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Iteration of Partially Specified Target Matrices: Applications in Exploratory and Bayesian Confirmatory Factor Analysis

Tyler M. Moore

Department of Psychiatry, Perelman School of Medicine, University of Pennsylvania

Steven P. Reise

Department of Psychology, University of California, Los Angeles

Sarah Depaoli

Department of Psychology, University of California, Merced

Mark G. Haviland

Department of Psychiatry, Loma Linda University School of Medicine

We describe and evaluate a factor rotation algorithm, iterated target rotation (ITR). Whereas target rotation (Browne, 2001) requires a user to specify a target matrix a priori based on theory or prior research, ITR begins with a standard analytic factor rotation (i.e., an empirically informed target) followed by an iterative search procedure to update the target matrix. In Study 1, Monte Carlo simulations were conducted to evaluate the performance of ITR relative to analytic rotations from the Crawford-Ferguson family with population factor structures varying in complexity. Simulation results: (a) suggested that ITR analyses will be particularly useful when evaluating data with complex structures (i.e., multiple cross-loadings) and (b) showed that the rotation method used to define an initial target matrix did not materially affect the accuracy of the various ITRs. In Study 2, we: (a) demonstrated the application of ITR as a way to determine empirically informed priors in a Bayesian confirmatory factor analysis (BCFA; Muthén & Asparouhov, 2012) of a rater-report alexithymia measure (Haviland, Warren, & Riggs, 2000) and (b) highlighted some of the challenges when specifying empirically based priors and assessing item and overall model fit.

Exploratory factor analysis (EFA) plays a crucial role in scale development and revision (Floyd & Widaman, 1995; Reise, Waller, & Comrey, 2000), theory generation and development (Preacher & MacCallum, 2003), comparison of data structures across populations (Caprara et al., 2000), data reduction (Fabrigar et al., 1999; Ford, MacCallum, & Tait, 1986), and preparation for confirmatory factor analysis (CFA; Gerbing & Hamilton, 1996; Gorsuch, 1997; van Prooijen & van der Kloot, 2001; Thompson, 2004). In all of these applications,

the first step in EFA is to extract m orthogonal dimensions, where m is determined by the researcher. These unrotated dimensions, typically, are not psychologically interpretable, which necessitates rotation of the extracted factors to a more meaningful criterion.

In the present study, we propose, evaluate, and apply an automated iterative version of a rotation technique, iterated target rotation (ITR), originally suggested in Browne (2001). In a partially specified target rotation (Browne, 2001), a researcher must define a target pattern matrix of specified (usually zeros) and unspecified (?) loadings a priori either according to theory or prior data analysis. Although one subsequently can decide whether to modify the target in light of the results, as Browne (2001) noted, no formal mechanisms

Correspondence concerning this article should be addressed to Tyler M. Moore, Ph.D., M.Sc., Department of Psychiatry, Neuropsychiatry Section, Perelman School of Medicine, University of Pennsylvania, 3400 Spruce Street - #1038, Philadelphia, PA 19104. E-mail: tymoore@upenn.edu

for doing so have been evaluated empirically. In ITR, as proposed here, one begins with a standard factor rotation method (e.g., Quartimax), defines a partially specified, empirically informed target matrix based on that rotation, and uses an iterative search procedure to update the target matrix.

ITR is expected to be most useful when data have a complex structure, that is, when commonly used analytic rotations are most problematic. Sass and Schmitt (2010), for example, observed positive bias in factor correlation estimates in data with complex structure using Geomin and Quartimin rotations. Moreover, ITR results can be used to guide the specification of a set of empirically based priors required for Bayesian confirmatory factor analysis (BCFA; Muthén & Asparouhov, 2012; see also Fong & Ho, 2014, for a recent application). In what follows, the logic underlying partially specified target rotations (Browne, 2001) and their iterated counterparts are reviewed after a brief overview of factor rotation. The rotation methods described below are important to review here because subsequently they were used to: (a) suggest an initial target matrix and (b) judge the relative accuracy of ITR versus standard analytic rotation.

Analytic Factor Rotation and Simple Structure

The ultimate goal of factor rotation is to identify interpretable and substantively meaningful dimensions that account for and explain the relationships among test items. Due to the indeterminacy of a factor solution, there are infinite ways to transform an initial factor pattern matrix (Λ) without changing the uniqueness (diagonal elements of Ψ) or the reproduced correlation matrix (Σ). For this reason, the most commonly applied analytic factor rotations aim to meet one or more of the simple structure criteria listed in Thurstone (1947).

As Sass and Schmitt (2010) pointed out in their review of rotation criteria, most researchers mistakenly assume that the only important choice in selecting a criterion is whether it allows factors to correlate (oblique vs. orthogonal rotation). In fact, as Sass and Schmitt demonstrated, the choice of rotation may not be entirely straightforward, because oblique criteria themselves can vary substantially in what they emphasize. Some criteria, for example, attempt to get as close to independent cluster structure (i.e., a pattern where each variable loads saliently on one factor and near zero on any other factor) as possible, whereas others are more likely to identify salient cross-loadings.

Specifically, Sass and Schmitt (2010) described the Crawford-Ferguson (CF) family of factor rotations [(Equation (1))] that vary in how much emphasis the rotation places on minimizing complexity in the variables (rows), as opposed to the factors (columns), depending on the value of a constant (k).

$$f(\Lambda) = (1 - k) \sum_{i=1}^p \sum_{j=1}^m \sum_{l \neq j, l=1}^m \lambda_{ij}^2 \lambda_{il}^2$$

$$+ k \sum_{i=1}^m \sum_{l=1}^p \sum_{j \neq l, j=1}^p \lambda_{ij}^2 \lambda_{lj}^2 \quad (1)$$

Where, p = the number of variables, m = the number of factors, k = the user-defined constant determining how much emphasis the criterion function places on column (vs. row) complexities, λ_{ij} = the factor loading corresponding to the i th variable (row) in the j th factor (column), and Λ = the factor loading matrix.

Quartimin ($k = 0$), for example, maximizes row simplicity and, thus, always will recover a population structure that contains perfect independent cluster structure. At the other extreme, Facparsim ($k = 1$) rotation minimizes the complexity of the factors (columns) and ignores the complexity of the variables (rows). Facparsim is unique among rotation criteria, because it places no emphasis on assigning variables (rows) to factors (columns) and assumes that the factors each account for the same amount of variance (Crawford & Ferguson, 1970). Browne (2001), therefore, considered the Facparsim criterion to be of theoretical interest only. Finally, the Parsimax rotation falls directly between the Quartimin and Facparsim rotations; in Parsimax, the term k is replaced by $(m - 1)/(p + m - 2)$, thus, guaranteeing rows (p) and columns (m) have equal weight.¹ Parsimax was created (Crawford & Ferguson, 1970) for the specific purpose of equalizing the influences of the first and second terms in Equation (1).

Iterated Target Rotation

Target rotations represent an alternative to the CF family of analytic simple structure rotations described above (Browne, 2001). In a target or Procrustes rotation, all elements of a factor loading matrix are specified (i.e., assigned numeric values; typically 1s for salient loadings and 0s otherwise), and then a complexity function is minimized that considers all elements of the loading matrix. Such rotations have a long history in the psychometric literature (Henricksen & White, 1964; McArdle & Cattell, 1994). Over 40 years ago, for example, Guilford and Hoepfner (1971) used target rotations in an attempt to validate the structure of intellect (SOI) model, a landmark study we will comment on in more detail in the discussion.

The idea of rotating to a partially specified target matrix began with Tucker (1944) and was expanded upon by Gruvaeus (1970), Browne, (1972a, 1972b), and ten Berge (1977). In a partially specified target rotation, a researcher needs to specify a pattern of specified loadings (typically zeros for non-salient loadings) and unspecified elements (? indicating that there are no empirical assumptions regarding the value of loadings) a priori based on theory or previous studies. The unspecified elements are ignored when minimizing the complexity function and, thus, have no effect on the rotation [see

¹The reason k does not equal .50 is that the number of rows is not the same as the number of columns; thus, k has to adjust for $m \neq p$ when weighting the sum.

Equation (2) below]. The initially extracted solution then is rotated by minimizing the rotation criterion function in Equation (2), or equivalently, minimizing the difference between the specified elements (typically zeros) of the target matrix and the rotated elements. Specifically,

$$f(L) = \sum_{j=1}^m \sum_{i \in I_j} (\lambda_{ij} - b_{ij})^2 \quad (2)$$

Where, b_{ij} = the element corresponding to the i th row in the j th column in the target matrix;

$f(L)$ = the complexity function that needs to be minimized; m = the number of factors; λ_{ij} = the factor loading corresponding to the i th variable (row) in the j th factor (column); and $i \in I_j$ indicates that only the specified elements (non ?) of the target matrix are used.

Browne (2001, p. 125) originated the idea of iterating partially specified target matrices based on experimenter judgment, suggesting that after an initial target rotation, “The target may be changed . . . This procedure may be repeated until the investigator is satisfied with the outcome.”²

In the present research, we propose two modifications. First, rather than starting with a theoretically chosen, partially specified target pattern, we begin with a standard analytic rotation method from the CF family. Second, using a factor loading cut-off criterion (e.g., rotated loading = .20), a new target matrix is formed by specifying all loadings below the cutoff as specified zeros and all values above the cut-off as non-specified. A new rotation then is performed based on this new target matrix, and the results again are evaluated in regard to the criterion value. When the target matrix does not change between iterations, the process stops.

In Table 1, we provide an example of ITR using a cut-off criterion of .15 in data with a very complex population structure (i.e., many items with nontrivial cross-loadings). In this example, the initial target matrix was purely random and not based on any preliminary analytic rotation. Observe that even using a random starting target matrix, where the probability of being a specified zero was .50, the ITR solution quickly converged to the correct population structure with RMSE of .001. In contrast, Quartimin, Parsimax, and Facparsim did not recover this pattern perfectly and yielded RMSE of .193, .140, and .137, respectively. As illustrated in Table 1, the results of ITR were data-driven, that is, no CF-family complexity function was minimized, and, other than selecting a cut-off criterion, no researcher judgments were made.

In what follows, we conducted two studies to demonstrate the potential utility of ITR. In Study 1, we performed a brief Monte Carlo demonstration to evaluate the feasibility and

potential strengths of the ITR method relative to CF rotations. In Study 2, we demonstrated the role that ITR can play in deriving prior distributions for use in a BCFA (Muthén & Asparouhov, 2012).

STUDY 1: PERFORMANCE OF ITR RELATIVE TO CF ANALYTIC ROTATIONS

The following simulation was designed to explore the relative advantage of ITR over CF rotations as a function of data complexity (i.e., departure from perfect independent cluster structure). Because ITR proceeds through multiple cycles of adaptation to the data, we expected ITR to recover a true population factor pattern better than any single, “one-shot” analytic rotation where k may or may not match the data complexity. The critical question in Study 1, thus, was not whether ITR is “better,” but rather how much better and how ITR performance was affected by data complexity. We also examined the degree to which the starting analytic rotation (i.e., the k value in CF rotations) affected the accuracy of the ITR results. In other words, we asked, does the initial analytic rotation used to suggest the target make any important difference on ITR results?

Simulation Design

The true population factor loading pattern (Λ) was specified to be 20 (items) by 4 (dimensions), and each factor was marked by five items with loadings varying between .50 and .60. The factors were allowed to correlate with the elements of Φ varied uniformly between .10 and .40, changing with every simulation.³

Three conditions were simulated to represent data that varied from mild to severe violations of independent cluster structure. For each factor, two of the five items per factor were specified to have cross-loadings of zero, so that the factors were always identified. Then, for each of the 36 remaining cells with zero loadings (three items by three possible cross-loadings, by four factors), we generated a random number from a uniform distribution ranging from 0 to 1. If that random number was below an a priori determined cut-off, then a loading of .25 was assigned to that cell. The cut-off values were .11 (4/36), .33 (12/36), and .66 (24/36), for Conditions A, B, and C, respectively. These cut-off values produced matrices with the expected number of salient cross-loadings of 4, 12, and 24, respectively.

Once the true population factor pattern matrix was specified, a population correlation matrix (Σ) was generated using the common formula $\Sigma = \Lambda \Phi \Lambda' + \Psi$, and the sim.structure

²Browne’s (2001) suggestion is similar to the hand rotations factor analytic researchers conducted between 1935 and 1970 (for lack of computer programs). One would do an original hand rotation of the unrotated factor matrix, inspect it to see what it looked like, and then engage in another hand rotation to “clean up” the solution or reorient the factors. This would continue until the researcher was satisfied with the result.

³Preliminary results suggested that the strength of the correlations among the factors had little to no influence on the relative abilities of the rotations to approximate the population factor structure *across conditions*, and, thus, they were not evaluated further.

TABLE 1
 Example of Perfect Target Iteration Convergence on a Complex Population Structure, Starting From a Random Target Matrix

Item	Population Structure				Random Target				Target Rotation 0				Target 1			
	F1	F2	F3	F4	F1	F2	F3	F4	F1	F2	F3	F4	F1	F2	F3	F4
1	.50		.40	.30	0	0	0	0	.38		.42	.25	?	0	?	?
2	.50	.40			?	0	0	0	.66		.14		?	?	0	0
3	.50				?	?	0	0	.48	-.20	.14		?	0	?	0
4	.50				0	0	?	0	.48	-.20	.14		?	0	?	0
5	.50		.20	.20	?	?	?	0	.41		.27	.22	?	0	?	?
6		.50		.40	?	?	?	?	.10	.52	-.30	.37	0	?	0	?
7	.20	.50	.40		?	?	?	?	.43	.57	.22	-.23	?	?	?	0
8	.20	.50			0	0	0	0	.42	.35	-.14		?	?	0	0
9		.50		.40	0	?	?	?	.10	.52	-.30	.37	0	?	0	?
10		.50		.30	0	?	0	0	.14	.49	-.27	.25	?	?	0	?
11	.20	.40	.50		?	?	?	?	.38	.54	.35	-.25	?	?	?	0
12	.20		.50	.40	0	?	?	0		.29	.41	.28	0	?	?	?
13		.30	.50	.30	0	?	?	0		.61	.26		0	?	?	0
14			.50		0	0	?	0		.28	.45	-.21	0	?	?	0
15		.40	.50	.20	?	?	0	?	.13	.67	.24		?	?	?	0
16	.30		.40	.50	0	0	0	0	.13	.22	.32	.45	?	?	?	?
17	.30			.50	0	0	0	?	.12			.61	?	0	0	?
18				.50	?	0	?	?	-.16	.11	-.13	.57	0	?	0	?
19			.40	.50	0	?	0	?	-.16	.34	.23	.41	0	?	?	?
20	.30	.30	.30	.50	?	0	0	?	.27	.41	.11	.43	?	?	0	?
Item	Target Rotation 1				Target 2				Target Rotation 2				Target 3			
	F1	F2	F3	F4	F1	F2	F3	F4	F1	F2	F3	F4	F1	F2	F3	F4
1	.47		.34	.32	?	0	?	?	.50		.42	.29	?	0	?	?
2	.53	.39			?	?	0	0	.49	.41			?	?	0	0
3	.51				?	0	0	0	.49				?	0	0	0
4	.51				?	0	0	0	.49				?	0	0	0
5	.49		.14	.24	?	0	?	?	.50		.21	.20	?	0	?	?
6		.55		.33	0	?	0	?		.52		.37	0	?	0	?
7	.21	.55	.39		?	?	?	0	.19	.51	.41		?	?	?	0
8	.23	.50			?	?	0	0	.19	.51			?	?	0	0
9		.55		.33	0	?	0	?		.52		.37	0	?	0	?
10		.54		.23	0	?	0	?		.51		.27	0	?	0	?
11	.20	.46	.49		?	?	?	0	.19	.40	.51		?	?	?	0
12	.16		.47	.37	?	0	?	?	.20		.52	.36	?	0	?	?
13		.39	.49	.20	0	?	?	?		.31	.52	.24	0	?	?	?
14			.52		0	0	?	0			.52		0	0	?	0
15		.49	.50		0	?	?	0		.41	.52	.13	0	?	?	?
16	.26		.35	.49	?	0	?	?	.30		.42	.47	?	0	?	?
17	.28			.54	?	0	0	?	.30			.51	?	0	0	?
18				.50	0	0	0	?				.49	0	0	0	?
19			.38	.46	0	0	?	?			.42	.46	0	0	?	?
20	.28	.37	.24	.46	?	?	?	?	.30	.31	.31	.47	?	?	?	?

Note. Converged solution (Target rotation 3, not shown) is identical to population structure (RMSE < .0001); Population inter-factor correlations (phi) set to .30; loadings with absolute value < .10 omitted; Random target generated such that each element had a 50% binary probability (0,1); Target rotation 0 is based on random target.

command in the *psych* (Revelle, 2012) R library (R Development Core Team, 2012) was used to simulate raw data matrices. For each condition, 1,000 simulated data matrices were created for each of three sample sizes: $N = 250$, $N = 500$, and $N = 1,000$.

For each dataset, maximum likelihood factor extraction was used, and the factanal function in the *stats* library in R performed seven CF rotations: $k = 0$ (Quartimin), $m - 1/(p + m - 2)$ (Parsimax) .20, .40, .60, .80, and 1 (Facparsim). These

seven rotations then formed the basis for specifying a set of specified (0) and unspecified (?) elements for an initial target matrix. That is, each CF rotation (Quartimin, and so forth) was used to create a first target matrix for its own series of iterated targets.

To convert a factor solution to a partially specified target matrix, a threshold value for deciding whether a loading is “substantial” (and, therefore, should not be part of the rotation criterion function) must be specified. Herein, we used a

cut-off value of .10 for all simulations. Thus, if the estimated loading was .10 or greater, it was unspecified (“?”) and if less than .10 it was specified to be zero (“0”). A target rotation then was performed using the comprehensive exploratory factor analysis program (CEFA;⁴Browne, Cudeck, Tateneni, & Mels, 2008), and the resulting solution then was used to create a new target matrix with the same rule as was applied in the previous target creation. Subsequent iterations continued until the target matrix produced was the same as one of the previous target matrices. Such a solution was said to have “converged.” Preliminary simulations suggested that seven iterations was the maximum likely to be useful in the present study, so the *R* program stopped after seven iterations.

Finally, the seven CF rotations and the iterated-target rotation were compared in terms of the RMSE between the true population structure and the estimated structure. To ensure that the RMSEs in the present study were calculated using the same factor order for both the population and exploratory solutions, they were calculated using every possible reordering of the exploratory solution, and then the lowest RMSE was taken to be the one corresponding to the most congruent reordering.

Simulation Results

Although we planned to provide a detailed description of ITR convergence rates, they were so high as to prohibit meaningful analysis. That is, almost all iterated target solutions converged before reaching the maximum iterations, and there were no meaningful patterns (hypothesized or discovered) in convergence rates across conditions. Preliminary analysis suggested, however, that the number of iterations required for convergence increases as sample size becomes small.

Table 2 displays the results of the 63 simulated conditions from above. The table shows the median RMSE of the rotated factor solutions from their corresponding population structures. “Initial” solutions were the CF rotations, and “converged” solutions were the iterated target rotations using the indicated CF rotation as a starting point (first target matrix). Four important summary points can be drawn from Table 2. First, as expected, the ITR method always outperformed the initial CF rotation. Second, and more importantly, although all solutions were worse under the most complex data structure, the relative advantage of ITR over any CF rotation increased as a function of data complexity. Third, the starting rotation had very little influence on the accuracy of the final ITR solution. Finally, more accurate results were obtained using any method as sample size increased.

⁴Rotation to a partially specified target matrix programs also are available in the *R* GPArotation package (Bernaards & Jennrich, 2008); software available from Lorenzo-Seva and Ferrando (2006), and *Mplus* (Muthén & Muthén, 2012).

STUDY 2: APPLICATION OF ITR IN BCFA

In Study 2, we demonstrated the application of ITR as a tool for deriving prior distributions for a BCFA (Muthén & Asparouhov, 2012) of a rater-report alexithymia measure (Haviland, Warren, & Riggs, 2000). Muthén and Asparouhov (2012) presented a flexible method for handling cross-loadings that are theorized to be zero (or very near zero) via the Bayesian estimation framework. Within this framework, cross-loadings hypothesized to be near zero do not need to be fixed exactly to zero, but rather fixed values of zero can be replaced with *approximate* zeros. These approximate zeros are defined through the use of Bayesian prior distributions that are placed on the factor loadings. Typically, in BCFA, a researcher uses theory or prior analyses to define an independent cluster pattern. Then, diffuse priors are specified for the factor loadings for items expected to load on a particular factor; the diffuse priors essentially specify the loadings to be freely estimated. Informative priors, centered at zero and with $\sigma = .10$ to mimic an approximate zero without fixing parameters in the model, are specified for all other cross loadings for items not expected to load onto a factor. Specifying diffuse priors for factor loadings using default settings in programs such as *Mplus* 7.11 (Muthén & Muthén, 1998–2012), however, may not be optimal for some datasets as we show below.

On its face, ITR appears to be an excellent exploratory tool to use in conjunction with BCFA. The results of an ITR can be used to: (a) alert the researcher to items with salient loadings on multiple factors and to adjust the model accordingly (as opposed to fitting the independent cluster structure model and then finding problems in fit post hoc) and (b) suggest empirically informed means and standard deviations for the prior distribution for all elements of the loading and factor intercorrelation matrices.

For our example, we used clinical and people-in-general data ($N = 1,485$) from the Observer Alexithymia Scale (OAS; Haviland, Warren, & Riggs, 2000), a 33-item observer scale that measures expressions of emotion regulation deficits. Items are rated on a 4-point scale ranging from 0 (*never; not at all like the person*) to 3 (*all of the time, completely like the person*). Item content, written in lay terms, is from the California Q-set alexithymia prototype (Haviland & Reise, 1996). Correlated traits modeling suggests a five-factor structure, distant (unskilled in interpersonal matters and relationships), un insightful (lacking good stress tolerance and insight and self-understanding), somatizing (excessive health worries), Humorless (colorless and uninteresting), and rigid (inflexibility and excessive self-control) (Haviland, Warren, & Riggs, 2000), whereas bifactor modeling shows a relatively strong general factor (alexithymia) (Reise, Moore, & Haviland, 2010).

For purposes of simplicity and clarity, we used 19 items (six distant, six un insightful, three humorless, and four rigid). We dropped all somatizing items (the subscale with the

TABLE 2
Median Root Mean Square Error (RMSE) for Each of the Seven Initial Crawford Rotations and Their Converged Iterated-Targets Solutions (threshold = .10) for Three Sample Sizes

Initial Rotation	N = 1000					
	Secondary Loadings = 4		Secondary Loadings = 12		Secondary Loadings = 24	
	Initial	Converged	Initial	Converged	Initial	Converged
k = 0 (Quartimin)	.040	.032	.053	.032	.073	.031
k = .136 (Parsimax)	.040	.032	.045	.032	.053	.031
k = .2	.041	.032	.044	.032	.051	.031
k = .4	.043	.032	.044	.032	.048	.031
k = .6	.043	.032	.044	.032	.046	.031
k = .8	.044	.032	.044	.032	.046	.031
k = 1 (Facparsim)	.044	.032	.045	.032	.045	.031
	N = 500					
	Secondary Loadings = 4		Secondary Loadings = 12		Secondary Loadings = 24	
Initial Rotation	Initial	Converged	Initial	Converged	Initial	Converged
k = 0 (Quartimin)	.053	.048	.064	.046	.079	.047
k = .136 (Parsimax)	.052	.048	.056	.046	.061	.045
k = .2	.052	.048	.055	.046	.059	.044
k = .4	.054	.048	.055	.046	.057	.044
k = .6	.055	.048	.055	.046	.056	.044
k = .8	.055	.048	.055	.046	.055	.044
k = 1 (Facparsim)	.056	.048	.055	.046	.055	.044
	N = 250					
	Secondary Loadings = 4		Secondary Loadings = 12		Secondary Loadings = 24	
Initial Rotation	Initial	Converged	Initial	Converged	Initial	Converged
k = 0 (Quartimin)	.072	.071	.081	.071	.093	.074
k = .136 (Parsimax)	.071	.071	.073	.070	.076	.069
k = .2	.071	.071	.073	.070	.075	.068
k = .4	.073	.071	.073	.070	.073	.068
k = .6	.074	.071	.073	.070	.072	.068
k = .8	.075	.071	.073	.070	.071	.068
k = 1 (Facparsim)	.075	.071	.073	.070	.071	.068

Note. Simulations = 1000; Loadings < .1 were converted to zeros in the target matrix; Loadings > .1 were converted to “?” (unknowns) in the target matrix.

weakest relationships with OAS total and subscale scores as well as with external correlates). We also dropped eight redundant items and the item, “likes to touch or be touched,” the one skipped most often by raters, particularly clinicians. The OAS is an especially good choice for the present examples; the Bayesian approach can account for the demonstrated salient cross-loadings, thus, eliminating the need to parcel (Haviland, Warren, & Riggs, 2000) or to condemn the scale because an item-level analysis fails to meet entirely arbitrary CFA “fit” standards (Meganck, Vanheule, Desmet, & Inslegers, 2010).

ITR of the OAS

The total sample ($N = 1,485$) was randomly split into bins to create exploratory ($N = 1,000$) and confirmatory ($N = 485$) samples. We decided to create an approximate 2/3 split so that the exploratory analyses used to define prior distributions would be as accurate as possible and allow a reasonable sample size for final formal model testing. Table 3 displays the item content for this 19-item, 4-factor version of the

OAS; in theory, Items 1–6 are distant markers, Items 7–12 are un insightful markers, Items 13–15 are humorless markers, and 16–19 are rigid markers. For illustrative purposes, in Table 4, we show the mean- and variance-adjusted weighted least squares (WLSMV in *Mplus*) factor results for the exploratory sample using CF rotations with $k = 0$ (Quartimin), .136 (Parsimax), and 1 (Facparsim), respectively.

Several important findings stand out in this table. First, regardless of rotation, several items have loadings on a dimension other than their theorized dimension (i.e., salient cross-loadings). In fact, at least two items appear to belong *primarily* to a dimension other than their theorized dimension. Experienced researchers will recognize immediately that these cross-loadings would cause problems in “fit” if an independent cluster structure CFA model were to be specified based on prior theory/analyses. Second, although the rotations provided mostly the same substantive message, more salient cross-loadings were derived with the Facparsim solution. Moreover, observe that as k increases, primary loadings tended to be larger, and factors were estimated to be more correlated (see also Sass & Schmitt, 2010, for their

TABLE 3
OAS Subscales and Items: Theoretical Factors With CF Loadings/Secondary Loadings (Facparsim, k = 1)

Factors	
Distant	
1.	<i>Is a warm person</i> (secondary loading on humorless)
2.	<i>Has compassion</i> (secondary loading on humorless)
3.	<i>Is good at relationships</i> (secondary loadings on un insightful and humorless)
4.	<i>Likes to explore his or her feelings</i> (secondary loading on rigid)
5.	<i>Is imaginative; creative</i> (secondary loading with higher loading on humorless)
6.	<i>Likes to have close friends</i> (secondary loadings on humorless and rigid)
Un insightful	
7.	Falls apart when things are really tough
8.	Becomes frustrated in the face of uncertainty
9.	Has strong emotions that he or she cannot explain
10.	<i>Seems to lack a sense of purpose</i> (secondary loading on distant)
11.	<i>Has trouble finding the right words to describe his or her feelings</i> (secondary loadings on distant and rigid)
12.	<i>Understands his or her needs very well</i> (secondary loading with higher loading on distant)
Humorless	
13.	Has a good sense of humor
14.	Is playful
15.	<i>Is colorless; uninteresting</i> (secondary loading with higher loading on rigid)
Rigid	
16.	Is too self-controlled
17.	Is stiff; rigid
18.	Sees things only as black or white
19.	Puts off enjoying the good things in life; even when it is not necessary to do so

Note. Items with secondary loadings in italic type.

TABLE 4
CF Rotations of the 19-Item OAS Using k = 0 (Quartimin), k = .136 (Parsimax), and k = 1 (Facparsim)

Item	k = 0 Quartimin				k = .136 Parsimax				k = 1 Facparsim			
	D	U	H	R	D	U	H	R	D	U	H	R
Factor Loadings												
1	.76				.66		.28		.64		.32	
2	.78				.69		.23		.66		.26	
3	.65	.24			.57	.26			.55	.25	.23	
4	.63				.56				.54			.20
5	.31		.37		.24		.43		.23		.44	
6	.44		.20		.37		.27	.22	.35		.30	.23
7		.82				.80				.79		
8		.71				.69				.68		
9		.62				.60				.59		
10	.35	.46			.31	.46			.31	.45		
11	.26	.39	-.24		.24	.38		.21	.23	.37		.22
12	.44	.32			.39	.33			.37	.32		
13			.78				.82				.82	
14			.68				.73				.73	
15			.26	.37			.32	.38			.34	.40
16				.75				.74				.73
17				.60				.62				.62
18	.21			.53				.55				.55
19				.52				.51				.52
Factor Correlations (phi matrices)												
D	—				—				—			
U	.34	—			.24	—			.21	—		
H	.55	.31	—		.46	.26	—		.42	.20	—	
R	.38	.37	.47	—	.29	.32	.46	—	.26	.29	.42	—

Note. Loadings less than .20 not shown. D is distant, U is un insightful, H is humorless, and R is rigid.

TABLE 5
Initial Target Matrix Based on Theory and Initial Target Rotation Results

Item	D	U	H	R	D	U	H	R
1	?				.77	.05	.14	-.01
2	?				.79	.03	.09	-.06
3	?				.60	.31	.08	-.04
4	?				.63	-.11	-.12	.15
5	?				.35	-.05	.35	.13
6	?				.47	-.04	.18	.18
7		?			-.14	.87	.16	-.10
8		?			-.24	.75	.11	.09
9		?			-.09	.67	-.13	.13
10		?			.26	.52	-.02	-.08
11		?			.16	.44	-.22	.15
12		?			.37	.38	.00	-.04
13			?		.14	.09	.76	.00
14			?		.19	.00	.66	.13
15			?		.18	.13	.26	.35
16				?	-.13	-.05	.08	.76
17				?	.18	.11	.09	.59
18				?	.17	.12	-.10	.53
19				?	-.09	.07	.16	.52

Note. Loadings > = .20 shown in bold. D is distant, U is uninsightful, H is humorless, and R is rigid.

commentary on factor correlation estimation in the CF family of rotation). Of course, these rotations were mathematically equivalent and had the same fit (CFI = .966, RMSEA = .067, and SRMR = .035), but each solution, nevertheless, provided a somewhat different picture of the structure of the OAS.

For the sake of illustration, instead of using one of the CF rotations shown in Table 4 to suggest an initial target matrix, in this application, we started with the theoretical structure that has been described in the literature. Thus, the initial 19 × 4 target matrix placed a ? in the pattern matrix where each item was expected to have its primary loading and 0 everywhere else. Setting the number of factors to 4, an initial unrotated factor pattern was extracted using WLSMV and then rotated using the initial target. The results are shown in Table 5.

We then elected to use a .20 cut-off value for updating the target matrix based on these results. Thus, if the rotated solution had a loading of .20 or above, it was unspecified (i.e., coded as a ? in the target matrix), and below .20 it was a specified zero. The cut-off of .20 was chosen for two reasons: (a) loadings above this value would fall out of the range of the BCFA normal prior with a mean of zero and standard deviation of .10 used for cross-loadings theorized to be zero in continuous data (Muthén & Asparouhov, 2012), and (b) a loading below .20 would not be of sufficient magnitude, in our opinion, to warrant serious consideration as a trait marker or substantively important cross-loading.

Using the .20 cut-off, the new target matrix and subsequent rotated solution are shown in Table 6. Results suggested

TABLE 6
Second-Iteration Target Matrix and Results

Item	D	U	H	R	D	U	H	R
1	?				.76	.07	.14	-.02
2	?				.79	.05	.09	-.07
3	?	?			.64	.31	.07	-.05
4	?				.61	-.09	-.12	.14
5	?		?		.32	-.05	.35	.15
6	?				.44	-.03	.18	.18
7		?			-.03	.84	.14	-.10
8		?			-.15	.71	.10	.10
9		?			-.01	.64	-.15	.13
10	?	?			.33	.51	-.03	-.09
11		?			.22	.43	-.23	.15
12	?	?			.42	.38	.00	-.05
13			?		.11	.08	.77	.03
14			?		.15	-.01	.67	.15
15			?	?	.17	.12	.26	.37
16				?	-.18	-.08	.08	.80
17				?	.16	.08	.09	.62
18				?	.16	.10	-.11	.55
19				?	-.12	.04	.16	.55

Note. Loadings > = .20 shown in bold. D is distant, U is uninsightful, H is humorless, and R is rigid.

that seven elements previously specified as 0 needed to be unspecified (i.e., coded as ?) in the new target. Items 3 and 5 displayed salient cross-loadings on either the uninsightful or humorless factors. Item 15 had a salient cross-loading on rigid. Item 5, in fact, had the same loading on humorless as on its theoretically intended factor. Items 10 and 12 also were identified as having salient cross-loadings on distant. Table 6 displays the updated target matrix and the subsequent results. Observe that results based on this updated target showed one additional cross-loading (Item 11 loaded 0.22 on distant). Finally, Table 7 shows the last iteration. A new target matrix based on these results led to the exact same target as before, and, thus, the solution had converged. The above results, including standard errors of the factor loadings and correlations among the factors, were used in the subsequent BCFA.

Application of BCFA Using ITR Results as Priors

In this section, we first present results from a BCFA with default diffuse (non-informative) priors on the primary and secondary factor loadings, as well as default diffuse priors on the loadings hypothesized to be zero. This model was estimated to assess the effect of default diffuse prior settings on the loading estimates. Next, we present results from a BCFA where informative, or empirically derived, priors are implemented. We found that the former model did not converge and that more informative priors were needed in this modeling context.

The *Mplus* version 7.11 software program (Muthén & Muthén, 1998–2012) was used to implement the Bayesian

TABLE 7
Third-Iteration Target Matrix and Results

Item	D	U	H	R	D	U	H	R
1	?				.77	.06	.14	-.03
2	?				.79	.04	.09	-.08
3	?	?			.66	.30	.07	-.05
4	?				.62	-.10	-.13	.14
5	?		?		.31	-.05	.36	.14
6	?				.44	-.04	.18	.18
7		?			.01	.82	.15	-.09
8		?			-.12	.70	.10	.11
9		?			.04	.62	-.15	.13
10	?	?			.37	.50	-.03	-.09
11	?	?			.26	.41	-.24	.15
12	?	?			.45	.37	-.01	-.05
13			?		.08	.08	.78	.03
14			?		.13	-.01	.68	.15
15			?	?	.17	.11	.26	.37
16				?	-.17	-.08	.08	.79
17				?	.17	.08	.09	.61
18				?	.19	.10	-.12	.54
19				?	-.12	.04	.16	.54

Note. Loadings $> .20$ shown in bold. D is distant, U is uninsightful, H is humorless, and R is rigid.

model estimation. In the Bayesian analyses, the model parameters receiving priors were the factor loadings and the logit thresholds for these polytomous items. The normal distribution, $N(\mu, \sigma^2)$, was used as the prior for all model parameters. Specifically, the hyperparameters μ and σ^2 represent the mean and the variance of the normal prior, respectively.

An initial model was specified for the confirmatory sample ($N = 485$) via the Bayesian estimation framework using default diffuse (i.e., non-informative) priors as implemented in the software program. Each item was allowed to load freely onto each factor, and the default settings for prior distributions were implemented for all primary and secondary factor loadings, as well as loadings hypothesized to be zero. Specifically, the default distributions were as follows: factor loadings for categorical items were distributed $N(0,5)$, categorical item thresholds were distributed $N(0,10^{10})$, factor variances were distributed inverse-Wishart denoted $IW(1,5)$, and factor covariances were distributed $IW(0,5)$. Using this initial model with the default prior settings, we attempted to obtain Markov chain Monte Carlo (MCMC) chain convergence through the following. We estimated the model using the default settings in *Mplus*, which specified 2 MCMC chains and a maximum of 50,000 iterations (with the first half discarded as the unstable, burn-in phase of the chain). We then estimated the model with 100,000 MCMC iterations and 2 chains, with the first 50,000 iterations discarded as the burn-in. Finally, we estimated this model with 100,000 iterations (50,000 as burn-in) and only a single MCMC chain to assess whether between-chain convergence problems were presenting convergence problems. None of these estimation scenarios resulted in convergence.

Given that salient loadings and loadings hypothesized to be zero were estimated freely in this model, the lack of convergence was likely not due to model misspecification (i.e., salient loadings were not fixed to zero in this model). Instead, problems with obtaining convergence may be linked to the use of default diffuse priors. The variance hyperparameter values for the default diffuse priors specified on the factor loadings ($\sigma^2 = 5$), and item thresholds ($\sigma^2 = 10^{10}$) were relatively large. These default diffuse priors may have been improper priors for some of the model parameters, which can make convergence difficult to obtain. These non-convergence results using default diffuse priors presented a compelling case for specifying more informative priors within BCFA.

In an attempt to specify more reasonable and informative priors for the factor loadings, empirically informed (or data-driven) priors were implemented based on ITR results obtained previously.⁵ Perhaps the most common method for specifying a data-driven prior is to use estimates from a previous analysis to drive the hyperparameter values (e.g., see Berger, 2006; Brown, 2008; Candel & Winkens, 2003; van der Linden, 2008). For illustration, we used the WLSMV estimates resulting from ITR (shown in Table 7) to determine the hyperparameter values for each prior specified for these loadings. The WLSMV estimate was used as the mean hyperparameter, and the standard error of the estimate was used as the variance hyperparameter. Typically, the squared value of the standard error of the estimate would be deemed more comparable to the variance hyperparameter. Because these standard errors all were in decimal form below 1.0, however, squaring the value would decrease the hyperparameter variance value, thus, increasing the precision of the prior to an unrealistic (or excessive) degree. In an attempt to use a relatively weakly informative, normal prior where the precision of the prior was not increased to an unreasonable (or excessive) level, the WLSMV standard error of the estimate was directly used as the variance hyperparameter.

For Bayesian estimation, the Gibbs sampling algorithm was used to construct the MCMC chain. The default number of MCMC chains (2) was requested, and 25,000 iterations were requested in the burn-in phase and an additional 25,000 iterations in the post-burn-in phase of the chain (i.e., the posterior distribution).

Chain convergence was monitored by visually examining the MCMC trace (or convergence/history) plots for each model parameter. All model parameters had trace plots that showed tight, horizontal bands, thus, indicating no visual signs of non-convergence within the chains. Also, the Brooks, Gelman, and Rubin convergence diagnostic (Gelman, 1996; Gelman & Rubin, 1992a, 1992b) was examined. Within the *Mplus* software program, this convergence diagnostic creates a ratio of within- and between-chain variation. If this ratio is very near 1.0 (according to a preset bound), then

⁵Informative priors only were specified for the factor loadings to illustrate how ITR results can be used to inform priors for factor loadings. All other parameters were estimated with default diffuse priors as specified above.

TABLE 8
OAS 19 Bayesian Confirmatory Factor Analysis in Which Prior Distributions on Loadings and Cross-Loadings Were Determined by Iterated Target Rotation

Item	Factor Loadings				PPC Confidence Intervals and p Values	
	Distant (F1)	Uninsightful (F2)	Humorless (F3)	Rigid (F4)	95% CI	p Value
1	.70	-.02	.12	.07	-32.3, 35.8	.52
2	.82	.01	-.05	-.06	-31.0, 36.8	.52
3	.63	.18	.04	.08	-25.5, 28.4	.54
4	.64	-.04	-.03	-.01	-20.0, 30.0	.57
5	.37	-.01	.43	-.06	-23.7, 30.7	.51
6	.37	-.04	.22	.18	-26.5, 32.0	.50
7	-.02	.73	.08	-.02	-27.4, 33.9	.54
8	-.04	.57	.06	.09	-24.0, 31.4	.54
9	-.02	.63	-.10	.15	-14.5, 26.2	.56
10	.38	.57	-.06	-.17	-32.5, 39.0	.44
11	.16	.42	-.06	.08	-23.6, 35.2	.54
12	.40	.36	.12	-.05	-26.8, 34.0	.53
13	.17	.09	.65	.05	-27.3, 31.2	.57
14	.09	-.03	.72	.13	-22.2, 25.7	.49
15	.23	.11	.26	.32	-52.5, 45.2	.48
16	-.16	-.09	.04	.82	-22.4, 28.2	.53
17	.11	.13	.10	.62	-30.6, 34.7	.47
18	.34	.06	-.19	.45	-24.3, 28.8	.53
19	-.16	.02	.04	.68	-23.9, 39.9	.61
	Factor Correlations					
	F1	F2	F3	F4		
F1	—					
F2	.30	—				
F3	.65	.28	—			
F4	.49	.40	.55	—		

Note. Significant loadings bolded. CI = confidence interval; PPC = potential parameter change; F = factor.

the 2 MCMC chains are not fluctuating away from one another and the within-chain variation is stable; obtaining these results point toward chain convergence. Convergence was met for the present investigation based on this diagnostic.

Results for the factor loadings are presented in Table 8. The same loading patterns held across the four factors compared to the WLSMV results presented earlier (Tables 4 and 7). Notice, however, that the cross-loadings hypothesized to be zero are all very small and near zero. The model presented in Table 8 illustrates the added flexibility of Bayesian methods in that loadings hypothesized to be zero are allowed to approximate zero rather than be fixed to zero, which is common in traditional approaches.

When fitting a model via the Bayesian estimation framework, a common procedure for assessing model fit is called posterior predictive checking (PPC). Essentially, the PPC technique simulates data based on the proposed model. The fit of the model then is compared across the simulated data and the empirical data. This comparison is carried out through a discrepancy function (typically likelihood-ratio based). If there is a significant difference between the fit of the simulated and the fit of the empirical data, then model fit has not been obtained.

The PPC procedure specifically tests a null hypothesis that the difference between the fit to the simulated and empirical data is zero (i.e., the fit of the model is exactly the same for both data sets). The most interpretable result obtained via PPC is the 95% confidence interval for this measure of discrepancy. In particular, if the confidence interval does *not* contain the value zero, then evidence of model misfit has been obtained. For the technical details of the PPC procedure, see Berkhof, Mechelen, and Gelman (2003), Gelman (2003), or Stern and Cressie (2000).

The item-level fit results obtained via PPC are presented in Table 8. The 95% confidence intervals for the 19 items all contained the null value; the respective nonsignificant posterior predictive *p* values also are presented. These results showed that there was no evidence for model misfit at the item level.

DISCUSSION

Factor rotation to a partially specified matrix (Browne, 2001) falls between analytic rotations (i.e., no specified elements, and the rotation emphasizes one or more rules of simple

structure criteria) and Procrustes rotation (i.e., a fully specified target matrix). In a partially specified target rotation, the researcher identifies a subset of loadings that are expected to be near zero and leaves the other loadings free to be any value. The rotation criterion function involves minimizing only the differences between the specified elements of the target matrix and the final solution and, therefore, only the specified elements control the factor rotation.

Specified elements can be selected based on theory,⁶ previous factor analytic results, or as shown Study 1, an ordinary CF analytic rotation. Regardless, the target rotation results can be used to suggest a new target matrix, and additional target rotations may be performed in an iterated fashion. Browne (2001) suggested that ITR can be viewed as the interplay between the researcher and the data. We suggested automating the procedure by selecting a cut-off value. Admittedly, the selection of this cut-off is arbitrary; if a selected cut-off value is low (e.g., .05) there may be too few specified elements to identify the factors and define a meaningful solution. If set too high (e.g., .40), then many smaller but potentially salient loadings may be misspecified, which ultimately may distort the factor rotation. In our exploratory analyses of the OAS, we selected a cut-off of .20 to be consistent with the variance of the prior distribution for hypothesized zero loadings in BCFA as implemented in *Mplus*. In other research contexts, the determination of a cut-off value in ITR, clearly, is in need of further study. At this point, we suggest that researchers try multiple values (e.g., .30, .20, and .10) and explore the consistency of results.

In this article, we suggested and demonstrated two important roles for ITR. The first potential application of ITR is as an alternative or complement to analytic rotations in EFA (see also Asparouhov & Muthén, 2009, for application of target rotation in exploratory structural equation modeling). In Study 1, our Monte Carlo comparison of analytic rotations versus ITR in data that varied in factor complexity suggested that the ITR method holds promise for exploratory factor rotation. It appears to be reliable (very high convergence rates) and accurate (low RMSE) even when faced with data drawn from highly complex population structures.

Although the scope of our Monte Carlo investigation was limited, especially in terms of our ability to study systematically the recovery of factor correlations as in Sass and Schmitt (2010), we were able to draw several clear conclusions. As expected, ITR was “better” than any CF rotation, and its superiority improved as the structure became more complex. These results are not surprising given the somewhat unfair nature of the comparison; CF rotations are a single-shot procedure with a fixed criterion (k), whereas

ITR are, in a sense, self-correcting. Moreover, the starting point—the rotation method used to determine the initial target matrix—made little difference. Finally, sample size influenced the results; larger sample sizes yielded more accurate results for all procedures (for further commentary on sample size in exploratory factor analysis see Hogarty, Hines, Kromrey, Ferron, & Mumford, 2005, and MacCallum, Widaman, Zhang, & Hong, 1999).

We also believe that a second important application of ITR occurs in BCFA. BCFA requires the specification of prior distributions, and default values are provided in programs such as *Mplus*. These defaults (e.g., 10^{10} for the variance of factor loadings for continuous items, or 5 for the variance of factor loadings for categorical items) may not be appropriate for any particular dataset, and this issue of how to properly specify priors for primary loadings, secondary cross-loadings, and near zero cross-loadings under a variety of data conditions (sample size, degrees of communality) clearly needs more research.

In the Study 2 analyses of the OAS, ITR appeared to be useful in two important ways. First, it can be used to identify items that have salient loadings on more than one factor. Second, the results of the ITR can be used to suggest empirically informed priors. We used an ITR with a .20 criterion and found seven (of 19) items with salient loadings on more than one factor. When we ran *Mplus* using default priors to evaluate this structure, we did not obtain a converged solution for any of 3 different MCMC settings, but when we ran *Mplus* using empirically informed priors, we obtained a well-fitting solution. This suggests that more work on specifying priors and the evaluation of fit in BCFA is a worthwhile investment. For now, we suggest that researchers consider the use of empirically based priors, especially in situations like the present data where the sample is large enough to divide into exploratory and confirmatory parts.

Summary

In EFA, researchers have a myriad of analytic rotation options; many yield equivalent solutions but may present different ways of understanding the data structure. Rotations from the CF family, for example, vary only in their emphasis on different simple structure criteria by weighting rows and columns differentially [(Equation (1))]. Sass and Schmitt (2010), thus, suggested inspecting the results of multiple rotations, such that the researcher can decide which is “best.” Here, we add yet another approach for deciding on an optimal rotated solution by describing and applying an ITR methodology. ITR, in contrast to CF rotation, does not attempt to simplify rows or columns of a rotated factor matrix but rather seeks to find all salient loadings, where salient is defined by the researcher. On the other hand, Sass and Schmitt (2010) noted that the phenomenon of “factor collapse” is thought to be extremely rare in CF rotations. Whether this

⁶We note that if there is an a priori theory regarding a scale’s structure, target rotation—relative to any analytic rotation—provides the “fairest” exploratory evaluation of that structural theory; if the target rotation results are not consistent with the a priori theory, no other CF rotation method will be either.

is true for ITR under a variety of scenarios remains to be demonstrated.

In CFA contexts, Asparouhov and Muthén (2009) demonstrated the use of Geomin and Target rotations in exploratory structural equation modeling (see also, Marsh et al., 2009). We see no reason why an ITR cannot serve a similar role, given that it appears to be well suited for data with a complex structure where items may have meaningful loadings on more than one factor. In fact, ITR may be most useful in exactly the data analytic contexts where exploratory structural equation modeling is most needed. Finally, ITR also is consistent with the practice of identifying potential modeling problems prior to fitting more restricted models and then conducting post hoc modifications (Browne, 2001). On the other hand, ITR changes the rotation method to be more and more consistent with the data with each iteration, based on a benchmark value for the loadings. It, therefore, also runs the risk of capitalizing on chance in terms of what elements are specified and non-specified.

Despite our relatively clear and encouraging results, we must warn against the possible misuse of iterated target rotations for corroborating theories of factor structure. In the introduction, we cited Guilford and Hoepfer (1971) as early users of an iterated target rotation approach. Specifically, these researchers used a series of target rotations to attempt to validate the SOI model. The iterated part of their procedure was to update a target so that the resulting factors would conform more closely to predictions from SOI theory. (Note: they used what now would be considered to be very odd target matrices, such as factors with only one or two indicators, orthogonal factors, and in one study, an additional “wastebasket” factor.) They then advanced the argument that their procedure produced pattern matrices highly consistent with SOI theory.

Horn and Knapp (1973, 1974), however, showed that, by using iterated target rotations, they could validate pattern matrices produced by even randomly generated theories. Clearly, the Guilford and Hoepfer (1971) rotations did not provide strong, unequivocal evidence for SOI theory, which, as Horn and Knapp stated, is not to say that SOI theory is wrong, but rather it was not convincingly supported by this rotation technique. In short, Horn and Knapp demonstrated that iterated target rotations can be used to find almost anything, if not conducted properly. We believe that ITR, as suggested in the present article, does not suffer from the same problems as the Guilford and Hoepfer approach because: (a) we begin with results from an analytic rotation to define the initial target (not a theory of structure), and (b) our iterations are based on an empirical criterion (not a subjective one). The superiority of ITR compared to other CF rotations, however, as well as the benefits of deriving priors for BCFA from ITR results, should be studied further so that we can better realize the potential of these approaches.

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