On the Boundary Problems in Diagnostic Classification Models

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On the Boundary Problems in Diagnostic Classification Models**Abstract**

In diagnostic classification models, parameter estimation sometimes provides estimates that stick to the boundaries of the parameter space, which is called the boundary problem and may lead to extreme values of standard errors. However, the relationship between the boundary problem and irregular standard errors has not been analytically explored. In addition, prior research has not shown how maximum-a-posteriori estimates avoid the boundary problem and affect the standard errors of estimates. To analyze these relationships, the expectation-maximization algorithm for maximum-a-posteriori estimates and a complete data Fisher information matrix are explicitly derived for a mixture formulation of saturated diagnostic classification models. Theoretical considerations show that the emptiness of attribute mastery patterns causes both the boundary problem and the inaccurate standard error estimates. Furthermore, unfortunate boundary problem without emptiness causes shorter standard errors. A simulation study shows that the maximum-a-posteriori method prevents boundary problems. Moreover, this method with monotonicity constraint estimation improves standard error estimates more than unconstrained maximum likelihood estimates do.

Keywords: diagnostic classification models, maximum a posteriori estimation, expectation maximization algorithm, standard error

Capturing the progress of students' learning is important to effectively improve their learning. Diagnostic classification models (DCMs; Rupp, Templin, & Henson, 2010), also known as cognitive diagnostic models (CDMs; Leighton & Gierl, 2007), provide information about the state of students' knowledge. Various types of DCMs have been developed: the widest class of DCMs such as the log-linear cognitive diagnostic model (LCDM; Henson, Templin, & Willse, 2009), the generalized deterministic input noisy "and" gate (G-DINA) model (de la Torre, 2011), and the general diagnostic model (GDM; von Davier, 2008) that includes many sub-models. The principle purpose of DCMs is to estimate the state of students' knowledge, which are conceived as attribute mastery patterns in the context of DCMs. Attributes are latent binary variables that represent a student's ability mastery status. Attribute mastery patterns are permutations of the assumed attributes. For example, when two attributes, for example, "solving equations skill" and "calculating skill," are assumed in a mathematics test, the possible patterns are (00), (01), (10), and (10) and each pattern represent the attributes mastered or not. Given their main purpose, DCMs can be employed in small sample size situations, such as classroom achievement tests.

However, the parameter estimates of DCMs are not always trustworthy. Templin and Bradshaw (2014, pp. 322–323) pointed out that the parameter estimates might take their boundary values even if the true parameters are not on their boundaries. In other words, the parameter estimates stuck on their boundary. Templin and Bradshaw (2014) also pointed out standard errors (SEs) become inaccurate when there are several empty or nearly empty attribute mastery patterns in a numerical example. The parameter estimates on their boundaries and their inaccurate SE problems are named "boundary problems" and the emptiness of attribute mastery patterns is a likely cause of these problems. This emptiness can happen not only in small sample-size situations, a typical DCM application setting, but also large sample-size situations because as the number of attributes increases, the number of attribute mastery patterns increases exponentially. For example, Lee, Park, and Taylan (2011) assumed 15 attributes, leading to $2^{15} = 32768$ attribute mastery patterns. In this situation, a large number of attribute mastery

patterns will be empty even if the sample size is in thousands. In addition, the attributes are strongly correlated with each other in real data (e.g., von Davier, 2008), meaning that the distribution of attribute mastery patterns is not uniform. The analyzed data in Templin and Bradshaw (2014) contained 2,922 students but indicated emptiness of attribute mastery patterns. Thus, parameter estimation problem is a commonly occurring problem in DCM analysis.

The emptiness and irregular SEs estimate problems relate to each other, but the relationship between them has not yet been mathematically or systematically assessed. Not only the emptiness of attribute mastery pattern and irregular SEs but also the boundary problems that arise when the estimates stick to the boundaries of the parameter space (DeCarlo, 2011; Garre & Vermunt, 2006; Maris, 1999) can happen at the same time. For example, if all students belonging to a specific attribute mastery pattern correctly answer for an item, its correct item response probability becomes one, which is a boundary problem. Similarly, if all students of the pattern incorrectly answered an item, the correct response probability of all incorrect responses of the pattern is zero. This is again a problematic correct boundary problem situation, which becomes possible if a test item is too easy or too difficult to the specific attribute mastery pattern. As Templin and Bradshaw (2014) explained, the SEs of correct response probability may not be appropriately estimated. Therefore, the boundary problem is strongly connected to the emptiness and irregular SEs.

The study aimed to mathematically analyze the emptiness and irregular SE estimates from perspective of boundary problems. We also employ a maximum a posteriori (MAP; Ma & Jiang, 2021) estimation methodology that is considered a solution to the boundary problem (DeCarlo, 2011; Garre & Vermunt, 2006; Maris, 1999) for model parameters. The MAP method uses prior distributions, which can be thought as a regularization term in maximum likelihood (ML) estimation context. Therefore, the prior distributions prevent parameter estimates from sticking to their bounds. One mechanism is that prior information of correct item response probabilities works as pseudo correct response or incorrect response to empty patterns. Therefore, if emptiness is caused by sampling error, the MAP method works any time. However, if the

pattern is truly empty in the population, it may cause biased MAP estimation. The MAP works any time in principle, but is especially preferable in small sample size setting (Ma & Jiang, 2021). In addition, the MAP method is expected to improve SE estimation further than the ML method can. SE estimation is based on the inverse of the Fisher information matrix and irregular SEs indicate some problems in this matrix, such as its linear dependency. The MAP estimation prevents such linear dependency of information matrix as the similar mechanism of ridge estimation technique and makes it possible to calculate the inverse of the information matrix. However, SE estimation is based on asymptotical theory, and hence, the MAP estimation method may improve both point estimates and SEs more than the ML method, but it may be not enough. In this study, the effect of MAP estimates on both the boundary problem and SE estimates is assessed analytically as well as through simulation.

The contribution of this study is that it offers not only a practical solution to the emptiness, boundary problem, and irregular SEs but also a guideline for parameter estimation method selection in DCMs from a mathematically sound perspective. The remaining paper is structured as follows. In the next section, we review previous boundary problem literature and MAP estimation as a solution. In the third section, we introduce the mixture formulation of the saturated DCM—a sub-model of general mixture models (e.g., Gu & Xu, 2019; Yamaguchi, 2020; Yamaguchi & Okada, 2020a,b; Yamaguchi & Templin, 2022a), and set the priors. Furthermore, an expectation maximization (EM; Dempster, Laird, & Rubin, 1977) algorithm for the MAP estimator, for all model parameters in the saturated DCM, is developed in a mixture model manner. This derivation is needed to specify and recognize the model parameters in the general DCMs; note that there are two differences between the current study and the work of Ma and Jang (2021)—the latter’s consideration of SE estimation and their detailed derivation of MAP estimation for all parameters. In the fourth section, we derive an explicit formulation of the complete Fisher information matrix, and assess the effect of parameter estimates on the SEs. We also consider the situation of the monotonicity constraints (e.g., Henson, et al. 2009; Xu & Shang, 2018), which are important in both identifying the model and interpreting the parameter

estimates. The fifth section describes a simulation study to assess where the developed EM algorithm can recover the true parameters and prevent boundary problems and irregular SEs. The study also evaluates the effect of monotonicity constraints on parameters that is important in DCMs parameter estimation. The sixth section presents the discussion and concludes.

Boundary Problems and the Maximum-a-Posterior Estimation

A frequently mentioned problem with DCMs is the boundary problem that arises when the estimates stick to the boundaries of the parameter space (DeCarlo, 2011; Garre & Vermunt, 2006; Maris, 1999). This problem sometimes occurs with the ML estimation method in a small sample size setting (Philipp, Strobl, de la Torre, & Zeileis, 2018). The emptiness of the attribute mastery pattern has been identified as a cause of boundary problems (DeCarlo, 2011). Templin and Bradshaw (2014) also pointed out the relationship among the emptiness of attribute mastery patterns, boundary problems, and irregular SE estimation.

SEs may sometimes be inaccurate. Yamaguchi and Okada (2020b) showed that SE estimates for the correct item response probability parameters, which are expected to range from zero to one, are sometimes larger than one in the DINA model. If the SE values are less than zero, this means that the variation of estimates is negative, which is an oxymoron. In addition, if these values are greater than one, this indicates that the parameter estimates may take the outside of the parameter space, and this conclusion is equally meaningless.

To deal with the boundary problem in the ML method framework, an ad hoc procedure to set upper and lower bound of parameter estimates is necessary. This strategy is sometimes employed in DCM packages such as GDINA (Ma & de la Torre, 2017). Using an ad hoc method has no theoretical justification and package users may not realize so. However, using MAP estimates can naturally prevent boundary problem and irregular SEs in a theoretically explanatory way. In addition, we can control the strength of regularization explicitly, manipulating hyperparameters. Moreover, using MAP estimates can naturally incorporate previous information as priors. In summary, a theoretical analysis of the problems explains how

MAP is a theoretically sound method. Note that Bayesian estimation with the Markov chain Monte Carlo method (MCMC; e.g., Chen, Culpepper, Chen, & Douglas, 2018; Culpepper, 2015, 2019b; Culpepper & Chen, 2018; Culpepper & Hudson, 2018) is another practical solution of the boundary problem. The MCMC method is flexible and applicable to a very wide range of problems but computationally very heavy. In contrast, the MAP estimation procedure is generally a fast and realistic analysis option. Therefore, in this study, we focus on the classical MAP method that does not need heavy computation and provides analytically clear formulation.

Ma and Jiang (2021) proposed the MAP estimation method for DCMs but did not assess the relationship between MAP estimation and SEs. Therefore, we need to carefully check how the MAP method prevents the two problems from assessing the complete data Fisher information matrix that was converted to the observed Fisher information matrix. This provides us with the theoretical guarantee of MAP estimates as a solution to both the boundary problem and irregular SEs. Ma and Jiang (2021) designed the MAP estimation method specifically for item parameter as a modification of EM algorithm of the G-DINA model (de la Torre, 2011). However, Ma and Jiang (2021) were imperfect and did not provide a MAP estimation method for mixing parameters of attribute mastery patterns. As a related work, Latent GOLD (Vermunt & Magidson, 2005) can use the MAP estimation method for DCMs, but its application is restricted to sub-models of the general DCMs (e.g., Sen & Terzi, 2020). Moreover, the algorithm in Latent GOLD is intended for the general latent class model and does not provide an explicit representation of the MAP estimation algorithm for DCMs. In other words, previous studies did not derive an EM algorithm for the MAP estimation for all model parameters, and it is still unclear, from an analytical perspective, how the prior distribution for all parameters prevents the boundary problem.

Furthermore, not only point estimates but also SEs should be considered. The SEs of the parameter estimates in DCMs are obtained from the observed Fisher information matrix (Liu, Xin, Andersson, & Tian, 2019; Philipp, Strobl, de la Torre, & Zeileis, 2018). However, Philipp et al. (2018) and Liu et al. (2019) did not explicitly formulate the outer-product or Hessian

approximation of the observed Fisher information matrix. Although Liu et al. (2019) showed various types of estimation methods for the observed Fisher information matrix, they did not analyze the relationship between parameter and SE estimates. Moreover, Liu et al. (2019) did not explicitly show the element of the Fisher information matrix and did not focus on the theoretical connection of the boundary problem and irregular SEs. Generally speaking, the differential of the log marginal likelihood with respect to the parameters is difficult to derive (Meng & Rubin, 1991). This problem means that the relationship between the parameter and SE estimates remains a black box.

Furthermore, the Fisher information matrix analysis provides a perspective to assess the mathematical property of DCMs that has not been highlighted. The Fisher information determines the model statistical class (e.g., Watanabe, 2007, 2018), if it is regular or singular. When the Fisher information of a statistical model is not regular, the statistical model is singular, and because of this, parameter estimation fails. In addition, when statistical models with unobserved variables, such as the mixture model that includes DCMs, become singular, the DCMs run the risk of becoming singular. However, this point has not been underscored in the psychometrics field. This study provides insights into DCMs as a statistical model and helps deepen our understanding of them. We next provide a mathematical formulation of the saturated DCMs as a mixture formulation, to derive the parameter estimation procedure.

Saturated DCM in a Mixture Formulation

Item Response Function

First, we introduce latent class formulation and then the saturated DCM to modify latent class model, which is the binary observe data version of the mixture model. First, let $\mathbf{x}_i = (x_{i1}, \dots, x_{ij}, \dots, x_{iJ})^\top$ be the item response vector for an individual $i (= 1, \dots, I)$ for which each element x_{ij} is a realization of the random variable X_{ij} and a binary item response for the item $j (= 1, \dots, J)$, which takes the value of zero for incorrect and one for correct. In addition, let L be the number of latent class, when the latent class indicator vector $\mathbf{z}_i = (z_{i1}, \dots, z_{iL}, \dots, z_{iL})^\top$ is employed, which has only one element equal to one, and the other $L - 1$ elements are equal to

zero. Assuming local independence given the l th latent class, the item response probability is defined as

$$f(\mathbf{X}_i = \mathbf{x}_i | \mathbf{z}_i, \boldsymbol{\Theta}) = \prod_l \left[\prod_j \theta_{jl}^{x_{ij}} (1 - \theta_{jl})^{1-x_{ij}} \right]^{z_{il}}, \quad (1)$$

where θ_{jl} is the correct response probability parameter for item j in the l th latent class across individuals, and $\boldsymbol{\Theta}$ is a set of θ_{jl} .

In the context of DCMs, the latent class is called the attribute mastery pattern, which is the combination of the latent binary indicators of attribute α_k , $k(= 1, \dots, K)$. An attribute α_k represents the mastery status of a skill or ability in a test; if the k th attribute is mastered, then α_k takes the value of one; otherwise $\alpha_k = 0$. Thus, the number of attribute mastery patterns is $L = 2^K$, and the l th attribute mastery pattern vector $\boldsymbol{\alpha}_l$ is defined as $(\alpha_{l1}, \dots, \alpha_{lk}, \dots, \alpha_{lK})^\top$. The whole attribute mastery pattern set is represented by $\boldsymbol{\alpha}$. The saturated DCM requires more constraints on Equation 1. In the DCMs, a Q-matrix (Tatsuoka, 1983) is specified before data analysis, and an additional constraint on Equation 1 is assumed based on the Q-matrix of size $J \times K$. The elements of the Q-matrix, q_{jk} , are equal to one when attribute k is measured by item j and are zero otherwise.

This Q-matrix generates a systematic parameter equality constraint and is represented as a G-matrix (e.g., de la Torre, 2009a; Yamaguchi, 2020; Yamaguchi and Okada, 2020a). The G-matrix is defined for each item, and its size is $2^{\sum_k q_{jk}} \times 2^K$ because item j can only distinguish $2^{\sum_k q_{jk}}$ attribute mastery patterns. For example, let us assume that there are three attributes in a test and that an item measures the first and second attributes, implying that $\mathbf{q}_j = (1, 1, 0)^\top$, as shown in Table 1 (Yamaguchi & Okada, 2020a). The G-matrix is colored gray in Table 1. This item can determine four attribute mastery patterns, called item-specific attribute mastery patterns, given by $\boldsymbol{\alpha}_h^*$: $\boldsymbol{\alpha}_1^* = (0, 0, *)^\top$, $\boldsymbol{\alpha}_2^* = (1, 0, *)^\top$, $\boldsymbol{\alpha}_3^* = (0, 1, *)^\top$, and $\boldsymbol{\alpha}_4^* = (1, 1, *)^\top$, where “*” means to ignore the third attribute. These patterns are restricted attribute mastery patterns for item j . Thus, the attribute mastery patterns $\boldsymbol{\alpha}_1 = (0, 0, 0)^\top$ and $\boldsymbol{\alpha}_4 =$

$(0,0,1)^\top$ have the same item response probability; similarly, the pairs $\alpha_2 = (1,0,0)^\top$ and $\alpha_6 = (1,0,1)^\top$, $\alpha_3 = (0,1,0)^\top$ and $\alpha_7 = (0,1,1)^\top$, and $\alpha_5 = (1,1,0)^\top$ and $\alpha_8 = (1,1,1)^\top$ have the same correct item response probability parameters. The elements of $\mathbf{G}_j$, g_{jhl} , are defined by the indicator function $I(\cdot)$: $g_{jhl} = I(\alpha_h^* = \alpha_l)$ for all j, h , and l . The k th attributes satisfying $q_{jk} = 0$ are replaced by “*” in the l th attribute mastery pattern α_l when $I(\alpha_h^* = \alpha_l)$ is evaluated. This indicator function means that if the item-specific attribute mastery pattern is the same as the attribute mastery pattern when ignoring the irrelevant attributes in an item, then the corresponding element of the G-matrix is equal to one; if it is not, then this element is equal to zero. In other words, the G-matrix indicates which attribute mastery patterns should have the same item response probability.

A G-matrix converts attribute mastery pattern l to item-specific mastery pattern h in item j . The sub-models of the saturated DCMs are represented based on modified G-matrices. Employing the G-matrix notation, the saturated DCM item response function of individual i is represented as

$$P(\mathbf{X}_i = \mathbf{x}_i | \mathbf{z}_i, \boldsymbol{\Theta}, \mathbf{G}) = \prod_j \prod_{h=1}^{2^{\sum_k q_{jk}}} \prod_l \left\{ \left[\theta_{jh}^{x_{ij}} (1 - \theta_{jh})^{1-x_{ij}} \right]^{g_{jhl}} \right\}^{z_{il}}, \quad (2)$$

where θ_{jh} is the correct item response probability of the item-specific attribute mastery pattern h , $\boldsymbol{\Theta}$ is a set of all item parameters, and $\mathbf{G}$ is a set of the $\mathbf{G}_j$ -matrix. Equations 1 and 2, while quite similar, have some differences. First, the subscript of correct response probability θ_j changes from l to h because the correct response probabilities in the saturated DCM are defined not for original attribute mastery patterns but for item-specific patterns. Second, Equation 2 has g_{jhl} and the product over h . The g_{jhl} works as “a converter,” which means that the attribute mastery status represented as z_{il} changes to h through g_{jhl} .

It is important to clarify the model assumptions in this paper. For the item response model, we assume the same number of the most general DCMs, such as LCDM or GDINA. This is because the results of theoretical analysis are easily applicable to the sub-models. In addition,

the item response function is correctly specified. The Q-matrix is known in our setting. More precisely, for a given test, the number of attributes is known, and the elements of Q-matrix are correctly specified. This assumption may appear strong, but assuming fixed Q-matrix is still a common practice in analysis with DCMs (e.g., Chen & de la Torre, 2014; Li, Hunter, & Lei, 2016; Yamaguchi & Okada, 2018). The consequences of model misspecification are out of the scope of this study, but comprise future research topics.

Complete Data Likelihood and Full Joint Distribution

The distribution of the latent variable $\mathbf{z}_i$ is a categorical distribution with the mixing parameter $\boldsymbol{\pi}$:

$$P(\mathbf{z}_i|\boldsymbol{\pi}) = \prod_l \pi_l^{z_{il}}. \quad (3)$$

Exchangeability of individual is assumed and the complete data likelihood of $\mathbf{X}$ and $\mathbf{Z}$ that are sets of $\mathbf{x}_i$ and $\mathbf{z}_i$ across individuals is derived from Equations 2 and 3 as

$$\begin{aligned} P(\mathbf{X}, \mathbf{Z}|\boldsymbol{\Theta}, \boldsymbol{\pi}, \mathbf{G}) &= \prod_i P(\mathbf{X}_i = \mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\Theta}, \mathbf{G}) P(\mathbf{z}_i|\boldsymbol{\pi}) \\ &= \prod_i \prod_l \prod_j \left[\pi_l \prod_j \prod_{h=1}^{2^{\sum_k q_{jk}}} [\theta_{jh}^{x_{ij}} (1 - \theta_{jh})^{1-x_{ij}}]^{g_{jhl}} \right]^{z_{il}}. \end{aligned} \quad (4)$$

The marginal likelihood $P(\mathbf{X}|\boldsymbol{\Theta}, \boldsymbol{\pi}, \mathbf{G})$ is obtained by summing all possible latent class $\mathbf{Z}$: $\sum_{\mathbf{Z}} P(\mathbf{X}, \mathbf{Z}|\boldsymbol{\Theta}, \boldsymbol{\pi}, \mathbf{G})$.

Next, the priors for $\boldsymbol{\Theta}$ and $\boldsymbol{\pi}$ should be specified to derive the MAP algorithm. These priors are set as in Yamaguchi and Okada (2021). The prior for the parameter θ_{jh} is Beta distribution with hyperparameters $a_{jh}^0 > 0$ and $b_{jh}^0 > 0$, which is written as $\text{Beta}(a_{jh}^0, b_{jh}^0)$. We assume conditional independence of the parameters, and the joint distribution $P(\boldsymbol{\Theta}|\mathbf{A}^0, \mathbf{B}^0)$ of the parameter set $\boldsymbol{\Theta}$ under independent assumption is a product of $\text{Beta}(a_{jh}^0, b_{jh}^0)$, where $\mathbf{A}^0$ and $\mathbf{B}^0$ are sets of all hyperparameters a_{jh}^0 and b_{jh}^0 . Furthermore, prior distribution of $\boldsymbol{\pi}$ is the Dirichlet distribution with parameters $\boldsymbol{\delta}^0 = (\delta_1^0, \dots, \delta_l^0, \dots, \delta_L^0)^\top, \delta_l^0 > 0, \forall l$: $P(\boldsymbol{\pi}|\boldsymbol{\delta}^0) = \text{Dirich}(\boldsymbol{\delta}^0)$. The formulation of actual priors is shown in Supplemental Material A.

Using the complete data likelihood (Equation 4) and the priors, the log complete joint distribution is

$$\begin{aligned}
\log P(\mathbf{X}, \mathbf{Z}, \boldsymbol{\Theta}, \boldsymbol{\pi} | \mathbf{A}^0, \mathbf{B}^0, \boldsymbol{\delta}^0, \mathbf{G}) &= \log[P(\mathbf{X}, \mathbf{Z} | \boldsymbol{\Theta}, \boldsymbol{\pi}, \mathbf{G}) P(\boldsymbol{\pi} | \boldsymbol{\delta}^0) P(\boldsymbol{\Theta} | \mathbf{A}^0, \mathbf{B}^0)] \\
&= \sum_i \sum_j \sum_{h=1}^{2^{\sum_k q_{jk}}} \left(\sum_l g_{jhl} z_{il} \right) \{x_{ij} \log \theta_{jh} + (1 - x_{ij}) \log(1 - \theta_{jh})\} \\
&\quad + \sum_i \sum_l z_{il} \log \pi_l + \sum_l (\delta_l^0 - 1) \log \pi_l \\
&\quad + \sum_j \sum_{h=1}^{2^{\sum_k q_{jk}}} \{(a_{jh}^0 - 1) \log \theta_{jh} + (b_{jh}^0 - 1) \log(1 - \theta_{jh})\} + \text{const.},
\end{aligned} \tag{5}$$

where “const.” is a term containing the irrelevant terms of the model parameters.

EM Algorithm for MAP Estimation

In the mixture model, the E-step calculates the posterior expectation of z_{il} given current parameters $\boldsymbol{\Xi}^{\text{old}} = \{\boldsymbol{\Theta}^{\text{old}}, \boldsymbol{\pi}^{\text{old}}\}$,

$$\begin{aligned}
\mathbb{E}_{P(z_{il} | \mathbf{x}_i, \boldsymbol{\Xi}^{\text{old}})}[z_{il}] &= P(z_{il} | \mathbf{x}_i, \boldsymbol{\Xi}^{\text{old}}) \\
&= \frac{P(z_{il}, \mathbf{x}_i | \boldsymbol{\Xi}^{\text{old}})}{\sum_{l'} P(z_{il'}, \mathbf{x}_i | \boldsymbol{\Xi}^{\text{old}})} = \frac{\pi_l \prod_j \prod_{h=1}^{2^{\sum_k q_{jk}}} [\theta_{jh}^{x_{ij}} (1 - \theta_{jh})^{1-x_{ij}}]^{g_{jhl}}}{\sum_{l'} \pi_{l'} \prod_j \prod_{h=1}^{2^{\sum_k q_{jk}}} [\theta_{jh}^{x_{ij}} (1 - \theta_{jh})^{1-x_{ij}}]^{g_{jhl'}}}.
\end{aligned} \tag{6}$$

To shorten the notation, we define $\mathbb{E}_{P(z_{il} | \mathbf{x}_i, \boldsymbol{\Xi}^{\text{old}})}[z_{il}] = r_{il}$. In the M-step, $Q(\boldsymbol{\Xi} | \boldsymbol{\Xi}^{\text{old}})$, defined as

$$Q(\boldsymbol{\Xi} | \boldsymbol{\Xi}^{\text{old}}) = \mathbb{E}_{P(\mathbf{Z} | \mathbf{X}, \boldsymbol{\Xi}^{\text{old}})}[\log P(\mathbf{X}, \mathbf{Z}, \boldsymbol{\Theta}, \boldsymbol{\pi} | \mathbf{A}^0, \mathbf{B}^0, \boldsymbol{\delta}^0, \mathbf{G})], \tag{7}$$

is maximized with respect to $\boldsymbol{\Xi}$. If the convergence criterion is not satisfied, then the new parameters are substituted into $\boldsymbol{\Xi}^{\text{old}}$. The derivation of M-step is shown in Supplemental Material B and a new correct response parameter θ_{jh} is

$$\theta_{jh} = \frac{\sum_i \sum_l g_{jhl} r_{il} x_{ij} + a_{jh}^0 - 1}{\sum_i \sum_l g_{jhl} r_{il} + a_{jh}^0 + b_{jh}^0 - 2}, \tag{8}$$

which is a maximizer of $Q(\Xi|\Xi^{\text{old}})$. The element of mixing parameter π is updated as

$$\pi_l = \frac{\sum_i r_{il} + \delta_l^0 - 1}{I + \sum_l \delta_l^0 - 2^K}. \quad (9)$$

In summary, the update rule of the MAP algorithm is as follows. First, initialize the parameters Θ^{old} and π^{old} . Second, calculate the posterior of z_{il} with Equation 6 (E-step). Third, update the parameters with Equations 8 and 9 (M-step). Fourth, if the convergence criterion is satisfied, then output new parameters as the MAP estimates Ξ^* ; otherwise, substitute new parameters into Ξ^{old} and return to the second step. Essentially, the same update rule for Equation 8 can be seen in de la Torre (2009b, 2011) and Ma and Jiang (2021).

The meaning of the update rule for this algorithm is as follows. In Equation 8, $\sum_i \sum_l g_{jhl} r_{il}$ is the expected number of the item-specific pattern h in item j , and $\sum_i \sum_l g_{jhl} r_{il} x_{ij}$ is the expected correct response number of item j in item-specific pattern h . The numerator of Equation 8 is composed of the sum of the expected correct response numbers and the prior information for the correct response a_{jh}^0 . In addition, the denominator of Equation 8 is the sum of the expected numbers of the item-specific pattern and the prior parameters a_{jh}^0 and b_{jh}^0 . Thus, the update rule of the parameter expressed as Equation 8 is clearly in agreement with the meaning of the correct response probability. In addition, if the hyperparameters are $a_{jh}^0 = b_{jh}^0 = 1$, meaning that the prior is a uniform distribution, then Equation 8 is the same as the update rule of the usual EM algorithm developed by de la Torre (2011). a_{jh}^0 and b_{jh}^0 in Equation 8 are the hyper parameters and fixed before data analysis. The choice of hyper parameters affects the result, especially under a small sample size condition as discussed for long in Bayesian data analysis. The effects become small with increase of sample size. Note that if $\sum_i \sum_l g_{jhl} r_{il} x_{ij} = 0$, the update rule shown in Equation 8 becomes just $(a_{jh}^0 - 1)/(a_{jh}^0 + b_{jh}^0 - 2)$; this is the prior expected correct item response probability. In this case, the update rule no longer agrees with the correct item response probability mentioned above.

Similarly, the update rule mixing parameter π_l in Equation 9 is in agreement with the meaning of the parameter. $\sum_i r_{il}$ is the expected number of l th attribute mastery patterns.

Apparently, when the prior for the mixing parameters is the uniform distribution, which is $\delta_l^0 = 1, \forall l$, Equation 9 becomes the ratio of the expected number attribute mastery pattern to the total sample size. Equation 9 contains the prior information of each attribute pattern, which is expressed by the hyperparameter δ_l s. This is the definition of the mixing parameter π_l . From the above discussion, the update rule for the MAP estimates shows that Equations 8 and 9 are extensions of the usual EM algorithm update rule.

In addition, Equations 8 and 9 explain how the hyperparameters prevent the boundary problem and the emptiness of attribute mastery patterns. First, if some attribute mastery patterns are empty and $\sum_i \sum_l g_{jhl} r_{il}$ becomes almost zero, then $\sum_i \sum_l g_{jhl} r_{il} x_{ij}$ also becomes zero. In this situation, if the hyperparameters $a_{jh}^0 = b_{jh}^0 = 1$, then θ_{jh} becomes an unstable value because both the numerator and denominator are zero. Even in this situation, if $a_{jh}^0 > 1$ and $b_{jh}^0 > 1$, then the numerator and denominator are both positive and θ_{jh} can be calculated. Similarly, for the mixing parameter, even if $\sum_i r_{il}$ is almost zero, $\delta_l^0 > 1$ and $\sum_l \delta_l^0 > 2^K$ are satisfied, and π_l becomes positive. Of course, if the emptiness of the attribute mastery pattern holds in the population, then MAP provides biased estimates. However, if the emptiness is caused by random error, then MAP can avoid inappropriate parameter estimates. Note that the boundary problem in mixing parameters can be considered as shrinkage of some parameters to zero. In addition, if all individuals are classified into one attribute mastery pattern, the corresponding mixing parameter becomes one and the others become zero. However, this situation may not be realistic, and this study focuses only on the case of some mixing parameters sticking to zero.

Note that when several attribute mastery patterns are empty, a correct item response probability parameter estimate may become $\theta_{jh} = (a_{jh}^0 - 1)/(a_{jh}^0 + b_{jh}^0 - 2)$. Emptiness can take place in two cases: first, the attribute mastery patterns are truly empty in population, and second, emptiness is caused by sampling error. In the first case, MAP estimation provides biased estimates. In the second, MAP can provide better estimates and SEs than the ML method to prevent boundary problem. Furthermore, $\theta_{jh} = (a_{jh}^0 - 1)/(a_{jh}^0 + b_{jh}^0 - 2)$ is the parameter

estimate of correct item response probability without data, or prior expected correct response probability as mentioned above.

When we assign the same priors for several correct item response probability parameters of empty attribute mastery patterns, it will provide the same result. In this case, the estimates do not have any meaning of characteristics of items, and thinking about parameter estimate is fruitless. However, the items may be employed to estimate individual attribute mastery patterns because an item has several correct response parameters and has information to separate attribute mastery patterns, even if one of its parameters sticks to the bound.

Another note on priors for parameters is necessary. Priors work just the same as the smoothing technique in natural language processing such as latent Dirichlet allocation (e.g., Blei, Ng, & Jordan, 2003). This smoothing technique prevents failure of estimation and extracts information from data.

The update rule of Θ parameters is the same as Equation 4 in Ma and Jiang (2021). In addition, this algorithm is very similar to de la Torre's (2011) EM algorithm. However, Ma and Jiang (2021) did not provide an update rule for mixing parameter π , and de la Torre (2011) employed the marginal likelihood to develop his EM algorithm, which did not include prior information for the parameters. In addition, de la Torre (2011) did not explicitly include the updated part of the mixing parameters and converted the Θ parameters into the intercept, the main effects of the attributes, and the interaction effects among the attributes, meaning that the original parameter set was the first result. However, the mixture formulation clearly showed the dependency of the parameters in the saturated DCM and made it possible to consider an understandable meaning of the parameter update rule. Furthermore, this formulation considered all Θ and π parameters and their hyperparameters.

Parameter Estimation under Monotonicity Constraints

Henson et al. (2009, p.198) defined monotonicity constraint as “the property such that for any examinee that masters additional skills his or her probability of a correct response must be equal to or greater than the probability of a correct response prior to learning the additional

skills.” This constraint prevents label swapping of non-master and master, and ensures meaning of the correct response probability parameters. Rupp et al. (2010) demonstrated how to pose monotonicity constraint on LCDM with Mplus.

Hong, Chang, and Tsai (2016) proposed upward and downward modification methods for monotonicity constraint in G-DINA framework. These methods are ad hoc adjustments if monotonicity constraints are violated in EM iterations. Detailed modifications were described in Hong et al. (2016, pp.465–466). Ma and Jiang (2021) introduced a constraint matrix that represents monotonicity constraints and employed sequential quadratic programming techniques for M-step in EM algorithm. This procedure does not need ad hoc adjustments as Hong et al. (2016). In a Bayesian estimation framework, for example, Yamaguchi and Templin (2022a) developed an effective Gibbs sampling algorithm with monotonicity constraints for general DCMs in latent class formulation.

For standard error estimation, Hong et al. (2016, p. 466) employed usual asymptotical standard error estimation similar to the G-DINA framework even in monotonicity constraints situation. In a structural equation modeling context, Lüdtke, Ulitzsch, and Robitzsch (2021, p.3) obtained asymptotical SEs of contained maximum likelihood estimates to just substitute estimated parameters into the negative second partial derivatives of the log-likelihood function with respect to the model parameters. As a theoretical study, for asymptotical distribution of constrained models, Fukumizu, Kuriki, Takeuchi, and Akahira (2004, Chapter 2) discussed a class of singular models with constrained parameters. The class includes finite mixture models, monotonic regression models, and so on. The maximum likelihood estimator is $\sqrt{n}$ -consistency estimator. Here, the true parameter is inside the constrained parameter space. Fukumizu et al. (2004) also derived the asymptotical distribution of maximum likelihood estimator of the constrained model; it is (multivariate) normal distribution whose mean is the true parameter and covariance matrix is the inverse of Fisher information matrix. Therefore, the Fisher information matrix that will be derived in the next section will be employed under monotonicity constraint case.

Complete Data Fisher Information Matrix and the Effect of the Boundary Problem on SE Estimation

Complete Data Fisher Information Matrix

The observed Fisher information matrix can be estimated to adjust the complete data Fisher information matrix (Meng & Rubin, 1991) in mixture models. The complete data Fisher information matrix assumes both observed and latent variables, but the observed Fisher information employs only observed data. The complete data Fisher information matrix and the observed one have a close connection, and if the former has problems, then the latter too becomes problematic. The complete data Fisher information matrix is easier to derive than the observed data Fisher information matrix (Meng & Rubin, 1991). Thus, employing a mixture model formulation of DCMs and analyzing the complete data Fisher information matrix can provide clues about the relationship between emptiness and irregular SEs estimates from the perspective of boundary problems.

The asymptotic SEs of the parameter estimates Ξ^* are estimated by $\sqrt{\text{diag}(I_{obs}^{-1}(\Xi^*|\mathbf{X}))}$, where $I_{obs}(\Xi^*|\mathbf{X})$ is on the observed data Fisher information matrix and the $\text{diag}(\cdot)$ function takes the diagonal elements of its argument matrix. As mentioned above, the relationship between the parameter estimates and the SEs is not clear because of the complexity of $I_{obs}(\Xi^*|\mathbf{X})$. However, complete data Fisher information, which is written as $I_{comp}(\Xi^*|\mathbf{X})$, can be expressed as an explicit formulation of the parameter estimates. In addition, Meng and Rubin (1991) showed the relationship between $I_{obs}(\Xi^*|\mathbf{X})$ and $I_{comp}(\Xi^*|\mathbf{X})$ and developed an estimation method for $I_{obs}(\Xi^*|\mathbf{X})$ with $I_{comp}(\Xi^*|\mathbf{X})$, as shown in Supplemental Material C. From Equation 28 in Supplemental Material C, if $I_{comp}(\Xi^*|\mathbf{X})$ is singular, $I_{obs}(\Xi^*|\mathbf{X})$ also becomes singular. The inverse argument, however, does not always hold. In other words, we investigated sufficient conditions of the singularity of $I_{obs}(\Xi^*|\mathbf{X})$ by assessing $I_{comp}(\Xi^*|\mathbf{X})$. Here, $I_{comp}(\Xi^*|\mathbf{X})$ is derived based on the mixture formulation of the saturated DCM introduced in the previous section, and the connection between the parameter estimates and their SEs is revealed using $I_{comp}(\Xi^*|\mathbf{X})$.

$I_{comp}(\Xi|\mathbf{X})$ is approximated as

$$\begin{aligned} I_{comp}(\Xi^*|\mathbf{X}) &\approx \mathbb{E}_{\mathbf{P}(\mathbf{Z}|\mathbf{X}, \Xi^*)} \left[-\partial^2 \log \frac{\mathbf{P}(\mathbf{X}, \mathbf{Z}, \boldsymbol{\Theta}, \boldsymbol{\pi} | \mathbf{A}^0, \mathbf{B}^0, \boldsymbol{\delta}^0, \boldsymbol{\alpha}, \mathbf{G}, \mathbf{Q})}{\partial \Xi \partial \Xi^T} \right] \Big|_{\Xi=\Xi^*} \\ &= -\frac{\partial Q^2(\Xi|\Xi^*)}{\partial \Xi \partial \Xi^T} \Big|_{\Xi=\Xi^*}, \end{aligned} \quad (10)$$

where the exchangeability of expectation and derivation is assumed and $I_{comp}(\Xi|\mathbf{X})$ is evaluated with the estimated Ξ^* . The size of $I_{comp}(\Xi^*|\mathbf{X})$ is $p \times p$, and $p = \sum_j 2^{\sum_k q_{jk}} + 2^K - 1$ is the number of parameters in the saturated DCM. The elements of $I_{comp}(\Xi^*|\mathbf{X})$ are derived using Equation 10. The following equations provide the actual calculations of the elements.

First, the negative-signed second-order differential with respect to the item parameter is

$$-\frac{\partial Q^2(\Xi|\Xi^*)}{\partial^2 \theta_{jh}} = \frac{\sum_i \sum_l g_{jhl} r_{il} x_{ij} + a_{jh}^0 - 1}{\theta_{jh}^2} + \frac{\sum_i \sum_l g_{jhl} r_{il} (1 - x_{ij}) + b_{jh}^0 - 1}{(1 - \theta_{jh})^2}. \quad (11)$$

In addition, the first-order differential with respect to the mixing parameter is

$$\frac{\partial Q(\Xi|\Xi^*)}{\partial \pi_l} = \frac{\sum_i r_{il} + \delta_l^0 - 1}{\pi_l} - \frac{\sum_i r_{i2^K} + \delta_{2^K}^0 - 1}{1 - \sum_{l=1}^{2^K-1} \pi_l}, \quad (12)$$

and the negative-signed second-order differential is

$$-\frac{\partial^2 Q(\Xi|\Xi^*)}{\partial^2 \pi_l} = \frac{\sum_i r_{il} + \delta_l^0 - 1}{\pi_l^2} + \frac{\sum_i r_{i2^K} + \delta_{2^K}^0 - 1}{(1 - \sum_{l=1}^{2^K-1} \pi_l)^2}. \quad (13)$$

The differential with respect to different item parameters and the item and mixing parameters is

$$-\frac{\partial Q^2(\Xi|\Xi^*)}{\partial \theta_{jh} \partial \theta_{j'h'}} = -\frac{\partial Q^2(\Xi|\Xi^*)}{\partial \theta_{j'h'} \partial \theta_{jh}} = -\frac{\partial Q^2(\Xi|\Xi^*)}{\partial \theta_{jh} \partial \pi_l} = -\frac{\partial Q^2(\Xi|\Xi^*)}{\partial \pi_l \partial \theta_{jh}} = 0, \quad (14)$$

where $j' \neq j$ and/or $h' \neq h$. Finally, the differential with respect to two different mixing parameters is

$$-\frac{\partial^2 Q(\Xi|\Xi^*)}{\partial \pi_l \partial \pi_{l'}} = \frac{\sum_i r_{i2^K} + \delta_{2^K}^0 - 1}{(1 - \sum_{l=1}^{2^K-1} \pi_l)^2}, \quad (15)$$

where $l' \neq l$. Equations 11, 13, 14, and 15 are appropriately arranged and substituted into Equation 10, which is evaluated with the MAP estimate Ξ^* , and then, the complete data Fisher information matrix is calculated.

Effects of Parameter Estimates on SE Estimates

Equations 11, 13, and 15 show the non-zero elements of the completed data Fisher information matrix and are directly connected to the estimates of the SEs. For further analysis, Equation 8 is substituted into Equation 11; after some computation, the first $\sum_j 2^{\sum_k q_{jk}}$ th diagonal elements of $I_{comp}(\Xi^*|\mathbf{X})$ are

$$-\frac{\partial^2 Q^2(\Xi|\Xi^*)}{\partial^2 \theta_{jh}} = \left(\sum_i \sum_l g_{jhl} r_{il} + a_{jh}^0 + b_{jh}^0 - 2 \right)^2 \left\{ \frac{1}{\sum_i \sum_l g_{jhl} r_{il} x_{ij} + a_{jh}^0 - 1} + \frac{1}{\sum_i \sum_l g_{jhl} r_{il} (1 - x_{ij}) + b_{jh}^0 - 1} \right\}. \quad (16)$$

The first part of the right-hand side of Equation 18 is an important term. If $\sum_i \sum_l g_{jhl} r_{il} + a_{jh}^0 + b_{jh}^0 - 2$ is close to zero, some attribute mastery pattern may be almost empty, and $a_{jh}^0 + b_{jh}^0 = 2$, such that Equation 18 becomes zero. Furthermore, the complete data Fisher matrix becomes rank-deficient, and its inverse cannot be calculated, or, even if calculated, becomes very unstable, and the value becomes very large or infinite. This problem is a cause of irregularly large SEs for parameter estimates. In the next possible problematic situation, $\sum_i \sum_l g_{jhl} r_{il} + a_{jh}^0 + b_{jh}^0 - 2$ is not zero, but $\sum_i \sum_l g_{jhl} r_{il} x_{ij} + a_{jh}^0 - 1$ or $\sum_i \sum_l g_{jhl} r_{il} (1 - x_{ij}) + b_{jh}^0 - 1$ is close to zero. This is the case pointed out in the Introduction that the specific attribute mastery patterns are not zero but the students belonging to the patterns are all correct or incorrect for the item, that is, the item is too easy or difficult for the attribute mastery pattern. In this case, the emptiness of the attribute mastery pattern does not exist, or $a_{jh}^0 + b_{jh}^0 > 2$, but the boundary problem still occurs, which means that θ_{jh} is close to zero or one. In this situation, the right-hand side of Equation 16 is very large or infinite. Then, $I_{comp}(\Xi^*|\mathbf{X})$ does not become rank-deficient, and its inverse may be calculated, but the corresponding diagonal element becomes almost zero, and the SE of the corresponding parameter may also become almost zero. Thus, the boundary problem, if it unfortunately occurs, may cause very small SEs. In short, the emptiness of attribute mastery

patterns causes both boundary problem and irregularly large SEs and unfortunate boundary problems that are caused by all zero or one responses resulting in shorter SEs.

Equation 16 explains how hyperparameters prevent irregular SEs. If both hyperparameters, a_{jh}^0 and b_{jh}^0 , are larger than one, then the first term is always greater than zero, and the denominator of the second term never becomes zero. Thus, this setting prevents the rank defication of $I_{comp}(\Xi^*|\mathbf{X})$ and SEs that are almost equal to zero.

Next, to analyze the mixing parameter SEs, Equation 9 is substituted into Equations 13 and 15, and the following equations are obtained.

$$-\frac{\partial^2 Q(\Xi|\Xi^*)}{\partial^2 \pi_l} = \left(I + \sum_l \delta_l^0 - 2^K \right)^2 \left\{ \frac{1}{\sum_i r_{il} + \delta_l^0 - 1} + \frac{1}{\sum_i r_{i2^K} + \delta_{2^K}^0 - 1} \right\}, \quad (17)$$

$$-\frac{\partial^2 Q(\Xi|\Xi^*)}{\partial \pi_l \partial \pi_{l'}} = \frac{(I + \sum_l \delta_l^0 - 2^K)^2}{\sum_i r_{i2^K} + \delta_{2^K}^0 - 1}. \quad (18)$$

The first term on the right-hand side of Equation 17 and the numerator of Equation 18 are the same and positive except under unrealistic conditions. If both denominators on the right-hand side of Equation 17 are close to zero, then the corresponding diagonal element of $I_{comp}^{-1}(\Xi^*|\mathbf{X})$ becomes almost zero if the empty attribute mastery patterns do not affect Equation 18. This result implies that the SE of the attribute mastery pattern is almost zero. The hyperparameter δ_l^0 prevents such too-small SEs if we set $\delta_l^0 > 1, \forall l$, even if some $\sum_i r_{il}$ s are almost zero.

In summary, the emptiness of the attribute mastery patterns causes the rank deficiency of $I_{comp}(\Xi^*|\mathbf{X})$ and causes irregularly large SEs. The emptiness causes the boundary problem, but the boundary problem for correct response probabilities does not cause irregularly large SEs. The boundary problem may unfortunately occur when attribute mastery patterns are not empty, but item responses are all zero or one for some attribute mastery patterns. However, such boundary problem is not a trigger of rank deficiency of complete data Fisher information matrix, but the accidental boundary problem by sampling error causes too-small SEs for correct item response probability parameters. The irregularly large SEs for mixing parameters do not happen except in

unrealistic situations, but unfortunate emptiness by sampling error also causes too-short SEs for mixing parameters. If emptiness or a boundary problem occurs owing to sampling error, then the MAP procedure can prevent such irregular SEs. However, as in the discussion in the EM algorithm section, if the emptiness occurs or the true parameters are zero or one, the MAP procedure causes inappropriate SEs. The estimation procedure for actual SEs using EM algorithm is shown in Supplemental Material C.

The Simulation Study

Simulation Settings

The simulation study aimed to confirm the parameter recovery with the proposed algorithm and assess whether MAP estimates can avoid the boundary problem and inappropriate SE estimates. We also employed no-constrained estimation and monotonicity constrained for the MAP and ML methods because monotonicity constrained may be reduce the risk of boundary problems. Furthermore, we checked if boundary problems affected attribute mastery pattern recovery and what type of parameter estimation methods were recommended in DCMs. Because of space limitations, the results for mixing parameter results are omitted, following previous studies (e.g., de la Torre, 2009b).

We manipulated six factors: sample size, item quality (or strength of item discrimination), attribute correlation, number of attributes, Q-matrix complexity, and estimation method. Sample size conditions were 50, 200, 1000, and 4000. The sample size of 50 was the smallest number employed in Sen and Cohen (2021) that assessed parameter recovery of several diagnostic classification models in various sample size conditions. For a larger sample size condition, we assumed 200, as in Sen and Cohen (2021). Furthermore, Sessoms and Henson (2018) reviewed DCMs application studies and revealed that the sample size of the DCMs application was large, with a median of 1,255. Therefore, we assessed 1,000 and 4,000 sample size conditions.

As item parameter quality, we assumed high-quality and low-quality item conditions. Under the former, all non-mastering patterns have 0.1 correct item response probability for an

item and all mastering pattern have 0.9. This condition assumes large discriminations items. In contrast, low-quality items conditions set the correct item response probability for an item for all non-mastering pattern at 0.35 and for all mastering patterns at 0.65. The items in this condition were low discrimination powers. The other correct item response probabilities were generated as in Yamaguchi and Templin (2022a).

Three correlation conditions were defined: no correlation (0), moderate correlation (0.5), and high correlation (0.8). Attributes are correlated with each other, with very high correlation sometimes, with a value greater than 0.8 (e.g., Table 8 in von Davier, 2008). Therefore, no-correlation may not be realistic but can be seen as a reference condition. In addition, the number of attributes were three or five. The well-known Examination for the Certificate of Proficiency in English (ECPE; e.g., Templin & Bradshaw, 2014) data have three attributes, and Sen and Cohen (2021) also employed three attributes in their simulations. Sessoms and Henson (2018) found four attributes to be the most common in their review. We assumed a slightly more difficult situation and employed five attributes, as did Yamaguchi and Okada (2020a) in their simulation.

We also changed the Q-matrix, using simple and complex structures. The Q-matrices are shown in Tables 2 and 3 corresponding to three and five attributes. Tables 2 and 3 indicate simple (left part) and complex (right part) structures. In the simple structure, we assumed the item measures at two attributes. For example, items 13–15 in the left-hand-side of Table 2 and items 21–30 in the right-hand-side of Table 3 measure two attributes. The complex structure assumes that some items measure three attributes. For example, items 13–15 in the right hand-side of Table 2 and items 21–30 in the right-hand-side of Table 3 measure three attributes. The number of items were equal for both structures and all Q-matrices satisfied identifiability conditions.

The final manipulated factor was estimation methods. We assumed four conditions that are combination ML or MAP methods and unconstrained or monotonicity constraints: ML with no constraint, MAP with no constraints, ML with monotonicity constraints, and MAP with

monotonicity constraints. The estimation of monotonicity constraints was based on the supplemental material in Ma and Jiang (2021). The total number of conditions is $4 \times 2 \times 3 \times 2 \times 2 \times 4 = 384$.

The data generation procedure was similar to that of Chiu and Douglas (2013). First, three- (or five-) dimensional continuous latent variable vectors $\tilde{\alpha}_s (= (\tilde{\alpha}_1, \dots, \tilde{\alpha}_k, \dots, \tilde{\alpha}_K)^T)$ for each individual were generated from a multivariate normal distribution with mean $\mathbf{0}$, and the covariance matrix had ones as diagonal elements and the assumed attribute correlations as off-diagonal elements. Second, if $\tilde{\alpha}_k$ was greater than its threshold $\Phi^{-1}(k/(1+K))$, where $\Phi^{-1}(\cdot)$ is the inverse function of cumulative normal distribution, then α_k was equal to one (otherwise, it was equal to zero). This assumption reflected that the difficulty of mastery was different for each attribute and a large number of attributes caused more difficulty than a small number.

In the estimation setting, the maximum iteration number was fixed at 500, and the start values were generated randomly. In this study, the small positive number ϵ for the first-order Richardson extrapolation of the central difference method (REM; Tian, Cai, Thissen, & Xin, 2013; Jamshidian & Jennrich, 2000) was fixed at equal to 10^{-7} . For the hyperparameters for the MAP estimates, δ_l^0 s were all set equal to 1.1. This setting reflected almost zero knowledge of attribute mastery patterns. In other words, it was a difficult setting for mixing parameter estimation. The a^0 value was 1.01 for all non-mastery patterns, 2 for all mastery patterns, and 1.1 for others. In contrast, the b^0 value was 2 for all non-mastery patterns, 1.01 for all mastery patterns, and 1.1 for others. This setting implies that the prior expected correct response probability is less than 0.5 for all non-mastery patterns, greater than 0.5 for all mastery patterns, and 0.5 for other patterns. It is also expected to prevent the boundary problem and the rank deficiency of $I_{comp}(\Xi^*|\mathbf{X})$. All hyperparameters were set at equal to one for the ML estimates.

The simulation was repeated 200 times. The following were calculated for evaluation: the boundary problem rate, the mean absolute bias for correct item response parameters, root mean square error (RMSE), the mean absolute bias for SE calculated by taking the average of the

absolute difference between SE estimates and empirical SD over 200 simulation deprecation, and the correct attribute mastery rate. The attribute masteries were estimated patterns of maximize posterior probability with estimated correct item response probabilities and mixing parameters. In addition, in this study, the boundary problem of parameter estimates was operationally defined as the case in which the estimate is less than 10^{-5} or greater than $1 - 10^{-5}$. These values were set based on the GDINA function in the GDINA package (Ma & de la Torre, 2017) and the default settings of the function rounded estimates less than 10^{-4} or greater than $1 - 10^{-4}$ to 10^{-4} or $1 - 10^{-4}$, respectively. Our criteria for the boundary problem were stricter than those in the GDINA function setting. Parameter updating was stopped when absolute changes of all parameters were less than 10^{-4} . The ratio of the boundary problem for each parameter was calculated and averaged over correct item parameters. Moreover, to avoid numerical problems in the REM step, parameter estimates become smaller than 2×10^{-7} or greater than $1 - 2 \times 10^{-7}$. The simulation script was written in the R language and is available on the Open Science Framework page: <https://osf.io/rwe5t/>.

Simulation Results

Figure 1 shows the boundary problem rate for correct item response probability parameters. On clear result was that the MAP methods never provided boundary problems, but ML methods sometimes provided boundary problem solution. In the ML methods, monotonicity constraint reduced the boundary problem rate more than the unconstrained method. In addition, compared to low-quality items or simple Q-matrix, high-quality items and complex Q-matrix conditions tended to have boundary problems. Under high-quality items conditions, true parameters are close to the bound and, therefore, understandable. The sample size increment reduced the boundary problem rate. High attribute correlation can slightly increase the boundary problem rate, but its impact was not so large in general.

Figure 2 depicts the absolute bias of correct item response probability parameters. Monotonicity constraints reduced the absolute bias in this situation. As expected, sample size reduced absolute biases. Quality of items and complexity of Q-matrix also affected absolute

biases. Low-quality items and complex Q-matrix increased absolute biases. The effect of the number of attributes was not large, and the differences between the ML and MAP methods were very small in this simulation. Attribute correlations did not affect absolute biases either. In addition, complex Q-matrix conditions showed larger absolute biases.

Figure 3 shows the RMSE of correct item response probability parameters. Similar to absolute biases, large sample sizes tended to decrease RMSE. Complexity of Q-matrix increased RMSEs. The monotonicity also decreased RMSEs under all conditions but especially under complex Q-matrix conditions. The ML method showed worse RMSEs than the MAP method, especially in high-quality items and complex Q-matrix conditions. However, the differences among ML and MAP methods were much smaller than those among non-constrained and monotonicity constraints.

Figure 4 indicates the mean absolute biases of SE estimation of correct item response probability parameters. Monotonicity constrained estimation tended to be small absolute bias of SEs in low-quality items or five attributes and complex Q-matrix conditions. This means variability of monotonicity constrained parameter estimates were closer to the approximated SEs than the non-constrained. In other words, the approximated SEs employed in this study can mimic the variability of monotonicity parameter constraints, as theoretically expected. Furthermore, the MAP provided smaller absolute biases, for example, under high-quality and complex Q-matrix conditions.

Finally, Figure 5 shows the correct attribute mastery pattern recovery rates, which are strongly affected by quality of items. This means if the test consists of high-quality items, the attribute mastery pattern was clearly recovered but lower-quality items made attribute mastery pattern estimation difficult. In addition, compared to simple Q-matrix conditions, complex ones tended to lower attribute mastery pattern recovery rates. In this simulation, the effects of the estimation methods were relatively small and ignorable. Namely, the effects of the MAP method were the same as those of the ML method.

In summary, boundary problems happened especially in high-quality items and small sample size settings, with MAP preventing boundary problems. However, under the high-quality items conditions, attribute mastery pattern recovery rates were very high. This means that boundary problems do not provide problematic resultants in terms of attribute mastery probability recovery. However, under the condition that boundary problems sometimes occurred, absolute biases or RMSEs were sometimes not small. This means understanding item characteristics in such situations may not be appropriate. MAP estimation reduced RMSEs, and thus provided stable correct item response probability parameters. Furthermore, monotonicity constraint estimation also provided a stable estimation. SE estimates under monotonicity constraint generated smaller absolute biases. From these results, the MAP estimation with monotonicity constraints is the most recommended estimation method for both attribute mastery and correct item response probabilities estimations. This recommendation was consistent with Ma and Jiang's (2021).

Discussion and Conclusion

Boundary problems are likely to cause estimation problems but have not been assessed in detail. This study intended to reveal the mathematical relationship between emptiness of attribute mastery patterns and irregular SE estimation from the perspective of boundary problems. For this objective, the saturated type of DCM was reformulated and the EM algorithm for MAP estimates developed. Moreover, the complete Fisher information matrix was derived and the EM algorithm-based SE estimation method was developed.

By considering the complete data Fisher information matrix, the relationship between the boundary problem and inappropriate SE estimates can be explained. It was shown analytically that the true common cause of both problems has been the emptiness of the attribute mastery patterns. However, the boundary problems were not the direct cause of the problem of irregular SEs, as revealed by the mathematical formulation of asymptotical SEs. MAP estimations worked as a regularization term and prevented boundary problems and irregular SEs. The simulation study then showed that the boundary problems could be related to unstable

correct item response probability parameters estimation but did not cause serious results in terms of attribute mastery pattern recovery. This analysis also explains how monotonicity constraint estimation reduces the boundary-problem risk and provides a stable estimation. In the simulation, the RMSEs of the MAP estimates were smaller than those of the ML method, with the MAP estimation method providing smaller SE estimates than the ML method. Furthermore, monotonicity constraints provided stable parameter estimation and more accurate SEs estimation than non-constrained estimation did. In addition, MAP estimation was able to avoid boundary problems at any time, as evident from the comparison with ML estimates. Although in some situations, especially under small-sample conditions, neither the ML nor the MAP method had biases or incorrect SEs, the MAP method and monotonicity constraints improved the SE estimates. Based on the simulation study, the MAP method with monotonicity constraint was the best estimation method.

The MAP estimation algorithm enabled researchers to take prior knowledge of DCM analysis into account. The MAP estimation method is an extension of the ML method, and the priors can work as regularization terms in the ML method. These priors prevent not only the boundary problem but also unreasonable estimates of SEs; they also provide more stable estimates. Moreover, monotonicity constrained estimation also improved stability of correct item response probability parameters. These results were congruent with those of Ma and Jiang (2021). Theoretical considerations and a simulation supported these points. In addition, the priors in the proposed MAP estimation method work to keep the complete data Fisher information matrix at full rank, a point not considered by previous studies. The simulation study also revealed that boundary problems did not have serious consequences for the estimation of attribute mastery, again not pointed out in previous studies, including Ma and Jiang (2021).

However, that boundary problems are not a serious resultant of attribute mastery pattern estimation should be carefully considered. First, the result was that the specified DCM and Q-matrix are correct, but holding this situation could be difficult. In the DCM analysis, careful consideration steps of the Q-matrix setting or item parameters estimations are included.

To extract valid and understandable results of attribute mastery patterns, we need to think about item parameter estimations. In other words, we cannot trust the classification result based on item parameter estimations that are so problematic. Therefore, it may be important to recognize that item parameter estimates are the foundation of other statistics, including estimates of person parameters, item-fit index (e.g., Sorrel et al., 2017), differential item functioning (e.g., Ma et al., 2021), reliability index (e.g., Templin & Bradshaw, 2013), and external validity evidence (e.g., Sorrel et al., 2016) especially in small sample size setting. The statistics based on item parameters, however, use estimated values. In other words, the uncertainties of correct item response probability, represented as SEs, are practically ignored. Therefore, including estimation uncertainty is an area that needs future study. These topics are of current interest in the DCM field, where more detailed theoretical studies are needed.

Some implications for DCM use are as follows. One simple suggestion is to use the MAP method with monotonicity constraints. This estimation method provides more stable parameter estimates than the ML method and unconstrained estimation. Monotonicity constraints especially provide more accurate approximate SEs than unconstrained estimation. The estimation method employed this study did not provide notable difference. Therefore, if the focus of data analysis is only on the estimation of attribute mastery patterns, the estimation methods for items and structural parameters were not serious problem. However, in such case, the correct item response probabilities may not be trustworthy and interpreting the parameters may be questionable. For test construction, the simple Q-matrix is better than the complex one, which provides unstable parameter estimates especially for large number of attributes.

An important point of the DCM analysis from simulation is to avoid a small sample size. From our simulation study, 50 is too small a sample size for estimating correct item response probabilities. We recommend increasing the sample size as much as possible, at least to several hundreds. If it is difficult, set appropriate hyper parameters based on previous knowledge of test items. This will help accurate parameter estimation but if the hyper parameters were inappropriate, the results may be biased.

For the MAP method, we need to determine the hyperparameters of the priors, which can be arbitrarily specified. If we can use previously estimated parameter values, we can use them as a prior. One choice of hyperparameters is that the correct response probability increases according to the number of attributes in an item-specific pattern. Recalling an example in Table 1, the hyperparameters can be determined to satisfy the inequality $\theta_{j1} < \text{Min}\{\theta_{j2}, \theta_{j3}\} < \text{Max}\{\theta_{j2}, \theta_{j3}\} < \theta_{j4}$. For θ_{j1} , which is the correct response probability of all non-mastery patterns; setting $a_{j1}^0 = 1.01$ and $b_{j1}^0 = 2$ means that the prior mode correct response probability is .0099. Similarly, for θ_{j4} , the correct item response probability of all mastery patterns, setting $a_{j4}^0 = 2$ and $b_{j4}^0 = 1.01$ means that the prior mode correct response probability is .99. For the other patterns, θ_{j2} and θ_{j3} , $a_{j2}^0 = a_{j3}^0 = b_{j2}^0 = b_{j3}^0 = 1.1$ mean that the prior mode correct response probability is 0.5. For mixing probability, the hyperparameter δ_l^0 may better reflect the correlations among the attributes. For example, all non-mastery and mastery patterns are sometimes more observed than other patterns; thus, it may be better if the hyperparameters for these two attribute mastery patterns are greater than the others. These priors may be reasonable for real data analysis; however, clearer recommendations for prior design should be discussed in future research. Furthermore, if inappropriate hyper parameters are specified, the item parameters can be biased, which will lead to the misclassification results of attribute mastery patterns. Further analyses are thus needed to reveal when the MAP method does not work well.

The simulation results indicated that simpler Q-matrices provide smaller absolute biases of point estimates, RMSEs, and absolute biases of SEs. They give us the simple lesson to keep Q-matrix structure simpler. In the case of complex Q-matrices, some items have eight correct item response probability parameters but some items in simple Q-matrices have at the most four parameters. This parameter increase can cause unitability of parameter estimation as pointed out Templin and Bradshaw (2014). In addition, the complexity of the Q-matrix may have a larger effect than the number of attributes. Thus, using items that measure a few attributes is important for DCM users.

The limitations of the EM and MAP estimates are seen when the attributes are correlated and have different thresholds. Because of these assumptions, some attribute mastery patterns are almost empty, and it is difficult to estimate some correct item response probabilities. In addition, such correct response probabilities tend to have small SEs, theoretically and numerically. These estimation errors were also observed for the mixing parameters. These biases and inappropriate SEs have not been reported before, perhaps because previous studies assumed easy conditions for simulation purposes. However, real data analysis situations are more difficult than simulations, and more effective estimation methods for more severe settings (such as a small sample size, large and correlated attributes, and complex Q-matrix conditions) will be required. In addition, if more informative priors are employed, the biases and estimation errors of SEs might disappear; for this reason, the effects of priors should be examined in future research.

Another limitation of the MAP method may be seen when attribute hierarchy (e.g., Leighton, Gierl, & Hunka, 2004) is assumed behind the test. Attribute hierarchy is the dependency of attributes, and, thus, some attribute mastery patterns are not assumed. For example, to master the “fraction subtraction” attribute, the “four arithmetic operations” that underlie it should also be mastered. In other words, if students master “fraction subtraction,” they will also have mastered the “four arithmetic operations,” and a pattern of mastering “fraction subtraction” but not mastering “four arithmetic operations” is not reasonable. The attribute hierarchy may not always be given a priori, but some statistical methods to detect attribute hierarchy have been developed (e.g., Wang & Lu, 2020). Using such exploratory methods is helpful in determining attribute hierarchy. However, if a data analyst does not perceive such an attribute hierarchy and employs the MAP estimation method with unstructured attributes, the result may be biased; they may fail to discover such an attribute hierarchy because the MAP method makes estimates stick to their boundary. Thus, if the purpose of the analysis is exploring attribute hierarchies, ML estimation may be better than MAP estimation.

The effect of misspecification of attribute hierarchy on parameter estimates is an interesting topic from both theoretical and practical aspects. Assessing bias or boundary problem

under misspecified attribute hierarchy condition is difficult. One reason is that the misspecification of attribute hierarchy implies Q-matrix and item response function misspecification. Even if the attribute hierarchy is not assumed, the result of Q-matrix misspecification is not clear. Moreover, misspecification of attribute hierarchy sometimes includes the misspecification of the number of attributes; that is, the number of parameters in assumed model may be at discord with the real model. Therefore, defining bias or problematic boundary problems is difficult. Furthermore, finding out realistic misspecification is another challenge. As the misspecification study is beyond the scope of this study, revealing misspecified attribute hierarchy effect on parameter estimates is a priority future research topic.

It is important to note that MAP estimates have not only benefits but problems too. One risk is to hide the overfitting problem. The boundary problem may indicate the overfitting of model to the current data. Ma and Jiang (2021) empirically showed that the usual ML method will cause overfitting, and the MAP estimation prevents this phenomenon. Therefore, we strongly recommend checking model fit indices (e.g., Hartz & Roussos, 2008; Ma, 2019; Rupp et al., 2010) and carefully using the MAP estimator. The overfitting problem can be another interpretation of the emptiness of attribute mastery pattern. The MAP estimator is a kind of regularized estimator that prevents overfitting problem, when data size is small and the model has many parameters. This situation is very common in DCM analysis settings because DCMs can be used in a classroom test. In such a situation, we have to reduce the number of parameters or use a simplified model if we use ML estimation method. However, such simplification or crude attributes reduce the value of diagnosis information extracted from data. Moreover, changing model side not estimation method may not be appropriate when the attributes and Q-matrix specification are supported well by cognitive theories or content knowledge because such modification directly causes model misspecification. Even when ML estimation is difficult, MAP can provide a parameter estimate. In addition, if there is prior information, such as mixing parameter or part of item parameters, MAP can consider such information as priors. The data

analyst should understand that the MAP method has pros and cons, and the reliability of the parameter estimate should be carefully checked using model fit or other indices.

Another limitation of the MAP estimation method is that the Q-matrix should be known. Even when real data applications of DCMs are assuming known Q-matrices, the assumption is a clear flaw. Recently, exploratory version DCMs that estimate not only model parameters but also Q-matrix from data have been actively studied (e.g., Chen et al., 2018; Culpepper, 2019b; Culpepper & Chen, 2018). Combining the MAP estimation method with exploratory DCMs can be a potential research topic. Related to the assumption of Q-matrix, we also need to note the gradation of the Q-matrix misspecification. This means that the percentage of element-wise misspecification is a more realistic discussion point. An initial Q-matrix can be validated with empirical data, according to Nájera et al. (2021), who reported that some Q-matrix validation methods could recover appropriate Q-matrix. Therefore, using empirical Q-matrix validation methods improves the utility of the MAP estimation method.

Moreover, MAP is not appropriate for the case of mismatch between the assumed model and true data generation mechanism as it produces biased estimates. If some parameters are truly on the bound of their bound, it is another case that MAP is not appropriate. This is because prior distributions block bounded estimation in finite sample size. We mentioned these points in the Introduction to clarify the limitations of the estimation method.

To deal with boundary problem, MAP is just one solution, and so are Hong et al.'s (2015) upward/downward algorithms. Their methods can be less meaningful if the estimates stick to the newly defined parameter bound with monotonicity constraint. In this case, we do not interpret the parameter estimates. As mentioned above, full Bayesian estimations, not discussed in this study, are also a solution (e.g., Yamaguchi & Templin, 2022b). One reason we employed the MAP estimation is that can be tractable in mathematical analysis. If the purpose is how to prevent the boundary problems, comparison of various methods is important, but it is not the primary purpose of this study and can only be a future research topic.

Finally, the emptiness of attribute mastery patterns is important from the perspective of the identifiability of models. Theoretical works on DCMs (Chen, Culpepper, & Liang, 2020; Culpepper, 2019a) assume non-emptiness of attribute mastery pattern. In future research, it is important to reveal the theoretical consequences of emptiness of attribute mastery pattern for model identifiability problem or related topics.

As a final note, the simulation settings were limited and we considered idealized situations, namely a correct simple structure of the Q-matrix and simple true item parameters. The result indicated the MAP method did not improve the classification results, but this does not mean this method is meaningless. As mentioned above, the item parameters and mixing parameter are important to ensure the attribute mastery estimation quality and a MAP estimation can provide stable parameter estimates. However, further analyses are needed to determine when the ML method fails and the MAP estimation can compensate the limitations of the ML method.

References

- Blei, D. M., Ng, A. Y., & Jordan, M. I. (2003). Latent Dirichlet allocation. *Journal of Machine Learning Research*, 3(Jan), 993–1022. <https://dl.acm.org/doi/10.5555/944919.944937>
- Cai, L. (2008). SEM of another flavour: Two new applications of the supplemented EM algorithm. *British Journal of Mathematical and Statistical Psychology*, 61, 309–329. <https://doi.org/10.1348/000711007X249603>
- Chen, J., & de la Torre, J. (2014). A procedure for diagnostically modeling extant large-scale assessment data: The case of the programme for international student assessment in reading. *Psychology*, 5(November), 1967–1978. <https://doi.org/10.4236/psych.2014.518200>
- Chen, Yinghan, Culpepper, S. A., Chen, Y., & Douglas, J. (2018). Bayesian estimation of the DINA Q matrix. *Psychometrika*, 83, 89–108. <https://doi.org/10.1007/s11336-017-9579-4>
- Chen, Yinyin, Culpepper, S., & Liang, F. (2020). A sparse latent class model for cognitive diagnosis. *Psychometrika*, 85(1), 121–153. <https://doi.org/10.1007/s11336-019-09693-2>
- Chiu, C. Y., & Douglas, J. (2013). A nonparametric approach to cognitive diagnosis by proximity to ideal response patterns. *Journal of Classification*, 30, 225–250. <https://doi.org/10.1007/s00357-013-9132-9>
- Culpepper, S. A. (2019a). An exploratory diagnostic model for ordinal responses with binary attributes: Identifiability and estimation. *Psychometrika*, 84(4), 921–940. <https://doi.org/10.1007/s11336-019-09683-4>
- Culpepper, S. A. (2019b). Estimating the cognitive diagnosis Q matrix with expert knowledge: Application to the fraction-subtraction dataset. *Psychometrika*, 84, 333–357. <https://doi.org/10.1007/s11336-018-9643-8>
- Culpepper, S. A., & Chen, Y. (2019). Development and application of an exploratory reduced reparameterized unified model. *Educational and Behavioral Statistics*, 4(1), 3–24. <https://doi.org/10.3102/1076998618791306>

- Culpepper, S. A., & Hudson, A. (2018). An improved strategy for Bayesian estimation of the reduced reparameterized unified model. *Applied Psychological Measurement*, 42, 99–115. <https://doi.org/10.1177/0146621617707511>
- de la Torre, J. (2009a). A cognitive diagnosis model for cognitively based multiple-choice options. *Applied Psychological Measurement*, 33, 163–183. <https://doi.org/10.1177/0146621608320523>
- de la Torre, J. (2009b). DINA model and parameter estimation: A didactic. *Journal of Educational and Behavioral Statistics*, 34, 115–130. <https://doi.org/10.3102/1076998607309474>
- de la Torre, J. (2011). The generalized DINA model framework. *Psychometrika*, 76, 179–199. <https://doi.org/10.1007/S11336-011-9207-7>
- DeCarlo, L. T. (2011). On the analysis of fraction subtraction data: The DINA model, classification, latent class sizes, and the Q-matrix. *Applied Psychological Measurement*, 35, 8–26. <https://doi.org/10.1177/0146621610377081>
- Dempster, A. P., Laird, N. M., & Rubin, D. (1977). Maximum likelihood from incomplete data via the EM algorithm. *Journal of the Royal Statistical Society. Series B (Methodological)*, 39, 1–38. <https://doi.org/10.2307/2984875>
- Ferguson, T. S. (1996). A course in large sample theory. London: Chapman and Hall.
- Fukumizu, K., Kuriki, S., Takeuchi, K., & Akahira, M. (2004). 特異モデルの統計学[Statistical theory of singular models]. Chiyoda: Tokyo, Iwanami. (in Japanese)
- Garre, F. G., & Vermunt, J. K. (2006). Avoiding boundary estimates in latent class analysis by Bayesian posterior mode estimation, 33(1), 43–59. <https://doi.org/10.2333/bhmk.33.43>
- Gu, Y., & Xu, G. (2019). Learning attribute patterns in high-dimensional structured latent attribute models. *Journal of Machine Learning Research*, 20(115), 1–58. <https://www.jmlr.org/papers/volume20/19-197/19-197.pdf>

- Hartz, S., & Roussos, L. (2008). The fusion model for skills diagnosis: Blending theory with practice. *ETS Research Report Series*, 08–71, 1–57.
<https://www.ets.org/Media/Research/pdf/RR-08-71.pdf>
- Henson, R. A., Templin, J. L., & Willse, J. T. (2009). Defining a family of cognitive diagnosis models using log-linear models with latent variables. *Psychometrika*, 74, 191–210.
<https://doi.org/10.1007/S11336-008>
- Hong, C. Y., Chang, Y. W., & Tsai, R. C. (2016). Estimation of generalized DINA model with order restrictions. *Journal of Classification*, 33(3), 460–484.
<https://doi.org/10.1007/s00357-016-9215-5>
- Jamshidian, M., & Jennrich, R. I. (2000). Standard errors for EM estimation. *Journal of the Royal Statistical Society. Series B (Statistical Methodology)*, 62, 257–270. Retrieved from
<https://www.jstor.org/stable/3088858>
- Lee, Y.-S., Park, Y. S., & Taylan, D. (2011). A cognitive diagnostic modeling of attribute mastery in Massachusetts, Minnesota, and the U.S. national sample using the TIMSS 2007. *International Journal of Testing*, 11, 144–177.
<https://doi.org/10.1080/15305058.2010.534571>
- Leighton, J. P., Gierl, M. J., & Hunka, S. M. (2004). The attribute hierarchy method for cognitive assessment: A variation on Tatsuoaka's rule space approach. *Journal of Educational Measurement*, 41(3), 205–237. <https://doi.org/10.1111/j.1745-3984.2004.tb01163.x>
- Leighton, J. P., & Gierl, M. J. (Eds.). (2007). *Cognitive diagnostic assessment for education: Theory and applications*. New York, NY: Cambridge University Press.
- Li, H., Hunter, C. V., & Lei, P.-W. (2016). The selection of cognitive diagnostic models for a reading comprehension test. *Language Testing*, 33(2012), 1–35.
<https://doi.org/10.1177/0265532215590848>
- Liu, Y., Xin, T., Andersson, B., & Tian, W. (2019). Information matrix estimation procedures for cognitive diagnostic models. *British Journal of Mathematical and Statistical Psychology*, 72(1), 18–37. <https://doi.org/10.1111/bmsp.12134>

- Lüdtke, O., Ulitzsch, E., & Robitzsch, A. (2021). A comparison of penalized maximum likelihood estimation and Markov Chain Monte Carlo techniques for estimating confirmatory factor analysis models with small sample sizes. *Frontiers in Psychology, 12*. <https://doi.org/10.3389/fpsyg.2021.615162>
- Ma, W. (2020). Evaluating the fit of sequential G-DINA model using limited-information measures. *Applied Psychological Measurement, 44*(3), 167–181. <https://doi.org/10.1177/0146621619843829>
- Ma, W., & de la Torre, J. (2017). GDINA: The generalized DINA model framework. Retrieved from <https://cran.r-project.org/package=GDINA>
- Ma, W., & Jiang, Z. (2021). Estimating cognitive diagnosis models in small samples: Bayes modal estimation and monotonic constraints. *Applied Psychological Measurement, 45*(2), 95–111. <https://doi.org/10.1177/0146621620977681>
- Ma, W., Terzi, R., & de la Torre, J. (2021). Detecting differential item functioning using multiple-group cognitive diagnosis models. *Applied Psychological Measurement, 45*(1), 37–53. <https://doi.org/10.1177/0146621620965745>
- Maris, E. (1999). Estimating multiple classification latent class models. *Psychometrika, 64*, 187–212. <https://doi.org/10.1007/BF02294535>
- Meng, X. L., & Rubin, D. B. (1991). Using EM to obtain asymptotic variance-covariance matrices: The SEM algorithm. *Journal of the American Statistical Association, 86*, 899–909. <https://doi.org/10.1080/01621459.1991.10475130>
- Nájera, P., Sorrel, M. A., de la Torre, J., & Abad, F. J. (2021). Balancing fit and parsimony to improve Q-matrix validation. *British Journal of Mathematical and Statistical Psychology, 74*(S1), 110–130. <https://doi.org/10.1111/bmsp.12228>
- Philipp, M., Strobl, C., de la Torre, J., & Zeileis, A. (2018). On the estimation of standard errors in cognitive diagnosis models. *Journal of Educational and Behavioral Statistics, 43*, 88–115. <https://doi.org/10.3102/1076998617719728>

- Rupp, A. A., & Templin, J. (2008). Unique characteristics of diagnostic classification models: A comprehensive review of the current state-of-the-art. *Measurement: Interdisciplinary Research & Perspective*, 6, 219–262. <https://doi.org/10.1080/15366360802490866>
- Rupp, A. A., Templin, J. L., & Henson, R. A. (2010). *Diagnostic measurement: Theory, methods and applications*. New York, NY: Guilford Press.
- Sen, S., & Cohen, A. S. (2021). Sample size requirements for applying diagnostic classification models. *Frontiers in Psychology*, 4050. <https://doi.org/10.3389/fpsyg.2020.621251>
- Sen, S., & Terzi, R. (2020). A comparison of software packages available for DINA model estimation. *Applied Psychological Measurement*, 44(2), 150–164. <https://doi.org/10.1177/0146621619843822>
- Sessoms, J. & Henson, R. A. (2018) Applications of diagnostic classification models: A literature review and critical commentary. *Measurement: Interdisciplinary Research and Perspectives*, 16(1), 1–17, <https://doi.org/10.1080/15366367.2018.1435104>
- Sorrel, M. A., Abad, F. J., Olea, J., de la Torre, J., & Barrada, J. R. (2017). Inferential item-fit evaluation in cognitive diagnosis modeling. *Applied Psychological Measurement*, 41(8), 614–631. <https://doi.org/10.1177/0146621617707510>
- Sorrel, M. A., Olea, J., Abad, F. J., de la Torre, J., Aguado, D., & Lievens, F. (2016). Validity and reliability of situational judgement test scores: A new approach based on cognitive diagnosis models. *Organizational Research Methods*, 19, 506–532. <https://doi.org/10.1177/1094428116630065>
- Tatsuoka, K. K. (1983). Rule space: An approach for dealing with misconceptions based on item response theory. *Journal of Educational Measurement*, 20, 345–354. <https://doi.org/10.1111/j.1745-3984.1983.tb00212.x>
- Templin, J., & Bradshaw, L. (2013). Measuring the reliability of diagnostic classification model examinee estimates. *Journal of Classification*, 30, 251–275. <https://doi.org/10.1007/s00357-013-9129-4>

- Templin, J., & Bradshaw, L. (2014). Hierarchical diagnostic classification models: A family of models for estimating and testing attribute hierarchies. *Psychometrika*, 79(2), 317–339.
<https://doi.org/10.1007/s11336-013-9362-0>
- Tian, W., Cai, L., Thissen, D., & Xin, T. (2013). Numerical differentiation methods for computing error covariance matrices in item response theory modeling an evaluation and a new proposal. *Educational and Psychological Measurement*, 73, 412–439.
<https://doi.org/10.1177/0013164412465875>
- Vermunt, J. K., & Magidson, J. (2005). *Technical guide for Latent GOLD 5.1: Basic, advanced and syntax* [Computer software and manual]. Belmont, CA: Statistical Innovations.
- von Davier, Matthias. (2008). A general diagnostic model applied to language testing data. *The British Journal of Mathematical and Statistical Psychology*, 61(Pt 2), 287–307.
<https://doi.org/10.1348/000711007X193957>
- Wang, C., & Lu, J. (2020). Learning attribute hierarchies from data: Two exploratory approaches. *Journal of Educational and Behavioral Statistics*, 1–27.
<https://doi.org/10.3102/1076998620931094>
- Watanabe, S. (2007). Almost all learning machines are singular. *Proceedings of the 2007 IEEE Symposium on Foundations of Computational Intelligence*, 383–388.
<https://doi.org/10.1109/FOCI.2007.371500>
- Watanabe, S. (2018). *Mathematical theory of Bayesian statistics*. Chapman and Hall/CRC.
- Xu, G., & Shang, Z. (2018). Identifying latent structures in restricted latent class models. *Journal of the American Statistical Association*, 113(523), 1284–1295.
<https://doi.org/10.1080/01621459.2017.1340889>
- Yamaguchi, K. (2019). DINA モデルの再定式化と推定アルゴリズムの直接的導出 [A re-formulation of the DINA model and a direct derivation of estimation algorithms]. *Japanese Journal for Research on Testing*, 15, 21–43. (in Japanese)
- Yamaguchi, K. (2020). Variational Bayesian inference for the multiple-choice DINA model. *Behaviormetrika*, <https://doi.org/10.1007/s41237-020-00104-w>

- Yamaguchi, K., & Okada, K. (2018). Comparison among cognitive diagnostic models for the TIMSS 2007 fourth grade mathematics assessment. *PLoS ONE*, *13*, e0188691.
<https://doi.org/10.1371/journal.pone.0188691>
- Yamaguchi, K., & Okada, K. (2020a). Variational Bayes inference algorithm for the saturated diagnostic classification. *Psychometrika*, *85*(4), 973–995.
<https://doi.org/10.1007/s11336-020-09739-w>
- Yamaguchi, K., & Okada, K. (2020b). Variational Bayes inference for the DINA model. *Journal of Educational and Behavioral Statistics*, <https://doi.org/10.3102/1076998620911934>
- Yamaguchi, K., & Templin, J. (2022a). A Gibbs sampling algorithm with monotonicity constraints for diagnostic classification models. *Journal of Classification*, *39*, 24–54.
<https://doi.org/10.1007/s00357-021-09392-7>
- Yamaguchi, K., & Templin, J. (2022b). Direct estimation of diagnostic classification model attribute mastery profiles via a collapsed Gibbs sampling algorithm. *Psychometrika*.
<https://doi.org/10.1007/s11336-022-09857-7>

Table 1.

A modified example of G-matrix for $\mathbf{q}_j = (1,1,0)^T$ shown in Yamaguchi and Okada (2021)

					Attribute mastery pattern (l)							
					1	2	3	4	5	6	7	8
Restricted attribute mastery pattern (h)	α_h^*	Attribute			G-matrix							
		1	2	3								
1	α_1^*	0	0	*	1	0	0	1	0	0	0	0
2	α_2^*	1	0	*	0	1	0	0	0	1	0	0
3	α_3^*	0	1	*	0	0	1	0	0	0	1	0
4	α_4^*	1	1	*	0	0	0	0	1	0	0	1

Note: Attribute mastery pattern 1 =(0,0,0), 2 = (1,0,0), 3 = (0,1,0), 4=(0,0,1), 5 = (1,1,0), 6 = (1,0,1), 7 = (0,1,1), and 8 =(1,1,1).

Table 2.

Q-matrices with three attributes employed in simulation study (left: simple structure, right: complex structure)

Item	Simple structure			Complex structure		
	Attribute			Attribute		
	1	2	3	1	2	3
1	1	0	0	1	0	0
2	0	1	0	0	1	0
3	0	0	1	0	0	1
4	1	0	0	1	0	0
5	0	1	0	0	1	0
6	0	0	1	0	0	1
7	1	0	0	1	1	0
8	0	1	0	1	1	0
9	0	0	1	1	0	1
10	1	0	0	1	0	1
11	0	1	0	0	1	1
12	0	0	1	0	1	1
13	1	1	0	1	1	1
14	1	0	1	1	1	1
15	0	1	1	1	1	1

Table 3.

Q-matrices with five attributes employed in simulation study (left: simple structure, right: complex structure)

Item	Simple structure					Complex structure				
	Attribute					Attribute				
	1	2	3	4	5	1	2	3	4	5
1	1	0	0	0	0	1	0	0	0	0
2	0	1	0	0	0	0	1	0	0	0
3	0	0	1	0	0	0	0	1	0	0
4	0	0	0	1	0	0	0	0	1	0
5	0	0	0	0	1	0	0	0	0	1
6	1	0	0	0	0	1	0	0	0	0
7	0	1	0	0	0	0	1	0	0	0
8	0	0	1	0	0	0	0	1	0	0
9	0	0	0	1	0	0	0	0	1	0
10	0	0	0	0	1	0	0	0	0	1
11	1	0	0	0	0	1	1	0	0	0
12	0	1	0	0	0	1	0	1	0	0
13	0	0	1	0	0	1	0	0	1	0
14	0	0	0	1	0	1	0	0	0	1
15	0	0	0	0	1	0	1	1	0	0
16	1	0	0	0	0	0	1	0	1	0
17	0	1	0	0	0	0	1	0	0	1
18	0	0	1	0	0	0	0	1	1	0
19	0	0	0	1	0	0	0	1	0	1
20	0	0	0	0	1	0	0	0	1	1
21	1	1	0	0	0	1	1	1	0	0
22	1	0	1	0	0	1	1	0	1	0
23	1	0	0	1	0	1	1	0	0	1
24	1	0	0	0	1	1	0	1	1	0
25	0	1	1	0	0	1	0	1	0	1
26	0	1	0	1	0	1	0	0	1	1
27	0	1	0	0	1	0	1	1	1	0
28	0	0	1	1	0	0	1	1	0	1
29	0	0	1	0	1	0	1	0	1	1
30	0	0	0	1	1	0	0	1	1	1

Figure 1.

Boundary problem ratio of correct item response probability parameters

Note: Plot characters “○” and “△” indicate maximum likelihood estimation (ML) and maximum-a-posteriori estimation (MAP). Solid line and break line mean unconstrained (unconst.) and monotonicity constraints (mono-const.), respectively, in estimation procedures. Colors distinguish attribute correlation conditions.

Figure 2.

Absolute bias of correct item response probability parameters

Note: Plot characters “○” and “△” indicate maximum likelihood estimation (ML) and maximum-a-posteriori estimation (MAP). Solid line and break line indicate unconstrained (unconst.) and monotonicity constraints (mono-const.), respectively, in estimation procedures. Colors distinguish attribute correlation conditions.

Figure 3.

Root mean square error of correct item response probability parameters

Note: Plot characters “○” and “△” indicate maximum likelihood estimation (ML) and maximum-a-posteriori estimation (MAP). Solid line and break line indicate unconstrained (unconst.) and monotonicity constraints (mono-const.), respectively, in estimation procedures. Colors distinguish attribute correlation conditions.

Figure 4.

Absolute bias of standard error estimates of correct item response probability parameters

Note: Plot characters “○” and “△” indicate maximum likelihood estimation (ML) and maximum-a-posteriori estimation (MAP). Solid line and break line indicate unconstrained (unconst.) and monotonicity constraints (mono-const.), respectively, in estimation procedures. Colors distinguish attribute correlation conditions.

Figure 5.

Correct recovery rate of attribute mastery pattern

Note: Plot characters “○” and “△” indicate maximum likelihood estimation (ML) and maximum-a-posteriori estimation (MAP). Solid line and break line indicate unconstrained (unconst.) and monotonicity constraints (mono-const.), respectively, in estimation procedures. Colors distinguish attribute correlation conditions.

Supplemental Material A. Prior distribution of Θ and π

The priors for Θ and π should be specified to derive the MAP algorithm. These priors are set as in Yamaguchi and Okada (2021). The Beta distribution with hyperparameters $a_{jh}^0 > 0$ and $b_{jh}^0 > 0$ is appropriate for the prior for the parameter θ_{jh} because θ_{jh} is a probability parameter and is bounded by zero and one. Thus, for all j and h ,

$$\text{Beta}(a_{jh}^0, b_{jh}^0) = P(\theta_{jh} | a_{jh}^0, b_{jh}^0) \propto \theta_{jh}^{a_{jh}^0 - 1} (1 - \theta_{jh})^{b_{jh}^0 - 1}. \quad (19)$$

In addition, the conditional independence of the parameters is assumed, and the joint distribution of Θ is

$$P(\Theta | \mathbf{A}^0, \mathbf{B}^0) \propto \prod_j \prod_{h=1}^{2^{\sum_k q_{jk}}} \theta_{jh}^{a_{jh}^0 - 1} (1 - \theta_{jh})^{b_{jh}^0 - 1}, \quad (20)$$

where $\mathbf{A}^0$ and $\mathbf{B}^0$ are sets of all hyperparameters a_{jh}^0 and b_{jh}^0 . Furthermore, π is also a probability parameter, but it has more than two elements, so the Dirichlet distribution with parameters $\boldsymbol{\delta}^0 = (\delta_1^0, \dots, \delta_l^0, \dots, \delta_L^0)^\top, \delta_l^0 > 0, \forall l$ is suitable for the prior:

$$P(\pi | \boldsymbol{\delta}^0) \propto \prod_l \pi_l^{\delta_l^0 - 1}. \quad (21)$$

Supplemental Material B. Derivation of maximization step in EM algorithm

The maximization step is derived by using $Q(\Xi|\Xi^{\text{old}})$. The actual functional form of $Q(\Xi|\Xi^{\text{old}})$ is represented as

$$\begin{aligned} Q(\Xi|\Xi^{\text{old}}) = & \sum_j \sum_h^{2^{\sum_k q_{jk}}} \left\{ \left(\sum_i \sum_l g_{jhl} r_{il} x_{ij} + a_{jh}^0 - 1 \right) \log \theta_{jh} \right. \\ & + \left(\sum_i \sum_l g_{jhl} r_{il} (1 - x_{ij}) + b_{jh}^0 - 1 \right) \log(1 - \theta_{jh}) \Big\} \\ & + \sum_l \left(\sum_i r_{il} + \delta_l^0 - 1 \right) \log \pi_l + \text{const.} \end{aligned} \quad (22)$$

To maximize $Q(\Xi|\Xi^{\text{old}})$, the partial differentials with respect to θ_{jh} and π_l are set equal to zero:

$$\frac{\partial Q(\Xi|\Xi^{\text{old}})}{\partial \theta_{jh}} = \frac{\sum_i \sum_l g_{jhl} r_{il} x_{ij} + a_{jh}^0 - 1}{\theta_{jh}} - \frac{\sum_i \sum_l g_{jhl} r_{il} (1 - x_{ij}) + b_{jh}^0 - 1}{1 - \theta_{jh}} = 0. \quad (23)$$

Then, we solve Equation 23 with respect to θ_{jh} and obtain a new correct response parameter:

$$\theta_{jh} = \frac{\sum_i \sum_l g_{jhl} r_{il} x_{ij} + a_{jh}^0 - 1}{\sum_i \sum_l g_{jhl} r_{il} + a_{jh}^0 + b_{jh}^0 - 2}. \quad (24)$$

π is bound by the constraint $\sum_l \pi_l = 1$, and, thus, Lagrange's method of the undetermined multiplier λ is introduced, and the partial differential of π_l is

$$\frac{\partial}{\partial \pi_l} \left\{ Q(\Xi|\Xi^{\text{old}}) + \lambda \left(1 - \sum_l \pi_l \right) \right\} = \frac{\sum_i r_{il} + \delta_l^0 - 1}{\pi_l} - \lambda = 0, \quad (25)$$

and

$$\lambda = I + \sum_l \delta_l^0 - L. \quad (26)$$

Equation 26 is substituted into Equation 25 and solved with respect to π_l ; the new parameter is

$$\pi_l = \frac{\sum_i r_{il} + \delta_l^0 - 1}{I + \sum_l \delta_l^0 - L}. \quad (27)$$

Equations 24 and 27 are employed in the M-step.

Supplemental Material C. Estimation of the Fisher information matrix based on the EM algorithm

To confirm the theoretical analysis of the complete Fisher information matrix, an estimation method for the observed Fisher information matrix using the EM algorithm was derived. The supplemental EM (SEM) algorithm (Cai, 2008; Meng & Rubin, 1991) is a famous method of estimating an observed Fisher information matrix using the EM algorithm. Another easy-to-use method is the first-order Richardson extrapolation of the central difference method (REM; Tian, Cai, Thissen, & Xin, 2013; Jamshidian & Jennrich, 2000). These EM algorithm-based methods can avoid expectations of all possible item response patterns, which exponentially increase the computational cost based on the number of items, to calculate the expected Fisher information. Such EM-based information matrix estimate methods have sometimes been employed in item response theory studies (Cai, 2008). Application to the DCM context has been limited to the DINA model (Yamaguchi, 2019).

We show here an estimation method for $I_{obs}(\Xi^*|\mathbf{X})$ used to gain asymptotic SEs of the parameter estimates, using $I_{comp}(\Xi^*|\mathbf{X})$ and the EM algorithm as an extension of Yamaguchi (2019). Meng and Rubin (1991) showed that the asymptotic variance-covariance matrix of estimated the parameters Ξ^* can be approximated as

$$[I_{obs}(\Xi^*|\mathbf{X})]^{-1} = [I_{comp}(\Xi^*|\mathbf{X})]^{-1} [\mathbf{I}_p - \Delta(\Xi^*)]^{-1}, \quad (28)$$

where $I_{obs}(\Xi^*|\mathbf{X})$ is the information matrix based on the log likelihood of the observed data. In addition, $\mathbf{I}_p$ is the $p \times p$ identity matrix, and $\Delta(\Xi^*)$ is a Jacobian of the EM mapping written as $M(\Xi^*)$. Thus far, the unknown term in Equation 28 is $\Delta(\Xi^*)$. The SEM and REM are types of numerical differential methods to calculate $\Delta(\Xi^*)$ using the EM algorithm. Note that the indicator subscripts in this section are different from those in the previous sections. The element d_{ij} , ($i, j = 1, \dots, p$) of $\Delta(\Xi^*)$ is denoted as

$$d_{ij} = \frac{\partial M_j(\Xi^*)}{\partial \Xi_i}, \quad (29)$$

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where $M_j(\Xi^*)$ is the j th element of the output of the EM map and Ξ_i is the i th element of the parameter vector.

The problem is calculating Equation 29 using the EM algorithm. Let the perturbation of the parameter be $(\xi_1^*, \dots, \xi_{i-1}^*, \xi_i^* + \epsilon, \xi_{i+1}^*, \dots, \xi_p^*) = \Xi^* + \epsilon \mathbf{e}_i$, where ϵ is a small positive number and $\mathbf{e}_i$ is a unit vector whose i th element is one. In REM, an element of d_{ij} is approximated as

$$d_{ij}^*(\epsilon) = \frac{M_j(\Xi^* - 2\epsilon \mathbf{e}_i) - 8M_j(\Xi^* - \epsilon \mathbf{e}_i) + 8M_j(\Xi^* + 2\epsilon \mathbf{e}_i) - M_j(\Xi^* + 2\epsilon \mathbf{e}_i)}{12\epsilon}. \quad (30)$$

Taking the limit of h to zero, the definition of the differential, $d_{ij}^*(\epsilon)$, then becomes

$$\lim_{\epsilon \rightarrow 0} d_{ij}^*(\epsilon) = d_{ij} = \frac{\partial M_j(\Xi^*)}{\partial \Xi_i}. \quad (31)$$

The order of approximation is $O(\epsilon^4)$ (Jamshidian & Jennrich, 2000, p. 260). One EM step can calculate the i th row of $\Delta(\Xi^*)$ at one time. Then, REM requires $4p$ additional EM steps after satisfying convergence. This computational cost gives us $\Delta(\Xi^*)$ without complex algebraic calculations. Finally, the estimated parameters are used to gain the observed data Fisher information matrix $I_{obs}(\Xi^*|\mathbf{X})$.