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Article in Applied Psychological Measurement · March 2020

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# Running head: IMPROVING ROBUSTNESS IN Q-MATRIX VALIDATION

1	This article should be cited as:
2	Nájera, P., Sorrel, M.A., de la Torre, J., & Abad, F. J. (in press). Improving robustness in Q-
3	matrix validation using an iterative and dynamic procedure. Applied Psychological
4	Measurement. doi:10.1177/0146621620909904
5	
6	Improving Robustness in Q-Matrix Validation using an Iterative and Dynamic Procedure
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16	This research was partially supported by Grant PSI2017-85022-P (Ministerio de
17	Ciencia, Innovación y Universidades, Spain).
18	The author(s) declared no potential conflicts of interest with respect to the research,
19	authorship, and/or publication of this article.
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# Improving robustness in Q-matrix validation using an iterative and dynamic procedure Abstract

27 In the context of cognitive diagnosis models, a Q-matrix reflects the correspondence between attributes and items. The Q-matrix construction process is typically subjective in nature, 28 which may lead to misspecifications. All this can negatively affect the attribute classification 29 accuracy. In response, several methods of empirical O-matrix validation have been developed. 30 The general discrimination index (GDI) method has some relevant advantages, such as the 31 possibility of being applied to several CDMs. However, the estimation of the GDI relies on 32 the estimation of the latent groups sizes and success probabilities, which is made with the 33 original (possibly misspecified) Q-matrix. This can be a problem, especially in those 34 situations in which there is a great uncertainty about the Q-matrix specification. To address 35 36 this, the present study investigates the iterative application of the GDI method where only one item is modified at each step of the iterative procedure, and the required cutoff is updated 37 38 considering the new parameter estimates. A simulation study was conducted to test the performance of the new procedure. Results showed that the performance of the GDI method 39 improved when the application was iterative at the item level and an appropriate cutoff point 40 was used. This was most noticeable when the original Q-matrix misspecification rate was 41 high, where the proposed procedure performed better 96.5% of the times. The results are 42 illustrated using Tatsuoka's fraction-subtraction dataset. 43

44 *Key words*: CDM, G-DINA, Q-matrix, validation, GDI.

### 46 Improving robustness in Q-matrix validation using an iterative and dynamic procedure

In the context of cognitive diagnosis assessment, cognitive diagnosis models (CDMs) 47 are latent class multidimensional statistical models that classify examinees as masters or non-48 49 masters of different skills. Those skills are often referred to as attributes. Several CDMs have been developed in the last years, which can be categorized as either reduced or general 50 models. The reduced models are the most specific ones; they provide low generalization but 51 high parsimony. The deterministic input noise and gate (DINA; Haertel, 1984; Junker & 52 Sijtsima, 2001), the deterministic input noise or gate (DINO; Templin & Henson, 2006), and 53 the noisy input, deterministic output and gate (NIDA; Maris, 1999; Junker & Sijtsima, 2001) 54 are some of the most widely known reduced models. Reduced models are usually preferred 55 because of the less number of parameter estimates and ease of interpretation. However, they 56 57 make strong assumptions about the data and model fit is therefore compromised. Reduced models are nested in the general models, which allow for greater flexibility, but with more 58 demanding requirements (e.g., larger sample sizes). The general diagnosis model (GDM; von 59 Davier, 2005) and the generalized DINA model (G-DINA; de la Torre, 2011) are two 60 examples of general models. These models are preferred when there is not enough evidence to 61 assume a specific response process underlying the item responses. 62 The estimation of a CDM typically requires two inputs: the item responses of the 63 examinees and a Q-matrix (Tatsuoka, 1983). The Q-matrix is a J (number of items)  $\times K$ 64

65 (number of attributes) matrix that reflects which attributes are measured by each item. Thus,

each item will have a q-vector  $(\mathbf{q}_j)$ , in which each q-entry  $(\mathbf{q}_{jk})$  will adopt a value of 1 or 0

67 denoting if attribute k is relevant for correctly answering item j or not, respectively.

68 The original Q-matrix construction process should have a theoretical foundation, and 69 thus it is usually performed after a literature review, by analyzing examinees' reports, or by 70 domain experts. These processes are subjective in nature and can lead to some

misspecifications in the Q-matrix. These Q-matrix misspecifications negatively affect the
estimation of the model parameters and the accuracy of the attribute profile classification
(Gao, Miller & Liu, 2017; Rupp & Templin, 2008). For this reason, in the last years, several
empirically-based methods of Q-matrix validation have been developed with the aim of
detecting and correcting misspecified entries in a Q-matrix.

The present paper will focus on the general discrimination index (GDI) method, also 76 known as the general method of Q-matrix validation, developed for the G-DINA framework 77 by de la Torre and Chiu (2016). The structure of the paper will be the following. First, the G-78 79 DINA model will be briefly introduced, followed by a description of the GDI method and its advantages and limitations. Second, an item-level iterative procedure for the GDI method is 80 proposed and described. Third, the performance of the iterative procedure is compared to that 81 82 of the GDI method by means of Monte Carlo simulation. Fourth, a real data illustration is conducted. Finally, a discussion of the results is provided, as well as future research insights 83 and comments on the advantages and limitations of the proposed procedure. 84

#### 85 Review of the G-DINA model

The G-DINA model (de la Torre, 2011) is a general, saturated CDM that subsumes most of the reduced models (e.g., DINA, DINO, *A*-CDM). In its original formulation, the probability of success can be decomposed into the sum of the effects due to the presence of specific attributes and their interactions:

$$P(\boldsymbol{\alpha}_{lj}^{*}) = \delta_{j0} + \sum_{k=1}^{K_j^{*}} \delta_{jk} \alpha_{lk} + \sum_{k'=k+1}^{K_j^{*}} \sum_{k=1}^{K_j^{*}-1} \delta_{jkk'} \alpha_{lk} \alpha_{lk'} \dots + \delta_{12\dots K_j^{*}} \prod_{k=1}^{K_j^{*}} \alpha_{lk} , \quad (1)$$

90 where  $\boldsymbol{\alpha}_{lj}^*$  is the reduced attribute vector whose elements are relevant for solving the item *j*; 91  $\delta_{j0}$  is the intercept of item *j*;  $\delta_{jk}$  is the main effect due to  $\alpha_k$ ;  $\delta_{jkk}$ , is the interaction effect due 92 to  $\alpha_k$  and  $\alpha_{k'}$ ; and  $\delta_{12...K_j^*}$  is the interaction effect due to  $\alpha_1, ..., \alpha_{K_j^*}$ , where  $K_j^*$  is the number 93 of attributes specified for item *j*.

94

## The GDI method of empirical Q-matrix validation

The GDI method of empirical Q-matrix validation (de la Torre & Chiu, 2016) is a
generalization of the δ-method (de la Torre, 2008) that was developed for the DINA model.
The GDI method has been shown to perform well under both reduced and general CDMs at
detecting and modifying misspecifications in the Q-matrix. Apart from its great flexibility and
generalization, this method is included in the GDINA package (Ma & de la Torre, 2018) of the
R software (R Core Team, 2018) with a low computational cost. This makes it one of the
most accessible and easily applicable methods.

102 This validation method relies on the general discrimination index (GDI; usually 103 represented as  $\varsigma_j^2$ ), which is the variance of the probabilities of success of the different latent 104 groups that are possible for an item weighted by the posterior distribution of those groups:

$$\varsigma_j^2 = \sum_{l=1}^{2^{K_j^*}} \omega(\boldsymbol{\alpha}_{lj}^*) [P(\boldsymbol{\alpha}_{lj}^*) - \bar{P}(\boldsymbol{\alpha}_{lj}^*)]^2$$
(2)

where  $2^{K_j^*}$  is the number of possible latent groups for item j,  $\omega(\boldsymbol{\alpha}_{lj}^*)$  is the posterior probability of examinees in group  $\boldsymbol{\alpha}_{lj}^*$ ,  $P(\boldsymbol{\alpha}_{lj}^*)$  is the probability of success for examinees in this group, and  $\overline{P}(\boldsymbol{\alpha}_{lj}^*)$  is the weighted mean probability of success across all the  $2^{K_j^*}$  possible latent groups for item j.

The method is based on the rationale that the correctly specified q-vector will lead to the highest possible item discrimination value; that is, the correct q-vector for an item will be the one that maximizes  $\varsigma_j^2$ . When comparing nested q-vectors, the specification of more attributes in the q-vector will lead to a higher  $\varsigma_j^2$ , and thus a criterion needs to be included so that the suggested q-vector for all items is not the one containing all the attributes ( $\varsigma_{q_j^{1:K}}^2$ ). De la Torre and Chiu (2016) defined the *proportion of variance accounted for* (PVAF), which is computed as PVAF<sub>jc</sub> =  $\varsigma_{q_j^2}^2 / \varsigma_{q_j^{1:K}}^2$ , where *c* reflects each of the 2<sup>K\*</sup> – 1 possible q-vectors

116 (note that the zero q-vector, with no attributes specified, is not plausible). The inclusion of spurious attributes is prevented by determining a cutoff point ( $\epsilon$ , also referred as *EPS* for 117 epsilon), so the suggested q-vector would be the simplest one (i.e., the one with less attributes 118 specified) among those that fulfill PVAF > *EPS*. 119

Despite the good performance of the validation method, the original study was not 120 without limitations, as de la Torre and Chiu (2016) noted. For instance, the authors did not 121 justify the election criterion for the value of the EPS, which was set to 0.95. This aspect of the 122 method was examined by Nájera, Sorrel, and Abad (2019), who found that the GDI method 123 124 showed a good performance under a wide set of conditions, given that an optimal EPS for each specific condition was used. Specifically, they provided a predictive formula for the 125 optimal *EPS* as a function of the average item quality (IQ), the sample size (N), and the 126 127 number of items (*J*):

 $EPS = \text{inv.}\log(-0.405 + 2.867 \cdot IQ + 4.840 \cdot 10^{-4} \cdot N - 3.316 \cdot 10^{-3} \cdot J), \quad (3)$ 

where *inv.logit*( $\cdot$ ) represents the inverse function of the logit function, computed as 128

 $\exp(x)/(1 + \exp(x))$ . IQ is computed as the average item quality  $(IQ = \frac{1}{I}\sum_{j=1}^{J}IQ_j)$ , where 129  $IQ_i$  is the difference in the probability of success between the latent group that possesses all 130 the relevant attributes specified in item j,  $P_i(1)$ , and the one with none of them,  $P_i(0)$ . 131

There is another aspect of the GDI method that deserves specific attention. When 132 computing  $\varsigma_j^2$ , the method assumes that the Q-matrix is correctly specified:  $\varsigma_j^2$  relies on the 133 estimation of the latent group sizes and their success probabilities, which are estimated using 134 the provisional (misspecified) Q-matrix. As the authors point out, "it would be difficult, if not 135 impossible, for the same experts to correctly specify all the entries of the Q-matrix, 136 particularly when the test is long. Consequently, (b) [this assumption] is expected to always 137 be violated" (de la Torre & Chiu, 2016, p. 258). The authors state that the violation of the

138

assumption "does not automatically invalidate the viability of the proposed method. [...] the
proposed method appears to be robust when the misspecifications in the Q-matrix is
controlled at a reasonable rate, which justifies the usefulness of the method in practice" (de la
Torre & Chiu, 2016, p. 258). According to the favorable results found by them with 5% of
misspecifications, and with 10% of misspecifications by Nájera et al. (2019), the method
seems indeed to be robust when the misspecification rate is low.

However, relying on the experts to make few mistakes while specifying the Q-matrix 145 is another assumption that may not always be realistic or, at least, will remain uncertain. It is 146 147 reasonable to think that different knowledge domains may vary in terms of Q-matrix specification difficulty. For instance, the Q-matrix of a scholastic exam of mathematical 148 operations seems easier to specify (e.g., " $8 + 3 \times 2$ ", would be easily detected as measuring, 149 for example, "sum" and "multiplication", but not "subtraction" or "division") than the Q-150 matrix of a reading comprehension test, a clinical diagnostic test, or a test assessing students' 151 competencies (e.g., Sorrel et al. [2016] reported lower inter-rater reliability for more abstract 152 attributes like "Study attitudes" compared to attributes easier to objectivize like "Helping 153 others"). In fact, the Q-matrix of the popular fraction subtraction data set (Tatsuoka, 1990), 154 which does not belong to a particularly ambiguous knowledge domain, is still controversial 155 (Kang, Yang, & Zeng, 2019). Thus, the degree of uncertainty involved in the process could 156 reasonably be higher than what has been assumed, especially when the response processes of 157 158 the knowledge domain are somehow subjectively defined. Some authors have taken this point under consideration, and have used in their simulation studies misspecification rates up to 159 40% (e.g., Wang et al., 2018). In light of the above, it is expected that the GDI method 160 performance will be compromised if the misspecification rate is reasonably high, since the 161 noise entered by the large number of misspecified q-entries can disrupt the calculation of  $\zeta_i^2$ . 162

163 Iterative Q-matrix validation methods

One way of mitigating the pernicious effects that the violation of the true Q-matrix 164 assumption may provoke is to apply the validation method with an iterative procedure. Some 165 validation methods follow this rationale. The *iterative modified sequential search algorithm* 166 (IMSSA; Terzi & de la Torre, 2018a) and the *iterative general discrimination index* method 167 (iGDI; Terzi, 2017; Terzi & de la Torre, 2018b) are two validation methods in which all 168 proposed q-vector modifications are introduced in the Q-matrix in each iteration. In this 169 sense, they can be referred to as *test-level* iterative methods. On the other hand, the *Q-matrix* 170 refinement method (QRM; Chiu, 2013) and the data-driven approach proposed by Liu, Xu, 171 and Ying (2012) update the Q-matrix after each q-vector modification; that is, they modify 172 only one item in each iteration. Thus, they can be referred to as an *item-level* iterative method. 173 174 Even though *test-level* iterative methods can improve the performance of non-iterative 175 methods, it may be more precise to apply the iterative procedure at the item level. At the testlevel iteration, the first step will introduce several modifications based on the original and 176 presumably misspecified Q-matrix, and thus the probability of introducing wrong 177 modifications will be high. At the item-level, only the first item will be modified based on the 178 information of the original Q-matrix, while the rest of the items will be modified based on 179 progressively better specified Q-matrices. In the context of the GDI method, this will result in 180 a better recovery of  $\varsigma_i^2$  and a more precisely predicted *EPS* as the iterations take place. 181

In light of the above, an optimal method should take into consideration the following desired characteristics: first, it should be conducted iteratively; second, the iterations should be applied at the item level; third, if a cutoff point is required, it should be selected by empirical means and updated within each iteration; fourth, it should be applicable to both reduced and general models. Based on this, it is expected that an item-level iterative procedure based on the GDI method, applied with an optimal *EPS* that gets updated after each

188	iteration, will lead to promising results. The steps of the iterative procedure algorithm
189	evaluated in this paper are the following:
190	Step 1: Estimate the CDM according to the item responses and the provisional Q-
191	matrix ( <b>Q</b> ).
192	Step 2: Select the <i>EPS</i> value.
193	<b>Step 3</b> : Compute all items' $\varsigma_j^2$ (and PVAF) for each possible q-vector specification and
194	define, for each item, the set of <i>appropriate q-vector(s)</i> , which fulfill(s) $PVAF > EPS$ .
195	Step 4: Select, for each item, the simplest element(s) among all the appropriate q-
196	vectors.
197	<b>4.1</b> : If there is only one element, then it is defined as the <i>suggested q-vector</i> .
198	<b>4.2</b> : If there are more than one element, the one with the highest PVAF is defined
199	as the suggested q-vector.
200	<b>Step 5</b> : Define, for each item, $PVAF_j^0$ as the PVAF of the <i>provisional q-vector</i>
201	specified in <b>Q</b> , and $\text{PVAF}_{j}^{*}$ as the PVAF of the suggested q-vector.
202	<b>Step 6</b> : Calculate all items' $\Delta PVAF_j$ , defined as $\Delta PVAF_j =  PVAF_j^* - PVAF_j^0 $ .
203	<b>Step 7</b> : Define the <i>hit item</i> as the item with the highest $\Delta PVAF_j$ .
204	Step 8: Update Q by changing the provisional q-vector by the suggested q-vector of
205	the <i>hit item</i> .
206	<b>Step 9</b> : Iterate over Steps 1 to 8 until $\sum_{j=1}^{J} \Delta PVAF_j = 0$ .
207	Step 2 and Steps 6 and 7 are of special relevance for the iterative procedure. Step 2
208	dictates which q-vectors are going to become appropriate q-vectors in Step 3 and,
209	consequently, which q-vector is going to become the suggested q-vector in Step 4. If the EPS
210	value is improperly chosen, the suggested q-vectors will be more likely to be incorrect. Thus,
211	each iteration will probably increase the distance between the provisional Q-matrix and the
212	true Q-matrix in a sort of "snowball" effect (i.e., errors will lead to more errors), and the $\zeta_j^2$
213	will be worse specified. Hence, it is very important that the EPS election criterion is not
214	arbitrary. The predictive formula provided by Nájera et al. (2019; see Equation 3) showed a
215	good performance under a wide range of conditions. Furthermore, it can be easily

216 implemented in the iterative procedure and entails an additional benefit: as the prediction formula considers the average item quality (IO), which is computed after the model is 217 estimated, the EPS in Step 2 can be updated after each iteration. Step 7 is also very important, 218 219 because the election of the *hit item* can be neither be at random. Especially in the first iterations, in which the Q-matrix will presumably still have several misspecifications, the  $\zeta_i^2$ 220 is going to be calculated with some error. Steps 6 and 7 are used to select, for each iteration, 221 the q-vector that is more likely to be misspecified. These steps should optimize the 222 performance of the iterative procedure by increasing the probabilities of properly modifying a 223 q-vector in each iteration. The iterations would stop when all the *provisional q-vectors* and 224 suggested q-vectors are equal. 225

226

#### **Simulation study**

A simulation study was conducted to test if the proposed iterative procedure for the GDI method provides better results than the standard (non-iterative) procedure. Two hypotheses were stated: a) the iterative procedure will show a better performance than the standard procedure, especially when the misspecification rate is high, b) this will be true as long as the *EPS* value is properly chosen, based on the predictive formula. The performance of the iterative procedure based on an inappropriate *EPS* value is expected to be worse than that of the standard procedure, due to the "snowball" effect previously described.

234 Method

235 *Design*. The examinees' responses were simulated under the G-DINA model. The 236 number of attributes was fixed at K = 5, and the underlying distribution of examinees' 237 attribute patterns was uniform. The number of examinees was fixed at N = 1000, the average 238 item quality at IQ = 0.6, and the number of items at J = 30. Those values are considered to 239 be medium levels of each factor in applied contexts (Nájera et al., 2019). Table 1 shows the 240 Q-matrix used to simulate the examinees' responses ( $Q_{true}$ ). The Q-matrix was used in the

paper of de la Torre and Chiu (2016). It contains the same number of one-, two- and three-

- attribute items, and each attribute is measured by the same number of items. Its structure
- satisfies the required conditions to be a complete (Köhn & Chiu, 2017, 2018) and identifiable
- 244 (Gu & Xu, in press a, in press b) Q-matrix. Three variables were studied: the proportion of
- misspecified q-entries or misspecification rate (MR = 0.1, 0.2, 0.3, 0.4), the application
- procedure for the GDI method (iterative, standard), and the *EPS* value (predicted *EPS*, 0.95).
- 247 Thus, a total of 16 conditions resulted after combining the different factor levels (4
- 248 misspecification rates  $\times$  2 GDI application procedures  $\times$  2 *EPS* values).

249 Table 1

250 *Q-Matrix for the Simulated Data* 

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Item	$\alpha_1$	$\alpha_2$	α3	$\alpha_4$	$\alpha_5$	Item	$\alpha_1$	$\alpha_2$	$\alpha_3$	$\alpha_4$	$\alpha_5$	
1	1	0	0	0	0	16	0	1	0	1	0	
2	0	1	0	0	0	17	0	1	0	0	1	
3	0	0	1	0	0	18	0	0	1	1	0	
4	0	0	0	1	0	19	0	0	1	0	1	
5	0	0	0	0	1	20	0	0	0	1	1	
6	1	0	0	0	0	21	1	1	1	0	0	
7	0	1	0	0	0	22	1	1	0	1	0	
8	0	0	1	0	0	23	1	1	0	0	1	
9	0	0	0	1	0	24	1	0	1	1	0	
10	0	0	0	0	1	25	1	0	1	0	1	
11	1	1	0	0	0	26	1	0	0	1	1	
12	1	0	1	0	0	27	0	1	1	1	0	
13	1	0	0	1	0	28	0	1	1	0	1	
14	1	0	0	0	1	29	0	1	0	1	1	
15	0	1	1	0	0	30	0	0	1	1	1	

251

Data generation. The probabilities of success of the latent groups with all the relevant

attributes,  $P_i(1)$ , and the probabilities of success of the latent groups with none of them,

253  $P_j(\mathbf{0})$ , were manipulated to generate the item's quality  $(IQ_j)$ . Specifically,  $P_j(\mathbf{1}) =$ 

254 U(0.7, 0.9) and  $P_i(\mathbf{0}) = U(0.1, 0.3)$ , which results in average values of  $\overline{P}(\mathbf{1}) \cong 0.8$  and

255  $\overline{P}(\mathbf{0}) \cong 0.2$ , giving an average item quality of  $IQ = \overline{P}(\mathbf{1}) - \overline{P}(\mathbf{0}) \cong 0.6$ . For the other latent

256 groups (those with some of the relevant attributes), the probabilities of success were simulated

so that they increased as the number of mastered attributes grew (i.e., monotonicity

constraint). Thus, a latent group that masters more attributes than other will always havehigher probabilities of success.

Misspecifications in the Q-matrix were introduced randomly with two constraints: 260 261 first, all items measured at least one attribute, and second, the first five items were not modified. This latter constraint ensured the completeness of the Q-matrix, by assuring that 262 each attribute had, at least, one single-attribute item measuring it (Köhn & Chiu, 2017, 2018). 263 A total of 200 data sets were generated for each of the conditions. For each data set, 264 the  $IO_i$  were generated according to the aforementioned uniform distribution, and a different 265 misspecified Q-matrix ( $Q_{miss}$ ) was produced. All simulations and CDM analyses were 266 performed in R software, using the GDINA package. 267 Dependent variables. Two different types of dependent variables were used to assess 268 the performance of the validation method. First, the Q-matrix recovery rate (QRR) was used 269 to measure the quality of the Q-matrix specification recovery. It reflects the number of q-270 271 entries that the method correctly specifies divided by the total number of q-entries  $(J \times K)$ . Second, the proportion of correctly classified attributes (PCA) and the proportion of correctly 272 classified vectors (PCV) were used to reflect the accuracy of attribute profile classification 273 274 (Ma & de la Torre, 2018). The PCA measures the proportion of entries (i.e., attributes) correctly classified in the  $N \times K$  matrix of attribute profile classification, while the PCV 275 reflects the proportion of examinees' attribute profiles that are completely correctly classified 276 (i.e., correctly classified rows in the  $N \times K$  matrix of attribute classifications). Please note that 277 the PCV is a stricter measure than the PCA, and will usually obtain lower values. These 278 279 accuracy measures are of high relevance, since they provide information about the impact of the Q-matrix specification quality in the final output of a CDM. 280 When applying a Q-matrix validation method, the suggested Q-matrix might show 281

some attributes positions (i.e., columns) interchanged. The possibility of having interchanged

283 attributes increases as the misspecification rate is higher. Thus, for each replica, the suggested Q-matrix was compared with  $\mathbf{Q}_{true}$  by checking the similarity between both matrices' 284 columns. Specifically, the mean absolute difference between the columns was conducted, and 285 286 the suggested Q-matrix's attribute columns were presented in the order that minimized the difference with the corresponding  $Q_{true}$  attribute columns. This process is akin to a domain 287 expert labelling the factors when interpreting a factor analysis, where the order of the factors 288 is arbitrary. In the present case, the domain expert will evaluate whether the attributes are 289 290 correctly labelled.

291 Results

Before describing the main results, a brief comment about the iterative process (when 292 using the predicted EPS) is provided. No convergence problems were registered during the 293 294 simulation study. Table 2 shows the average number of iterations and number of items modified (with one or more modifications in their q-vector) for each misspecification rate 295 condition. As expected, both measures increased as the misspecification rate did. It is 296 297 important to note that the number of iterations is usually higher than the number of items modified, given that one item can be modified several times during the iteration procedure. 298 One item can be more properly modified at a later moment of the procedure, when the rest of 299 the Q-matrix is better specified. On the other hand, information about the average IQ and EPS 300 is given in Table 3. As expected, the initial IQ (i.e., the one estimated with the misspecified 301 302 Q-matrix) rapidly decreased as the misspecification rate increased. However, after the iterative procedure was completed, the final IQ was adequately recovered, even for the most 303 unfavorable condition (i.e., MR = 0.4). This had an impact on the predicted *EPS*, which also 304 showed an increase from the original misspecified Q-matrix to the final validated Q-matrix. 305 In the following results, the performance of the standard and iterative procedures, as 306 well as their interaction with the predicted *EPS* and the *EPS* of 0.95, will be described. Tables 307

308	4, 5, and 6 show the results for the different dependent variables and conditions of the
309	simulation study in conjunction with the results obtained with the true Q-matrix and the
310	misspecified Q-matrices, which serve as upper and lower baselines, respectively. The type of
311	misspecification error (under- or over-specification) is disaggregated in Table 4. Plots for the
312	distribution of the dependent variables across the 200 replicates per misspecification rate
313	condition are provided in the Online Appendix. The different tables presented here include the
314	median of the 200 replicates due to the existence of asymmetry in the results distributions.
315	Results regarding the QRR, the PCA, and the PCV were consistent and showed similar
316	patterns. Thus, unless otherwise indicated, results for the three measures are described

- 317 together.
- 318 Table 2

319 Average Number of Iterations and of Modified Items

	]	Numb	er of item	s modifi	ed*			
MR	Mean	SD	Min	Max	Mean	SD	Min	Max
0.1	16.9	2.4	10	24	14.6	2.1	9	20
0.2	23.2	2.8	17	31	19.4	1.9	14	23
0.3	29.4	5.0	20	53	22.4	1.8	18	27
0.4	35.3	5.3	26	62	24.2	1.6	19	28

Note. \* = with one or more modifications in their q-vector. MR = misspecification rate. This

321 information refers to the iterative procedure in conjunction with the predicted *EPS*.

#### 322 Table 3

<sup>323</sup> Average Item Quality (IQ) and Used EPS

	I	2	E	PS
MR	Initial	Final	Initial	Final
0.1	0.545	0.574	0.824	0.836
0.2	0.481	0.567	0.795	0.833
0.3	0.421	0.549	0.765	0.825
0.4	0.369	0.531	0.738	0.817

Note. MR = misspecification rate. Initial *IQ* and *EPS* values are obtained with the original

misspecified Q-matrix. Final *IQ* and *EPS* values are obtained with the validated Q-matrix

after the iterative procedure (using the predicted *EPS*) is completed. Items were simulated with an IQ of 0.60.

As can be seen from Tables 4 to 6, the iterative implementation used in conjunction

329 with the predicted *EPS* always led to the best results. The Q-matrix recovery was very close

to one when the initial misspecification rate was low (QRR = 0.940), and was still high even

331	when the initial misspecification rate was high ( $QRR = 0.893$ ). This procedure achieved the
332	highest QRR among the four presented procedures in most of the replicates, especially as the
333	misspecification rate increased. Thus, the iterative-predicted EPS implementation obtained the
334	highest QRR 62% of the times ( $MR = 0.1$ ), 85.5% ( $MR = 0.2$ ), 93.5% ( $MR = 0.3$ ), and 96.5%
335	(MR = 0.4). It is important to note that, in those replicas in which it did not obtained the
336	highest QRR, it still obtained a QRR close to the highest, with a maximum loss of 0.07
337	through all misspecification rates. On the other hand, it obtained a QRR up to 0.32 higher
338	than the next best procedure, which reflects the better overall Q-matrix recovery shown in
339	Table 4. According to the GDI method rationale, a higher <i>EPS</i> tends to suggest more complex
340	q-vectors (i.e., with more attributes specified), and vice versa; thus, in Table 4 it can be seen
341	that the EPS of 0.95 produced more over-specification errors, while the predicted EPS
342	produced more under-specifications. The accuracy measures obtained with the iterative-
343	predicted EPS procedure were generally close to the upper limit regardless of the
344	misspecification rate. This was especially true for PCA. The misspecification rate affected
345	more severely the rest of the procedures. For example, the range of the median PCA values
346	reported in Table 5 for the standard and iterative implementations used in conjunction with
347	the predicted EPS were 0.085 and 0.012, respectively.

348 Table 4

			Predicted EPS		EPS = 0.95	
MR	<b>Q</b> true	Qmiss	std	ite	std	ite
0.1	1	0.900	0.940	0.940	0.887	0.833
	1	(6, 9)	(8, 1)	(8, 0)	(1, 16)	(1, 24)
0.2	1	0.800	0.907	0.933	0.827	0.780
		(13, 17)	(11, 3)	(9, 1)	(2, 24.5)	(1, 32.5)
0.2	1	0.700	0.817	0.913	0.720	0.687
0.5	1	(19, 26)	(17, 11)	(11, 2)	(6, 36)	(1, 46)
0.4	1	0.600	0.740	0.893	0.627	0.610
	1	(26, 34)	(21, 18)	(13, 3)	(8.5, 47)	(0.5, 58)

349 Medians for the Q-Matrix Recovery Rate (QRR) Results

350 *Note*. MR = misspecification rate;  $\mathbf{Q}_{true}$  = true Q-matrix;  $\mathbf{Q}_{miss}$  = misspecified Q-matrix; std =

351 standard procedure; ite = iterative procedure. A grayscale has been used for interpretation

352 purposes. Highest QRRs among the validation methods for each MR are shown in bold.

353 Median values for the number of under- and over-specified q-entries, respectively, are shown

- in brackets. Q-matrices are formed by 150 q-entries.
- 355 Table 5

250		D /	( <b>C</b> 1	C1 'C' 1 A '1	$(\mathbf{D}\mathbf{C}\mathbf{A})\mathbf{D}1$
356	<i>Mealans for the</i>	Proportion o	f Correctly	<i>Classifiea</i> Attributes	(PCA) Results
		1 .	,		

			Predicted EPS		EPS = 0.95	
MR	Qtrue	$\mathbf{Q}_{\mathrm{miss}}$	std	ite	std	ite
0.1	0.910	0.895	0.907	0.907	0.900	0.894
0.2	0.911	0.867	0.901	0.906	0.894	0.889
0.3	0.911	0.813	0.862	0.903	0.868	0.880
0.4	0.910	0.764	0.822	0.895	0.807	0.864

357 *Note.* MR = misspecification rate;  $\mathbf{Q}_{true}$  = true Q-matrix;  $\mathbf{Q}_{miss}$  = misspecified Q-matrix; std =

standard procedure; ite = iterative procedure. A grayscale has been used for interpretation

359 purposes. Highest PCAs among the validation methods for each MR are shown in bold.

#### 360 Table 6

362

361 Medians for the Proportion of Correctly Classified Vectors (PCV) Results

			Predict	ed EPS	EPS = 0.95		
MR	Qtrue	Qmiss	std	ite	std	ite	
0.1	0.637	0.583	0.625	0.625	0.603	0.581	
0.2	0.642	0.484	0.604	0.623	0.586	0.560	
0.3	0.643	0.325	0.457	0.613	0.492	0.531	
0.4	0.639	0.227	0.337	0.579	0.335	0.483	

*Note*. MR = misspecification rate;  $Q_{true}$  = true Q-matrix;  $Q_{miss}$  = misspecified Q-matrix; std =

standard procedure; ite = iterative procedure. A grayscale has been used for interpretation 363 purposes. Highest PCVs among the validation methods for each MR are shown in bold. 364 The following comments can be made regarding the manipulated factors. First, as it 365 366 was expected, for both application procedures (standard vs. iterative) and EPS values 367 (predicted *EPS* vs. EPS = 0.95), results were worse as the misspecification rate increased. Second, for both the standard and iterative procedures, and in line with the conclusions of 368 Nájera et al. (2019), the predicted EPS provided better results than the EPS of 0.95. Third, 369 regarding the interaction between the application procedure and the EPS value, the iterative 370 procedure showed a better performance than the standard procedure only when the predicted 371 EPS was used. Results were very similar for both procedures when the misspecification rate 372

373 was low (MR = 0.1), but, as the misspecification rate was higher, the differences between both

374 procedures substantially increased favoring the iterative procedure. On the contrary, when the

- EPS of 0.95 was used, the QRR of the iterative procedure was lower for all misspecification
- 376 rates. As previously stated, these results were expected, since an inappropriate *EPS* increases

the probability of selecting an incorrect suggested q-vector, enlarging the distance between the provisional Q-matrix and the true Q-matrix, disrupting the calculation of  $\varsigma_j^2$ . However, regarding the PCA and the PCV, the iterative procedure, in conjunction with the *EPS* of 0.95, showed slightly worse results when the misspecification rate was low (*MR* = 0.1 or 0.2), but outperformed the standard procedure when the misspecification rate was high (*MR* = 0.3 or 0.4). All this reflects the fact that both an iterative procedure and a dynamic optimal *EPS* value are required in order to achieve optimal results.

384

### **Real Data Example**

## 385 Data and Analysis

In order to facilitate a direct comparison between the proposed procedure and the 386 original GDI method, we used the same dataset as de la Torre and Chiu (2016). It consists of 387 536 examinees' responses to 11 fraction-subtraction items (Tatsuoka, 1990) measuring four 388 389 attributes (see strategy b in Mislevy, 1996): (1) performing basic fraction-subtraction operation, (2) simplifying/reducing, (3) separating whole number from fraction, and (4) 390 borrowing one from whole number to a fraction. Table 7 shows the initial Q-matrix for these 391 data, which is the same as the one used by de la Torre and Chiu (2016). A higher-order G-392 DINA model (de la Torre & Douglas, 2004) was used to fit the data. 393

#### 394 **Results**

Table 7 shows the Q-matrix suggested by the iterative procedure. Six q-entries modifications were proposed, all of them switching from 1 to 0, and all of them involving attribute 2, with the exception of attribute 1 in Item 1. These results are somewhat congruent with those found by de la Torre and Chiu (2016), who reported three modifications in attribute 2 (Items 4, 5, and 11). According to the results found in the simulation results, the iterative procedure suggested a less complex Q-matrix (i.e., less attributes specified) than the original GDI method (see Table 4).

Regarding the original Q-matrix, attribute 2 (simplifying/ reducing) seems to have 402 theoretical relevance to solve the modified items. However, it is important to note that it 403 shows a great collinearity with attributes 3 and 4; that is, almost every time attribute 2 is 404 required, attributes 3 and 4 are also required. The only time that attribute 2 appears without 405 attributes 3 or 4 is in Item 6, which is the only one that retains attribute 2 in the suggested Q-406 matrix. Thus, even though this attribute makes theoretical sense and seems to be correctly 407 specified in the original Q-matrix, it cannot be properly separated from other attributes. Since 408 it cannot provide any additional value, it becomes an irrelevant attribute and almost 409 disappeared in the suggested Q-matrix. 410

411 Table 7

	412	Original and	suggested	Q-matrices	for the	fraction-	subtraction da	ta
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		Original Q-matrix			Suggested Q-matrix				
	Item	$\alpha_1$	$\alpha_2$	α3	α4	$\alpha_1$	$\alpha_2$	α3	$\alpha_4$
1	$3\frac{1}{2}-2\frac{3}{2}$	1	1	1	1	0*	0*	1	1
2	$\frac{\overline{6}}{7} - \frac{4}{7}$	1	0	0	0	1	0	0	0
3	$3\frac{7}{8} - 2$	1	0	1	0	1	0	1	0
4	$4\frac{4}{12}-2\frac{7}{12}$	1	1	1	1	1	0*	1	1
5	$4\frac{1}{3}-2\frac{4}{3}$	1	1	1	1	1	0*	1	1
6	$\frac{11}{8} - \frac{1}{8}$	1	1	0	0	1	1	0	0
7	$3\frac{4}{5}-3\frac{2}{5}$	1	0	1	0	1	0	1	0
8	$4\frac{5}{7}-1\frac{4}{7}$	1	0	1	0	1	0	1	0
9	$7\frac{3}{5}-\frac{4}{5}$	1	0	1	1	1	0	1	1
10	$4\frac{1}{10}-2\frac{8}{10}$	1	1	1	1	1	0*	1	1
11	$\frac{1}{4\frac{1}{3}} - 1\frac{5}{3}$	1	1	1	1	1	0*	1	1

413 *Note*. Q-entries modifications are highlighted with an asterisk.

414 Regarding Item 1, the first attribute is also removed in the suggested Q-matrix. This

415 item can be correctly solved by following different strategies:

416 (a) 
$$3\frac{1}{2} - 2\frac{3}{2} = \frac{7}{2} - \frac{7}{2} = 0$$
 (attributes 1 and 4);

417 (b) 
$$3\frac{1}{2} - 2\frac{3}{2} = 2\frac{3}{2} - 2\frac{3}{2} = 0$$
 (attributes 1, 3, and 4)

A mesaplot (Ma & de la Torre, 2018), which shows the PVAF related to each possible 418 q-vector specification, for Item 1 is presented in Figure 1. Four q-vectors (0011, 0111, 1011, 419 420 1111) clearly show a higher PVAF than the rest. Since their PVAF is higher than the EPS (0.903), they form the set of appropriate q-vectors. The q-vector of 0011 is chosen as the 421 suggested q-vector because it is the simplest one. This attribute specification is related to 422 strategy (b), although attribute 1 is missing. A possible explanation to this could be that the 423 subtraction required in Item 1 may be a very easy operation that almost every examinee can 424 solve, since it involves two identical elements. As a consequence, attribute 1 would no longer 425 426 provide additional information. Nevertheless, these are modification suggestions, and domain experts can seek among the appropriate q-vector in order to find the most suitable 427 specification. The last decision about the Q-matrix specification should rely on the judgment 428 of domain experts (de la Torre & Chiu, 2016). 429



430

*Figure 1.* Mesaplot for Item 1 of Tatsuoka's fraction-subtraction dataset included in Table 7.
The black dot represents the original q-vector specification (1111). The PVAF represents the
ratio of the GDI associated to a q-vector to the highest possible GDI that is obtained when all

the attributes are specified.

435

#### Discussion

CDMs rely on a correctly specified O-matrix to provide an accurate classification of 436 examinees' attribute profiles. Domain experts are expected to specify the Q-matrix along with 437 438 a theoretical background, but they may commit some errors while doing so, especially when the knowledge domain is particularly complex and ambiguous (e.g., mental pathologies, 439 reading comprehension, students' competencies). In this context, among the many Q-matrix 440 validation methods that have been developed in the last few years, de la Torre and Chiu 441 (2016) proposed the GDI method, which has some important advantages, such as its great 442 flexibility to be used with several reduced or general CDMs, its good performance at 443 modifying incorrectly specified q-vectors, and its low computational cost (Ma & de la Torre, 444 445 2018). Despite its benefits, the GDI method relies on the original Q-matrix, which may not be correctly specified in most applied contexts. Although the method seemed robust to the 446 violation of this assumption when the Q-matrix misspecification rate was low, it is expected 447 to show a poorer performance when validating Q-matrices with more misspecifications. 448 449 The present paper evaluated an item-level iterative with dynamic *EPS* implementation for the GDI method (this approach can be referred to as "ILD-GDI"). Considering past 450 research (e.g., Chiu, 2013; Liu et al., 2012; Nájera et al., 2019; Terzi & de la Torre, 2018ab), 451 we hypothesized that this implementation would lead to better results compared to the 452 existing procedures, especially when the misspecification rate is high. A simulation study was 453 454 conducted to test this hypothesis. Results showed that the new implementation did provide better results. The gain obtained increased as the misspecification rate was higher. 455 The iterative procedure was hypothesized to have a poorer performance than the 456 standard procedure when used in conjunction with an inappropriate EPS. However, even 457 though the iterative-0.95 EPS (ite95) obtained a lower QRR than the standard-0.95 EPS 458 (*std95*), it provided better attribute profile classification results when the misspecification rate 459

460 was high (MR = 0.3 or 0.4). A tentative explanation of this result could be related to the type of misspecification error. Some prior studies in the field (e.g., Gao, Miller, & Liu, 2017; Choi, 461 Templin, Cohen, & Atwood as cited in Kunina-Habenicht, Rupp, & Wilhelm, 2012) have 462 463 found that under-specifications have a greater impact in attribute profiles classification than over-specifications. This effect is logically expected, since removing a parameter with a 464 substantive effect from a model might dramatically disrupt the probabilities of success of the 465 affected item; on the other hand, a spurious parameter added to the model may obtain a 466 marginal effect estimate, mitigating its impact (as long as the sample size is big enough to 467 468 produce stable parameter estimates).

This effect can explain the aforementioned results regarding *ite95* and *std95*. Table 4 469 470 shows the information regarding the Q-matrix recovery, disaggregated by specification error type. On one hand, when MR = 0.1 or 0.2, *std95*'s QRR was higher than *ite95*'s. *Std95*'s PCA 471 and PCV were also higher than ite95's. However, PCA differences were not as big as QRR 472 differences, since the higher amount of misspecifications in *ite95* were mainly over-473 474 specifications, and both procedures had a similar number of under-specifications. On the other hand, when MR = 0.3 or 0.4, *std95*'s QRR was still higher than *ite95*'s. However, *ite95*'s PCA 475 and PCV were higher than *std95*'s. Here, the QRR differences between both procedures were 476 smaller than those obtained with MR = 0.1 or 0.2. In addition, the higher amount of 477 misspecifications in *ite95* were mainly over-specifications, while *std95* obtained more under-478 479 specifications. As previously stated, the latter might provoke a bigger disruption in the posterior probabilities estimates, causing a worse attribute classification. 480 The explanation given above is certainly conditioned by the total number of 481

misspecifications. Under-specifications may have a bigger impact than over-specifications as
 long as the total number of misspecifications remains at a similar range. The validation
 procedure proposed in the present work (iterative in conjunction with the predicted EPS)

showed a higher number of under-specifications than *std95* and *ite95*; however, it showed a
much better performance in terms of Q-matrix specification recovery, which resulted in a
higher classification accuracy. It is important to note that other factors may have a relevant
role in modulating the relation between Q-matrix specification and attribute classification,
such as the number of different q-vectors represented in the Q-matrix (Rupp & Templin,
2008) and the identifiability of the Q-matrix (Gu & Xu, in press a, in press b).

Finally, a reviewer proposed examining whether the proposed procedure performs also 491 well when the underlying attribute's distribution is non-uniform. The performance of the 492 493 procedures under a multivariate normal distribution ( $\rho = 0.25$ ; see Xu & Shang, 2018) and a higher-order distribution ( $\lambda_0 = (-1, -0.5, 0, 0.5, 1), \lambda_{1k} = 1.5$ ; see de la Torre & Chiu, 2016) 494 are provided in the Online Appendix. It was observed that the pattern of results was very 495 similar to the ones obtained with the uniform distribution. Thus, the interpretation of the 496 findings do not differ according to the underlying attribute distribution, and the proposed 497 498 procedure still showed the best Q-matrix recovery and classification accuracy.

In conclusion, the ILD-GDI method proposed in this paper outperformed the original 499 method developed by de la Torre and Chiu (2016), as well as the method with the optimized 500 501 EPS value election (Nájera et al., 2019). The proposed procedure showed good performance at detecting and modifying the Q-matrix even with a high misspecification rate (QRR  $\geq$ 502 0.893) and also at classifying attribute profiles (PCA  $\ge$  0.895; PCA<sub>Otrue</sub>  $\approx$  0.910), being the 503 only procedure that achieved a PCV higher than 0.5 under the worse misspecification rate 504 scenario (PCV  $\ge$  0.579; PCV<sub>Qtrue</sub>  $\approx$  0.640). The iterative procedure's computation time was 505 506 short. On a laptop computer with four 2.2-GHz processors and 7 GB of RAM memory, the average replica computation time under the worst condition (MR = 0.4) was 111 seconds. 507 The performance of the ILD-GDI method was also illustrated with Tatsuoka's 508

509 fraction-subtraction data. De la Torre and Chiu (2016) found that the standard GDI method

510 with an EPS of 0.95 proposed three modifications. These modifications were congruent with the ones suggested by the ILD-GDI method. The suggestions of the ILD-GDI should be 511 considered rather than the GDI method's ones, since it provides a better recovery of the Q-512 513 matrix, as shown in the simulation study. However, two consideration should be noticed. First, even though Q-matrix validation methods are helpful in the search for the best possible 514 specified Q-matrix, some misspecifications may remain after their application. Second, 515 attribute positions in the Q-matrix are arbitrary just as factors are in a factor analysis; thus, 516 when two attributes (i.e., Q-matrix columns) have a similar specification through the items 517 518 and / or the number of misspecifications in the original Q-matrix is high, there exists the possibility that the suggested Q-matrix shows interchanged positions for these attributes with 519 520 respect to the original Q-matrix. These considerations emphasize the role of domain experts in 521 the review of the validated Q-matrix. They should reject those suggested modifications that lack a theoretical interpretation and check that the attributes maintain their original meaning. 522 Also, if they consider that several strategies can be followed to answer the items, multiple-523 524 strategy models may be of help (e.g., de la Torre & Douglas, 2008; Ma & Guo, 2019). These considerations may provide the most useful Q-matrix specification, since a tradeoff between 525 theoretical interpretation and data fit can be more easily achieved. 526

Further research is needed to extend the applicability of the ILD-GDI method. Even though the performance of the GDI method was deeply studied under a wide range of conditions by Nájera et al. (2019), the performance of the ILD-GDI method has only been tested under a limited set of conditions. Further research would help to know whether it is robust when the conditions are less favorable (e.g., small sample size, short test length, low item quality). In this sense, other factors can be added to the study design, such as the number of attributes or the underlying CDM (e.g., DINA).

534	Furthermore, it would be interesting to study whether the inclusion of model fit indices
535	to the iterative procedure could improve its performance. For instance, Kang et al. (2019)
536	used the item-level version of the RMSEA, which provided good results under the DINA
537	model. For the general CDMs framework, the Akaike's information criterion (AIC; Akaike,
538	1974) and the Bayesian information criterion (BIC; Schwarzer, 1976), which have been
539	previously used as fit indices in CDMs (e.g., Chen, de la Torre, & Zhang, 2013), could be
540	good candidates at selecting the suggested q-vector. One important drawback of this approach
541	would be the dramatic computational cost increment, since one additional model should be
542	estimated for each q-vector for each hit item. In this vein, the Wald test for model comparison
543	has also been recently used for Q-matrix validation under the sequential G-DINA model (Ma
544	& de la Torre, 2019).

#### 545 **Final remarks**

The authors want to emphasize that empirical validation methods suggest 546 modifications, and cannot derive a true Q-matrix in empirical settings. The suggested Q-547 matrix represents a model with empirical support. The purpose of Q-matrix validation should 548 not be to replace experts from the Q-matrix specification process, but to "provide 549 supplemental information for improving model-data fit, and consequently, increasing the 550 validity of inference from cognitive diagnosis assessments" (de la Torre & Chiu, 2016, p. 551 268). Especially in those contexts in which there is a certain degree of uncertainty involving 552 553 the Q-matrix, modification suggestions may help to understand which cognitive processes are involved in responding each item. Also, as has been shown in the real data illustration, 554 validation methods can help detecting problems regarding the structure of the Q-matrix (e.g., 555 attributes collinearity). Thus, we recommend applying three steps during the Q-matrix 556 specification process. First, construct the original Q-matrix with the help of domain experts. 557 In this step, the Delphi methodology can be of great help, facilitating the debate and 558

559 subsequent agreement between the judges (see Sorrel et al., 2016). It is also useful to track the degree of uncertainty involved in each q-entry during the process. Second, apply an empirical 560 Q-matrix validation method, in order to detect any possible misspecifications made in the first 561 562 step. Third, gather again the panel of experts to debate the theoretical viability of the suggested modifications and the meaning of the attributes after the process is completed. The 563 degree of uncertainty involving each q-entry recorded in the first step can be of help at this 564 point; a q-entry in which all experts showed a total agreement should probably not be 565 modified even though the validation method suggests the opposite. In conclusion, the authors 566 567 are of the opinion that the theory should be the main guide in the Q-matrix specification process. Empirical validation methods' role should be to support the domain experts' 568 judgements. 569 570 References Akaike, H. (1974). A new look at the statistical identification model. IEEE Transactions on 571 Automated Control, 19, 716–723. 572 Chen, J., de la Torre, J., & Zhang, Z. (2013). Relative and absolute fit evaluation in cognitive 573 diagnosis modeling. Journal of Educational Measurement, 50, 123-140. 574 Chiu, C.-Y. (2013). Statistical refinement of the Q-matrix in cognitive diagnosis. Applied 575 Psychological Measurement, 37(8), 598–618. 576 de la Torre, J. (2008). An empirically based method of Q-matrix validation for the DINA 577 model: Development and applications. Journal of Educational Measurement, 45, 343-578 362. 579 de la Torre, J. (2011). The generalized DINA model framework. Psychometrika, 76, 179–199. 580 de la Torre, J., & Chiu, C.-Y. (2016). A general method of empirical Q-matrix validation. 581 Psychometrika, 81(2), 253–273. 582

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