0	11	0	1	1	0	11	0	1	1	0
12	0	1	1	0	12	0	1	1	0	12	0	1	1	0
13	0	1	1	0	13	0	1	1	0	13	0	1	1	0
14	0	1	1	0	14	0	1	1	0	14	0	1	1	0
15	0	1	1	1	15	0	1	1	1	15	0	1	1	1
16	0	1	1	0	16	0	1	1	0	16	0	1	1	0
17	1	1	1	0	17	1	1	1	1	17	1	1	1	0

Table B2: The Q-matrices for the comparison in the ECPE dataset

Proposed method				Gibbs sampler (Chung, 2019)				EM-based algorithm (Chen et al., 2015)			
	Attributes				Attributes				Attributes		
Item	A1	A2	A3	Item	A1	A2	A3	Item	A1	A2	A3
1	1	1	0	1	1	1	0	1	1	1	0
2	0	1	0	2	0	1	0	2	0	1	0
3	1	1	0	3	1	1	1	3	1	0	1
4	0	0	1	4	0	0	1	4	0	0	1
5	0	0	1	5	0	0	1	5	0	0	1
6	0	0	1	6	0	0	1	6	0	0	1
7	1	1	0	7	1	1	0	7	1	0	1
8	0	1	0	8	0	1	0	8	0	1	0
9	1	0	1	9	1	0	1	9	1	0	0
10	1	0	0	10	1	0	0	10	1	0	0
11	1	0	1	11	1	0	1	11	1	0	1
12	1	0	1	12	1	0	1	12	1	0	1
13	1	0	0	13	1	0	0	13	1	0	0
14	1	1	1	14	1	1	1	14	1	0	0
15	0	1	0	15	0	1	0	15	0	0	1
16	1	0	0	16	1	1	0	16	0	0	1
17	0	1	0	17	0	1	0	17	0	1	1
18	0	1	0	18	0	1	0	18	0	0	1
19	0	0	1	19	0	0	1	19	0	0	1
20	1	0	1	20	1	0	1	20	1	0	1
21	0	1	0	21	0	1	0	21	0	1	0
22	0	0	1	22	0	0	1	22	0	0	1
23	0	1	0	23	0	1	0	23	0	1	0
24	0	1	1	24	0	1	1	24	1	1	1
25	1	1	0	25	1	1	1	25	1	0	0
26	0	1	1	26	0	0	1	26	0	0	1
27	1	0	0	27	1	0	0	27	1	0	0
28	0	0	1	28	0	0	1	28	0	0	1

Table B3: The estimated Q-matrix from the TIMSS 2003 mathematics dataset

Proposed method

Item	Attributes												
	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13
1	1	0	0	0	0	0	0	0	0	0	1	0	1
2	1	0	0	0	0	0	0	0	0	0	0	0	0
3	0	1	0	0	0	0	1	0	0	0	0	0	0
4	0	0	0	0	0	0	1	0	1	0	1	0	0
5	0	0	0	0	0	1	0	0	0	1	0	1	0
6	0	0	0	0	0	1	1	0	0	0	0	0	0
7	1	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	1	0	0	0	1	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0	1	0	0
10	0	0	0	0	0	1	0	0	0	0	0	1	1
11	0	1	0	0	0	0	0	1	0	0	0	0	0
12	0	0	1	0	0	0	0	0	0	0	0	0	1
13	0	0	0	0	0	1	0	0	1	0	0	0	0
14	0	1	0	0	0	0	0	0	0	0	1	0	1
15	0	1	0	0	0	0	0	0	0	0	0	1	0
16	0	0	0	0	1	0	0	0	0	0	0	0	0
17	0	1	0	1	0	0	0	0	0	0	1	0	0
18	1	0	0	1	0	1	0	0	0	0	0	0	0
19	0	1	0	0	1	1	0	1	0	0	0	0	1
20	0	1	1	1	0	0	0	1	0	0	0	0	0
21	0	0	1	0	0	1	0	0	0	0	0	0	0
22	0	1	0	0	0	0	0	0	0	0	0	0	0
23	0	0	0	1	0	0	0	0	1	0	0	0	0

Table B4: The Q-matrix reported in Su et al. (2003)

Expert knowledge (Su et al., 2003)													
Item	Attributes												
	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13
1	1	0	0	0	0	0	0	0	0	0	1	0	1
2	0	0	0	0	0	1	0	0	0	0	0	0	0
3	0	1	0	0	0	0	1	0	0	0	0	0	0
4	0	0	0	1	0	0	0	0	1	0	0	0	0
5	0	0	0	0	0	1	0	0	0	1	0	1	0
6	0	0	0	0	0	1	1	0	0	0	0	0	0
7	1	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	1	0	0	0	1	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0	1	0	0
10	0	0	0	0	0	1	0	0	0	0	0	0	0
11	0	1	0	0	0	0	0	1	0	0	0	0	0
12	0	0	1	0	0	0	0	0	0	0	0	0	1
13	0	0	0	0	1	0	0	0	0	0	0	0	0
14	0	0	0	0	0	1	0	0	0	0	0	0	0
15	0	1	0	0	0	0	0	0	0	0	0	1	0
16	0	0	0	0	1	0	0	0	0	0	0	0	0
17	0	0	0	1	0	0	0	0	0	0	0	0	0
18	0	0	1	0	0	0	0	0	1	0	1	0	1
19	0	1	0	0	0	0	0	0	0	0	0	0	0
20	1	0	0	0	0	0	0	0	0	0	0	0	0
21	0	0	0	0	1	0	0	0	0	0	0	0	0
22	0	1	0	0	0	0	0	0	0	0	0	0	0
23	0	0	0	1	0	0	0	0	1	0	0	0	0

Supplementary Material C

AIC and BIC under other DCMs

AIC and BIC were calculated given the estimated Q-matrix from the proposed method. The TIMSS 2003 mathematics dataset was used for a comprehensive comparison among other DCMs. The results indicated that, although the proposed method assumes the DINA model, its estimated Q-matrix yielded a better fit than the Q-matrix by the domain experts in terms of AIC for DINA, DINO, RRUM, ACDM, and GDINA models and in terms of BIC for DINA, DINO, ACDM, and GDINA models.

Table C1: The values of AIC and BIC given the five DCMs

AIC			
	Proposed method	Expert knowledge	Difference
DINA	35420.71	35743.76	−323.05
DINO	35671.89	35706.96	−35.07
RRUM	34206.34	34246.55	−40.21
ACDM	33960.71	34353.29	−392.58
GDINA	34356.91	34725.16	−368.25

BIC			
	Proposed method	Expert knowledge	Difference
DINA	73552.78	73875.83	−323.05
DINO	73803.95	73839.03	−35.07
RRUM	72477.28	72448.06	29.23
ACDM	72231.65	72554.79	−323.14
GDINA	72970.42	73051.65	−81.23

Note. The differences in relative model fit indices were computed by subtracting the value of *Expert knowledge* from that of *Proposed method.*

Supplementary Material D

Comparison between the proposed method and other Bayesian methods with identification constraints

To investigate the possibility in which the proposed method performs poorly compared with other Bayesian methods with identification constraints in situations where a true Q-matrix possesses a certain design yielding identified model parameters, we conducted an additional simulation study based on the specification adopted in Liu et al. (2020). Specifically, we considered the conditions of $K = 3$ or 4, $N = 500$, $J = 18$, and $\rho = 0$ or 0.25. The same attribute-pattern generation method as Liu et al. (2020) was employed in this simulation study. The true Q-matrices were also specified identical to Liu et al. (2020). Further, the same setting of the proposed method—as in the condition of $N = 500$ in our simulation study—was employed for our estimation. Table D1 presents the results of matrix- and element-wise recovery rates. They show that the recovery rates from the proposed method were highly comparable with those from Liu et al. (2020), despite the fact that our method estimated a Q-matrix without the knowledge of whether a true Q-matrix in the simulation condition holds an identified structure. This is in contrast to the methods in Liu et al. (2020) in the sense that they estimated a Q-matrix using the identification constraints when the true Q-matrix in the simulation conditions is known to have such a structure. Therefore, these results suggest that our method estimated an identified, true Q-matrix without any identification constraints in an accurate and fast manner from a much greater Q-matrix space than the space being considered by the methods with the identification constraints in Liu et al. (2020).

Table D1: Recovery rate under the simulation conditions specified in Liu et al. (2020).

				matrix-wise recovery (%)				element-wise recovery (%)			
K	N	ρ	J	cGibbs1	cGibbs20	cMHRM	Proposed Method	cGibbs1	cGibbs20	cMHRM	Proposed Method
3	500	0	18	99	100	100	100	99.6	100	100	100
3	500	0.25	18	100	100	100	100	100	100	100	100
4	500	0	18	96	98	98	98	99.4	99.96	99.96	99.72
4	500	0.25	18	98	99	99	98	99.7	99.99	99.99	99.72

Note. The recovery rates of cGibbs1, cGibbs20, and cMHRM were adapted directly from Liu et al. (2020).

Supplementary Material E

We considered three cases where the log-likelihood value of an unidentified, true Q-matrix equals that of another Q-matrix, whereas the ELBO value of the true one differs from that of another one.

The following settings were assigned to the three cases. The sample size was set to $N = 100,000$. The true values of the guessing and slip parameters for the DINA model were specified as in Table E1. To generate datasets, we used the `simGDINA` function in the `GDINA` R package (Ma & de la Torre, 2020). The stopping criteria for the proposed algorithm and marginal likelihood estimation with an EM algorithm were specified such that the iteration stopped when the maximum change in the ELBO or two-times the negative log likelihood became less than 10^{-6} or the number of iterations reached 3000. Lastly, non-informative prior distributions were assigned to structural and item parameters, and initial values of latent indicator variable z_{il} were set to be $1/L$ for the proposed method.

Table E1: Specification of guessing and slip parameters

	True Item Parameters	
Item	Guessing	Slip
1	0.290	0.227
2	0.262	0.236
3	0.057	0.100
4	0.231	0.169
5	0.239	0.096
6	0.073	0.294

Example 1: $K = 2$ and $J = 6$

Tables E2 and E3 show the details of Q-matrices in this example and their values of log likelihood and ELBO. Although the log-likelihood value of the true Q-matrix equals that of another one, the ELBO correctly prefers the true Q-matrix over another one.

Table E2: Q-matrices for the case with $K = 2$ and $J = 6$

$K = 2$					
True Q-matrix	Attribute		Another Q-matrix	Attribute	
Item	1	2	Item	1	2
1	1	0	1	1	0
2	1	0	2	1	0
3	1	0	3	1	0
4	1	1	4	1	1
5	1	1	5	0	1
6	1	1	6	0	1

Note. The red cell boxes denote the entries that changed from the true Q-matrix to another one.

Table E3: Values of log likelihood and ELBO

	Log Likelihood	ELBO
True Q-matrix	-320046.490	-320125.019
Another Q-matrix	-320046.490	-320128.646

Example 2: $K = 3$ and $J = 6$

Tables E4 and E5 show the details of Q-matrices in this example and their values of log likelihood and ELBO. Although the log-likelihood value of the true Q-matrix equals that of another one, the ELBO correctly prefers the true Q-matrix over another one.

Table E4: Q-matrices for the case with $K = 3$ and $J = 6$

K=3							
True Q-matrix	Attribute			Another Q-matrix	Attribute		
Item	1	2	3	Item	1	2	3
1	1	0	0	1	1	0	0
2	0	0	1	2	0	0	1
3	1	0	1	3	1	0	1
4	1	0	1	4	1	0	1
5	1	1	1	5	1	1	0
6	1	1	1	6	1	1	1

Note. The red cell box denotes the entries that changed from the true Q-matrix to another one.

Table E5: Values of log likelihood and ELBO

	Log Likelihood	ELBO
True Q-matrix	-347569.953	-347668.958
Another Q-matrix	-347569.953	-347671.755

Example 3: $K = 4$ and $J = 6$

Tables E6 and E7 show the details of Q-matrices in this example and their values of log likelihood and ELBO. Although the log-likelihood value of the true Q-matrix equals that of another one, the ELBO correctly prefers the true Q-matrix over another one.

Table E6: Q-matrices for the case with $K = 4$ and $J = 6$

K=4									
True Q-matrix	Attribute				Another Q-matrix	Attribute			
Item	1	2	3	4	Item	1	2	3	4
1	1	0	0	0	1	1	0	0	0
2	1	1	0	0	2	1	1	0	0
3	1	0	1	0	3	1	0	1	0
4	1	1	1	0	4	1	1	1	0
5	1	1	1	1	5	1	1	0	1
6	1	1	1	1	6	1	1	0	1

Note. The red cell boxes denote the entries that changed from the true Q-matrix to another one.

Table E7: Values of log likelihood and ELBO

	Log Likelihood	ELBO
True Q-matrix	-346630.739	-346763.324
Another Q-matrix	-346630.739	-346765.463

References

Liu, C.-W., Andersson, B., & Skrondal, A. (2020). A constrained Metropolis-Hastings Robbins-Monro algorithm for Q matrix estimation in DINA models. *Psychometrika*, *85*(2), 322–357. https://doi.org/10.1007/s11336-020-09707-4

Ma, W., & de la Torre, J. (2020). GDINA: An R package for cognitive diagnosis modeling. *Journal of Statistical Software*, *93*(14), 1–26. https://doi.org/10.18637/jss.v093.i14