



Incorporating Machine Learning Into Factor Mixture Modeling: Identification of Covariate Interactions to Explain Population Heterogeneity

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Methodology, 2023, Vol. 19(3), 303–322, <https://doi.org/10.5964/meth.9487>

Received: 2022-05-16 • **Accepted:** 2023-06-12 • **Published (VoR):** 2023-09-29

Handling Editor: Katrijn Van Deun, Tilburg University, Tilburg, The Netherlands

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Abstract

Factor mixture modeling (FMM) has been widely adopted in health and behavioral sciences to examine unobserved population heterogeneity. Covariates are often included in FMM as predictors of the latent class membership via multinomial logistic regression to help understand the formation and characterization of population heterogeneity. However, interaction effects among covariates have received considerably less attention, which might be attributable to the fact that interaction effects cannot be identified in a straightforward fashion. This study demonstrated the utility of structural equation model or SEM trees as an exploratory method to automatically search for covariate interactions that might explain heterogeneity in FMM. That is, following FMM analyses, SEM trees are conducted to identify covariate interactions. Next, latent class membership is regressed on the covariate interactions as well as all main effects of covariates. This approach was demonstrated using the Traumatic Brain Injury Model System National Database.

Keywords

factor mixture model, latent class, machine learning, structural equation model trees, covariate, interaction

- 1 Factor mixture modeling (FMM) has been increasingly used in social, behavioral, and
- 2 health sciences to examine unobserved population heterogeneity. It enables researchers
- 3 to model both dimension and typology simultaneously by integrating common factor
- 4 model and latent class analysis. such that latent classes (i.e., unobserved subgroups)
- 5 would emerge to capture differences in the common factor model. Latent classes that



6 encapsulate differences in the common factor model among individuals would emerge
7 from the FMM analyses. FMM has been applied with behavioral and health outcomes
8 to examine heterogeneity among psychological trauma victims based on posttraumatic
9 stress disorder symptoms (Elhai et al., 2011), breast cancer patients that reported fatigue
10 symptoms (Ho et al., 2014), and patients with eating disorders based on their emotion
11 regulation profiles (Nordgren et al., 2022), just to list a few.

12 Among FMM application, covariates (e.g., gender, race) play a critical role in FMM as
13 they are essential to understanding the formation and characterization of latent classes.
14 Specifically, covariates serve as the predictors of latent class membership via multinomial
15 logistic regression in which the log odds of the probability of belonging to a certain
16 class as opposed to a reference class are predicted by covariates. For example, Elhai et
17 al. (2011) found that patients that experienced more traumas and female patients were
18 more likely to be in a more severely symptomatic class as compared with the least
19 symptomatic class.

20 Despite the prevalence of covariate inclusion, interaction effects among covariates
21 have received considerably less attention. In the context of FMM, covariate interaction
22 refers to the interplay between covariates in affecting latent class membership. In oth-
23 er words, the relationship between latent class membership and one covariate might
24 depend on one or more other covariates. Take children's executive function skills as
25 a hypothetical example. From a developmental perspective, older children have more
26 developed executive function skills compared to their younger counterparts and thus are
27 more likely to be classified into a high executive function class versus a low executive
28 function class. However, this gap in classification between age groups might be smaller
29 for children with severe traumatic brain injuries (TBIs) as executive function skills of
30 both age groups would be negatively affected by the injuries. Therefore, examining
31 covariate interaction effects on latent class membership can offer us a more accurate
32 and nuanced understanding of population heterogeneity, as it is often the complex
33 and multifaceted interplay among factors that impact the outcome. In addition, the
34 identification of covariate interactions can guide the development and implementation
35 of tailored intervention programs that can improve individual outcomes more effectively.
36 For instance, an intervention program to improve the executive function of children
37 with TBIs can leverage the age by TBI severity interaction and tailor its design and/or
38 implementation accordingly.

39 Although it is critical to identify covariate interactions, they have not been consid-
40 ered or tested in substantive research based on a non-exhaustive review of fifty-nine
41 FMM applications we conducted. Such lack of investigation into covariate interactions
42 in FMM stands in stark contrast to the common testing of interaction effects in other
43 statistical models (e.g., regression) across applied research (Babikian et al., 2011; Ware
44 et al., 2020; Yeates et al., 2010). The lack of attention on covariate interactions in FMM
45 might be attributable to the fact that interaction effects cannot be identified in a straight-

46 forward fashion. That is, a major source of covariate selection has been theories or
 47 substantive knowledge of researchers; however, it can be a challenging task for applied
 48 researchers to come up with hypotheses regarding potential covariate interactions given
 49 the unobserved nature of heterogeneity in FMM (Brandmaier et al., 2013; Jacobucci et
 50 al., 2017). On the other hand, if an exploratory approach is taken to test all possible in-
 51 teractions, the number of interactions (including higher-order interactions) will increase
 52 exponentially as the number of covariates increases, which leads to a complicated model
 53 that is difficult to fit and interpret (Moons et al., 2015).

54 To address this gap in the literature, this study demonstrates the utility of a machine
 55 learning approach to identifying covariate interactions that might potentially explain
 56 the heterogeneity identified by FMM. Specifically, this study adopted the structural
 57 equation model or SEM trees which was proposed by Brandmaier et al. (2013) as a
 58 model-based decision tree approach to finding covariates and covariate interactions
 59 that impact parameter estimates of the specified model. SEM trees, as other decision
 60 tree approaches, have the capacity of automatically searching for covariate interactions
 61 (Arnold et al., 2021; Jacobucci et al., 2017). Leveraging this capacity, this study presents
 62 a novel integration of SEM trees into FMM for the purpose of identifying potential
 63 covariate interactions that explain latent class membership in FMM. This approach
 64 was demonstrated using the Traumatic Brain Injury Model System National Database
 65 (TBIMS-NDB April 2020 version), the country's largest multi-center database tracking
 66 the rehabilitation trajectories for individuals at least 16 years old treated for inpatient
 67 TBI rehabilitation. Through this demonstration, this study aims to provide an
 68 exploratory tool for FMM users to identify potential covariate interactions, which offers
 69 a more nuanced and sophisticated interpretation of heterogeneity and furthers the
 70 understanding of intersectionality.

71 Factor Mixture Modeling

72 Factor mixture modeling (FMM) is a combination of common factor model and latent
 73 class analysis (LCA), allowing us to model unobserved heterogeneity in parameters of
 74 the common factor model. The common factor model can be written as:

$$Y_{ik} = \tau_k + \Lambda_k \eta_{ik} + \varepsilon_{ik}. \quad (1)$$

75 Y_{ik} is a $\mathcal{J} \times 1$ vector of responses for an individual i that is assigned to class k ($k = 1, 2,$
 76 \dots, K), with \mathcal{J} denoting the number of items; τ_k is a $\mathcal{J} \times 1$ vector of item intercepts; Λ_k
 77 is a $\mathcal{J} \times R$ matrix of factor loadings and R refers to the number of factors; η_{ik} is a $R \times$
 78 1 vector of factor scores; and ε_{ik} a $\mathcal{J} \times 1$ vector of item residuals that are assumed to be
 79 normally distributed with a mean of zero and variance of Θ_k . According to Equation (1),
 80 item response is a function of intercepts, factor loadings, factor scores, and residuals, as

81 in a typical common factor model. However, the subscript k associated with the model
 82 parameters indicates that they are allowed to vary across latent classes except some
 83 constraints needed for model identification. That is, a commonly used identification
 84 strategy is to fix the first item loading to be one across classes and the factor mean of
 85 the last class is fixed to be zero. Factor scores are assumed to be normally distributed
 86 with α_k representing the vector of factor means and Ψ_k the covariance matrix of factors.
 87 Thus, the class-specific mean vectors and class-specific variance-covariance matrices can
 88 be expressed as:

$$\mu_k = \tau_k + \Lambda_k \alpha_k, \quad (2)$$

$$\Sigma_k = \Lambda_k \Psi_k \Lambda_k' + \Theta_k. \quad (3)$$

89 In FMM, the number of classes is often unknown a priori and needs to be determined
 90 by fitting models with varying numbers of classes and comparing model fit using infor-
 91 mation criteria (ICs), including Akaike information criterion (AIC; Akaike, 1974), Baye-
 92 sian information criterion (BIC; Schwarz, 1978), and sample size adjusted BIC (saBIC;
 93 Sclove, 1987). In addition to evaluating model fit, these ICs penalize model complexity
 94 by accounting for the number of parameters. Smaller IC values indicate a better trade-off
 95 between model fit and model complexity. Additionally, likelihood-based tests can be
 96 used in model selection, such as the Lo–Mendell–Rubin test (LMR; Lo et al., 2001), the
 97 adjusted LMR (aLMR; Lo et al., 2001), and the bootstrap likelihood ratio test (BLRT;
 98 McLachlan & Peel, 2000). These tests compare the fit of models with k and $(k-1)$ classes
 99 and a significant test result (e.g., $p < .05$) support the k classes over the $(k-1)$ classes.

100 In addition to the number of classes, measurement invariance (MI) is an important
 101 assumption of valid factor mean comparison across classes that needs to be tested (Clark
 102 et al., 2013; Kim et al., 2017; Lubke & Muthén, 2005; Wang et al., 2021). Models with
 103 different levels of equality constraints on measurement parameters can be constructed
 104 and compared, including configural invariance which requires the same factor structure
 105 across classes but factor loadings and intercepts are freely estimated, metric invariance
 106 that imposes the equality constraints on factor loadings across classes, and scalar invari-
 107 ance which adds additional equality constraints on intercepts. Note that scalar invariance
 108 is often considered as a sufficient prerequisite to factor mean comparison in FMM and
 109 multiple-group analyses (Lubke & Muthén, 2005; Meredith, 1993). Beyond MI testing on
 110 measurement parameters, the equality of other model parameters (i.e., residual variances,
 111 factor variances and covariances) across classes can also be tested to facilitate the under-
 112 standing and interpretation of latent classes and their differences (Clark et al., 2013).

113 Structural Equation Model (SEM) Trees

114 SEM trees integrate SEM into a model-based decision tree paradigm in which the data
 115 set is recursively partitioned into subsets based on the splitting of covariates so that
 116 differences in SEM parameter estimates are maximized across subsets (Brandmaier et
 117 al., 2013; Jacobucci et al., 2017). SEM trees are useful when researchers are interested in
 118 finding the influence of covariates and covariate interactions on the SEM model. SEM is
 119 a family of statistical procedures that has been widely adopted in social and behavioral
 120 sciences to model the relationships among multiple variables (Kline, 2015). One of the
 121 key features of SEM is its capacity to model latent constructs (or factors) that are meas-
 122 ured by a set of items (or observed variables) and take into account measurement errors.
 123 Examples of commonly used SEM procedures include path analysis, the common factor
 124 model, structural equation modeling (relationships among multiple factors), and latent
 125 growth curve models. Built on the SEM model, SEM trees serve as a tool for exploratory
 126 discovery of influences and interactions of covariates on SEM model parameters via the
 127 decision tree paradigm.

128 The decision tree is a supervised machine learning algorithm for prediction and
 129 classification (Gupta, 2014; Song & Lu, 2015). It grows a tree structure via recursive
 130 partitioning of the covariate space so that individuals classified into the same subset are
 131 relatively homogenous in terms of the outcome variable. Figure 1 presents an illustrative
 132 example of a scatterplot of a binary outcome variable, diagnosis of the Alzheimer's
 133 disease (triangles for Alzheimer's and squares for non-Alzheimer's) on the left and the
 134 resultant tree structure on the right, using age and education level as the covariates. The
 135 tree structure can be interpreted as a set of "if-then" statements. For instance, if age \leq
 136 65 and education level \leq 2, the predicted outcome is Alzheimer's diagnosis. The splitting
 137 of the data set can occur based on multiple criteria and the figure demonstrates a simple
 138 rule that constructs a decision tree with a minimal misclassification rate which is also
 139 referred to as an incorrect prediction rate (Gupta, 2014).

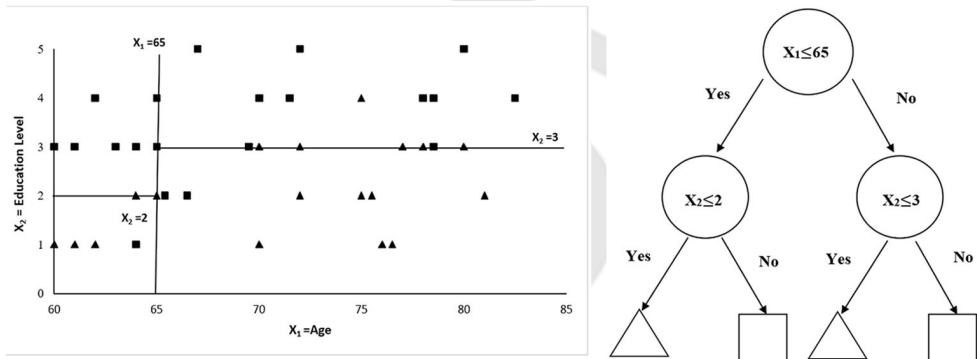
140 Algorithms

141 Integrating features of SEM and decision tree, Brandmaier et al. (2013) proposed SEM
 142 trees to partition the data set with respect to covariates to maximize difference in
 143 SEM parameters across subsets. SEM trees are performed in three steps. First, define a
 144 template SEM which is referred to as M , and fit M to the data set. The following equation
 145 shows the minimization of a fit function with q degrees of freedom via maximum
 146 likelihood estimation (Arnold et al., 2021):

$$\begin{aligned}
 &F_{ML}[\bar{Y}, S, \mu(\theta), \Sigma(\theta)] \\
 &= [\bar{Y} - \mu(\theta)]^T \Sigma(\theta)^{-1} [\bar{Y} - \mu(\theta)] + \text{tr}[S \Sigma(\theta)^{-1}] - \ln\{\det[S \Sigma(\theta)^{-1}]\} - p
 \end{aligned}
 \tag{4}$$

Figure 1

Example of Decision Tree



147 In this equation, \bar{Y} is a vector of observed means; S is the observed covariance matrix;
 148 p indicates the number of observed variables in SEM; θ is a vector of model parameter
 149 estimates; $\Sigma(\theta)$ is the model-implied covariance matrix; and $\mu(\theta)$ is a vector of model-
 150 implied means.

151 Second, to evaluate a possible split based on a covariate, the full data is partitioned
 152 into l subsets where $l = 1, 2, \dots, L$, and the template SEM model is fitted to each
 153 subset. Given that the subsets are non-overlapping, the fit of all SEMs across subsets is
 154 evaluated independently based on Equation (4) and these models are referred to as M_{SUB} .
 155 Then the fit of M_{SUB} and M is compared using the likelihood ratio test:

$$LR = (N - 1) \left\{ F_{ML}[\bar{Y}_F, S_F, \mu(\hat{\theta}_F), \Sigma(\hat{\theta}_F)] - \sum_{l=1}^L \frac{n_l}{N} F_{ML}[\bar{Y}_l, S_l, \mu(\hat{\theta}_l), \Sigma(\hat{\theta}_l)] \right\} \quad (5)$$

156 N and n_l refer to the sample size for the full data set and the subset l . LR follows the
 157 chi-square distribution with $(L - 1)q$ degrees of freedom. All possible splits are evaluated
 158 for each covariate, and the split with maximum increase in the LR is chosen.

159 Lastly, repeat the steps for each subset due to the chosen split to find further parti-
 160 tions that significantly improve the model fit; if the partition does not improve the model
 161 fit, then further partitioning is terminated. Results of SEM trees can be visualized as a
 162 tree structure with nodes. The inner node (i.e., node that has successors) represents a
 163 cut point with respect to a covariate, and leaf nodes are associated with an SEM that
 164 represents the induced subsamples of the data (Brandmaier et al., 2013).

165 **Model Constraints**

166 Similar to FMM, constraints on SEM model parameters can be imposed in SEM trees.
167 Specifically, there are two types of restrictions in a tree: a global restriction and a local
168 restriction. A global restriction can be imposed on any parameter(s) in the SEM model
169 in which the value for the constrained parameter is estimated with the full data set
170 and fixed across all subsequent models. A local restriction is imposed only for split
171 evaluation such that the parameters are equal across all models that share the same inner
172 node, but the resultant leaf nodes can have different values of the parameters. In other
173 words, parameters are allowed to be different across models, but their differences do not
174 contribute to the split evaluation.

175 **Integrating SEM Trees Into FMM**

176 Among a few applications of SEM trees that have been identified (Ammerman et al.,
177 2019; de Mooij et al., 2018; Li et al., 2021; Sagan & Łapczyński, 2020), interaction among
178 covariates was present. For instance, Li et al. (2021) included a total of 33 covariates
179 to examine their associations with students' attitudes towards collaboration, and found
180 that student gender affected the CFA model parameters of students' attitudes towards
181 collaboration, but only for those with above-average home educational resources, which
182 indicated an interaction effect between gender and home educational resources. Given
183 the advantage of SEM trees in automatically searching for covariate interactions, this
184 study proposes an integrated use of SEM trees and FMM such that covariate interactions
185 that are identified by SEM trees might potentially explain heterogeneity in FMM.

186 The proposed integrated use consists of the following five steps:

- 187 1. Identify constructs and items for the FMM analyses, as well as covariates that might
188 potentially explain the distinction among latent classes. Constructs refer to the
189 latent factors that are measured by a set of items, which is the basis of FMM analyses
190 as shown in Equation (1).
- 191 2. Conduct unconditional FMM analyses (without covariates) based on the identified
192 constructs and items. Specifically, given that the number of classes and the class-
193 varying parameters are unknown, a series of FMMs can be specified and fitted to the
194 data, including 1-class, 2-class configural, metric, and scalar invariance models, 3-
195 class configural, metric, and scalar invariance models, etc. The fitted models can be
196 compared in terms of fit based on multiple ICs, such as AIC, BIC, and saBIC¹. Model
197 with the smallest ICs can be chosen as the best-fitting model.

1) LMR, aLMR, and BLRT were not used because they are appropriate for determining the number of classes; however, compared models in the analysis involves different class-varying parameters in addition to the number of classes. Thus, the likelihood-based tests were not appropriate.

- 198 3. Examine the substantive interpretability of the best-fitting model based on
199 parameter estimates.
- 200 4. Conduct SEM trees analyses to identify covariate interactions that could potentially
201 explain latent class membership in FMM. To maximize the chance that covariate
202 interactions selected by the SEM trees would explain latent class membership in
203 FMM, we propose that the specification of parameter restrictions between these two
204 approaches should be matched. That is, the level of invariance (i.e., configural,
205 metric, or scalar) that is identified in FMM is also adopted in SEM trees via the global
206 constraint function.
- 207 5. Multinomial logistic regression is conducted with covariate interactions that are
208 detected by the SEM trees as well as all main effects to examine correlates of latent
209 classes. The three-step approach to covariate inclusion is adopted here, given that
210 the identification of latent classes is done without the influence of covariates, and
211 the impact of covariates and covariate interactions is examined while taking into
212 account classification errors (Asparouhov & Muthén, 2014; Vermunt, 2010).

213

Demonstration

214 This demonstration serves as example of the integrated use of FMM and SEM trees
215 via the five steps proposed above. The sample came from the [Traumatic Brain Injury](#)
216 [Model System National Database \(TBIMS-NDB\)](#) obtained as public datasets with version
217 date of April 2020. TBIMS-NDB was funded by the National Institute on Disability, Inde-
218 pendent Living, and Rehabilitation Research (NIDILRR) as a prospective, longitudinal,
219 multicenter database to examine the health outcomes of more than 17,000 individuals
220 who experienced TBIs that require inpatient rehabilitation in the United States. All data
221 were collected using surveys, with baseline data collected at the time of discharge from
222 inpatient rehabilitation settings and follow-up data collected at 1-, 2-, 5-, 10-, 15-, 20-,
223 25-, and 30-years post-injury. This demonstration used the 1-year post-injury data that
224 consisted of 9,741 individuals. A full description of the sociodemographic characteristics
225 of the sample as well as other descriptive statistics of the variables is provided in [Table 1](#).
226 Annotated codes for the following analyses are included in the electronic [Supplementary](#)
227 [Materials](#).

228 For Step 1, the 5-item Satisfaction with Life Scale (SWLS) was used as the outcome as-
229 sessment for life satisfaction levels among individuals following TBI (Diener et al., 1985;
230 Pavot & Diener, 1993). Each item scored from 1 (lowest life satisfaction) to 7 (highest life
231 satisfaction) asking different aspects of a patient's perception of his/her life conditions.
232 A total of seven covariates were identified, including Functional Independence Measure
233 (FIM) Cognitive on Admission (Linacre et al., 1994), pre-injury disability and pre-injury
234 limitations (National Research Council, 2004), TBI severity (Teasdale & Jennett, 1976) as
235 measured by patients' total Glasgow Coma Scores, age at injury, biological sex, race,

Table 1*Descriptive Statistics of Variables and Sample Sociodemographic Characteristics*

Variable/Characteristic	Statistic		
Life Satisfaction	N	M	SD
1. Ideal life	9717	4.06	2.08
2. Excellent life conditions	9728	4.06	2.08
3. Satisfaction with life	9729	4.60	2.05
4. Important things in life	9723	4.71	1.99
5. Life lived over	9709	3.84	2.22
Continuous Covariates	N	M	SD
TBI severity	5529	11.21	4.06
FIM Cognition	9695	16.03	7.58
Categorical Covariates	N	%	
Sex			
Females	2751	28.25	
Males	6988	71.75	
Race			
White	6897	70.82	
Black	1596	16.39	
Hispanic	849	8.72	
Others	397	4.08	
Age Group			
AYAs	2994	30.74	
Adults	5108	52.44	
Older Adults	1639	16.83	
Pre-Injury Employment Status			
Employed	6389	66.12	
Student	706	7.31	
Unemployed	2568	26.58	
Pre-Injury Impairment			
Yes	368	5.49	
No	6333	94.51	
Pre-Injury Physical Limitation			
Yes	491	7.33	
No	6206	92.67	

Note. Ideal life = In most ways my life is close to my ideal; Excellent life conditions = The conditions of my life are excellent; Satisfaction with life = I am satisfied with my life; Important things in life = I have gotten important things I want in life; Life lived over = If I could live my life over, I would change almost nothing. AYAs = adolescents and young adults.

236 and pre-injury employment status. All covariates were collected at baseline visit. Age at

237 injury was recoded as a categorical variable: adolescents and young adults (AYAs; ≤ 25),
 238 adults (26–59), and older adults or seniors (≥ 60).

239 For Step 2, unconditional FMM analyses were conducted with life satisfaction in
 240 *Mplus* 8.4² (Muthén & Muthén, 1998–2017). Table 2 presents model fit comparisons of
 241 FMMs. All fitted models converged except the 4-class configural and scalar models.
 242 Among converged models, AIC, BIC, and saBIC consistently showed that the 4-class
 243 metric model had a superior fit.

244 **Table 2**

245 *Model Fit Comparison of Factor Mixture Modeling*

Model	Parm	LL	AIC	BIC	saBIC	Entropy	Class Proportions
1-class	15	-94483	188996	189104	189056		
2-class conf	31	-88689	177440	177663	177565	.90	.72/.28
2-class metric	27	-88795	177644	177838	177753	.90	.73/.27
2-class scalar	18	-93401	186838	186967	186910	.92	.38/.62
3-class conf	47	-85263	170619	170957	170807	.91	.14/.58/.28
3-class metric	39	-85345	170769	171049	170925	.91	.14/.58/.28
3-class scalar	21	-93411	186863	187014	186947	.65	.40/.39/.21
4-class conf				Non-convergence			
4-class metric	51	-84430	168961	169328	169166	.87	.14/.25/.33/.28
4-class scalar				Non-convergence			

246 *Note.* conf = configural invariance; metric = metric invariance; scalar = scalar invariance; Parm = number of
 247 free parameters; LL = log-likelihood; AIC = Akaike information criterion; BIC = Bayesian information criterion;
 248 saBIC = sample size adjusted BIC.

249 For Step 3, interpretability of the 4-class metric model was examined. Table 3 presents
 250 the parameter estimates of this model by latent class. While loadings were constrained to
 251 be equal across classes, intercepts, factor mean, and factor variance were allowed to be
 252 freely estimated.³ Factor means were estimated to be -4.61, -3.01, and -1.98 for Classes 1,
 253 2, and 3 respectively, with Class 4 serving as the reference group (factor mean 0). Note
 254 that although factor mean comparison is not permitted with a metric invariance model,
 255 factor means of Classes 1, 2, and 3 were statistically significantly different from zero.
 256 Class 3 had the largest proportion, .33, followed by Class 4 (.28), Class 2 (.25), and Class 1
 257 (.14).

2) The EM algorithm was used to find the optimal parameter estimates via an iterative process until the convergence criterion (.00005 by default of *Mplus*) was met.

3) Exceptions were that intercept of the first item was constrained to be equal across classes and the factor mean of the last class (i.e., Class 4) in *Mplus* was fixed to be zero, for the identification purpose.

Table 3*Parameter Estimates of the Four-Class Metric Invariance FMM*

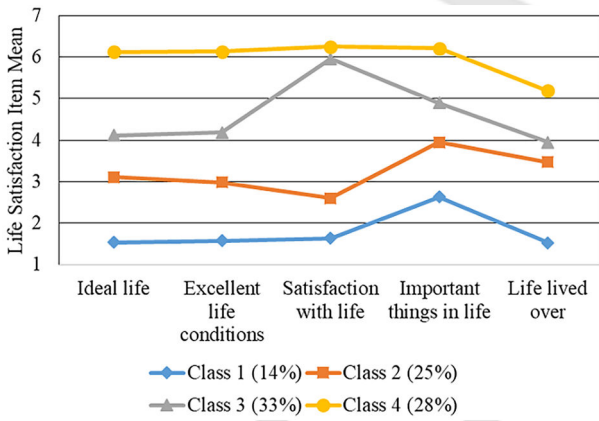
Item/Statistic	Loading	Intercept			
		Class 1	Class 2	Class 3	Class 4
Item					
Ideal	1.00	6.12	6.12	6.12	6.12
Cond	1.15	6.87	6.47	6.48	6.13
Satisfied	1.05	6.45	5.78	8.00	6.24
Important	.94	6.90	6.79	6.74	6.21
Live again	.88	5.57	6.16	5.64	5.23
Statistic					
Factor mean		-4.61	-3.01	-1.98	0
Factor variance		.23	.43	.34	.32
Class proportion		.14	.25	.33	.28

258 Distinction of the latent classes was further interpreted based on the life satisfaction
 259 item mean by class, as illustrated in Figure 2. ANOVAs with Bonferroni adjustment were
 260 conducted to compare the item means across classes and results showed statistically
 261 significant mean differences between any two groups. Class 4 had the highest mean
 262 across all items, followed by Class 3, Class 2, and Class 1. Of note is that Class 3 had
 263 relatively high mean on the item, “I am satisfied with my life”, which might correspond
 264 to the high item intercept in the 4-class metric invariance FMM.

265 For Step 4, SEM trees were performed in the *semtree* package in R (Brandmaier et
 266 al., 2021; R Core Team, 2021). A CFA model of life satisfaction measured by five items
 267 was specified and a total of 12 covariates were included. Given that a 4-class metric
 268 invariance model was supported in FMM, metric invariance was also established in SEM
 269 trees via the global constraints function such that factor structures and loadings were
 270 constrained to be equal across groups whereas intercepts, factor mean, and residual
 271 variances were freely estimated. The resulting tree was displayed in Figure 3. There were
 272 four splits among which the first two occurred on age and the other two on race. The
 273 first split divided the whole sample into two, older adults ($n = 1639$) versus the rest ($n =$
 274 8102). The second split further divided those that were not older adults into two, adults
 275 ($n = 5108$) versus AYAs ($n = 2994$). Each of these two groups was split again on whether
 276 or not the patient was Black. Therefore, there were a total of five groups as a result of
 277 SEM trees, older adults, Black adults, adults that were not Black, Black AYAs, and AYAs
 278 that were not Black, $n = 1639, 921, 4187, 502, 2490$ respectively.

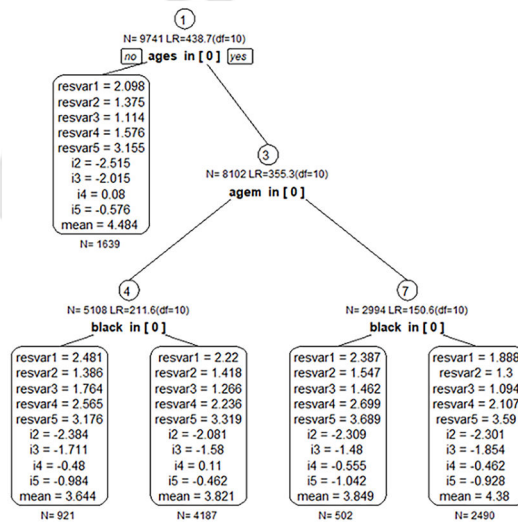
Figure 2

Life Satisfaction Item Mean by Latent Class



279 Figure 3

280 Tree Plot of SEM Trees



281

282 Note. N refers to the sample size at each split; LR is the likelihood ratio statistic with the difference in degrees of

283 freedom (*df*); ages and agem refer to older adults and adults, respectively; black refers to the race group of

284 Black.

Table 4*Results of Multinomial Logistic Regression via the Three-Step Approach*

Covariate	Class 1		Class 2		Class 3	
	Est (SE)	OR	Est (SE)	OR	Est (SE)	OR
TBI severity	-.04 (.02)	0.96*	-.01 (.01)	0.99	-.01 (.01)	0.99
FIM cognition	-.01 (.01)	0.99	-.02 (.01)	0.98*	-.01 (.01)	0.99
Adults	.63 (.18)	1.87***	.51 (.14)	1.66***	-.21 (.13)	0.81
Older Adults	-.56 (.24)	0.57*	-.06 (.18)	0.94	-.63 (.16)	0.54***
Female	.04 (.14)	1.04	.12 (.11)	1.12	.10 (.11)	1.10
Black	.72 (.18)	2.06***	.81 (.16)	2.24***	.54 (.16)	1.71**
Hispanic	.05 (.20)	1.05	.22 (.16)	1.24	-.10 (.16)	0.90
OtherRace	-.58 (.39)	0.56	.37 (.22)	1.44	-.28 (.24)	0.76
Student	-.10 (.33)	0.91	.07 (.24)	1.07	.04 (.22)	1.04
Unemployed	.64 (.15)	1.89***	.28 (.12)	1.32*	.29 (.11)	1.34**
Pre-impairment	-.22 (.27)	0.80	-.002 (.20)	1.00	.02 (.19)	1.02
Pre-phylimit	.38 (.22)	1.47	.16 (.18)	1.18	.18 (.18)	1.19
Older Adults*Black	-.82 (.52)	0.44	-.88 (.35)	0.42*	-.29 (.32)	0.75

Note. Pre-impairment = pre-injury impairment; pre-phylimit = pre-injury physical limitation; the missing groups for categorical covariates are the reference groups (i.e., AYAs, Male, White, and Employed). Est (SE) = estimated regression coefficient (standard error); OR = odds ratio.

* $p < .05$. ** $p < .01$. *** $p < .001$.

285 Given that split occurred on whether or not the patient was Black for both adults and
 286 AYAs but not older adults, an interaction effect was signified between the race category
 287 of Black and older adults. In other words, the impact of being Black on CFA model
 288 parameters was absent for older adults and present for the rest of the sample.

289 For Step 5, the interaction effect between older adults and Black that was detected
 290 by SEM trees was included in the multinomial logistic regression on top of all main
 291 effects. Results (see Table 4) showed that the interaction effect was significant for Class
 292 2, $B(SE) = -.88(.35)$, $p = .013$, which indicates that the impact of race on the likelihood
 293 of being assigned to Class 2, a somewhat satisfaction class, depended upon age group.
 294 That is, for individuals that were AYAs, the odds of being in Class 2 (versus Class 4, the
 295 reference group) for Black people were 2.24 times that of White people, controlling for all
 296 other covariates in the model. However, for older adults, Black individuals experienced a
 297 reduction of 7% in the odds of being in Class 2 compared to the White. In other words,
 298 seniority positively related with life satisfaction for Black individuals, and the Black
 299 AYAs were at a higher risk for life dissatisfaction.

300 The interaction between age group and race is further illustrated in Table 5 in which
 301 the composition of Classes 2 and 4 with regards to age group and race is presented.

Table 5*Age Group by Race Interaction Effect*

Race and Age Group	Class 2	Class 4
Black		
AYAs	119 (27.36%)	80 (29.52%)
Adults	283 (65.06%)	135 (49.82%)
Older Adults	33 (7.59%)	56 (20.66%)
Total	435 (100.00%)	271 (100.00%)
White		
AYAs	378 (23.46%)	664 (31.77%)
Adults	929 (57.67%)	926 (44.31%)
Older Adults	304 (18.87%)	500 (23.92%)
Total	1611 (100.00%)	2090 (100.00%)

Note. AYAs = adolescents and young adults.

302 That is, among 435 Black people that were assigned to Class 2, the somewhat satisfaction
 303 class, only 7.59% were senior, whereas 20.66% of Black people in Class 4, the high
 304 satisfaction class, were senior. The discrepancy in percentages was not as substantial
 305 as above for the Black AYAs, the White seniors, or the White AYAs. In addition to the
 306 interaction effect, adults were more likely to be in Class 2 than AYAs and those that were
 307 unemployed were associated with a higher likelihood of being in Class 2 than those that
 308 were employed.

309 For the other classes (i.e., Classes 1 and 3), despite the absence of a significant interac-
 310 tion effect, age, race, and unemployment all had significant impact on the latent class
 311 membership. That is, adults were more likely to be in Class 1 which were characterized
 312 by low life satisfaction, compared with AYAs. Older adults were less likely to be in
 313 Classes 1 and 3 which were the low and moderate life satisfaction classes, respectively,
 314 compared with AYAs. Individuals who were Black were more likely to be in Classes 1 and
 315 3 than Class 4, compared with those that were White. Those that were unemployed were
 316 associated with a higher likelihood of being in Classes 1 and 3 compared with those that
 317 were employed.

Discussion

318

319 This study aimed to demonstrate the utility of a machine learning approach, SEM trees,
320 for the identification of covariate interactions that potentially explain latent classes in
321 FMM. Specifically, this study tapped into the advantage of SEM trees in automatically
322 searching for covariate interactions and showed that covariate interaction that was
323 detected by SEM trees can be incorporated into FMM to explain the distinction among
324 latent classes. As demonstrated, SEM trees revealed the interaction between race and age
325 group, which provided a more nuanced understanding of how these factors interplayed
326 to affect life satisfaction. That is, the impact of being Black on individuals' likelihood
327 of being assigned to a somewhat satisfaction versus a high satisfaction class depended
328 on age group, which clearly indicates seniority as a protective factor against life dissatis-
329 faction. Retrospectively, this interaction effect is in alignment with the prior literature
330 on life satisfaction and other psychological and health outcomes (Ajrouch et al., 2001;
331 George et al., 1985; Phatak et al., 2013; Shaw et al., 2010). Overall, this demonstration
332 provides an example of how intersectionality can be examined and understood with an
333 integration of FMM and SEM trees.

334 Despite the utility of the SEM trees in identifying covariate interactions, there is no
335 guarantee that the interaction terms will turn out to be the sources of heterogeneity in
336 FMM. For example, the race by age group interaction was statistically significant in one
337 latent class, but not for the other two classes. This possible discrepancy between FMM
338 and SEM Trees occurred due to the drastic differences between the two approaches in
339 how heterogeneity is modeled (Jacobucci et al., 2017). That is, in FMM, latent classes
340 formed on the basis of the estimated model parameters (e.g., intercepts, loadings, factor
341 mean, factor variance), whereas splits of the sample in SEM trees depend upon covari-
342 ates. Note that although a conditional FMM might be more comparable to SEM trees
343 given that the contribution of covariates to the formation of latent classes is allowed,
344 we adopted unconditional FMM in our study which allows researchers to first examine
345 heterogeneity based on the outcome of interest and subsequently explore the impact
346 of covariates. This has been aligned with the vast majority of FMM applications (e.g.,
347 Babusa et al., 2015; Bernstein et al., 2013; Elhai et al., 2011).

348 The possible discrepancy between FMM and SEM trees in identifying covariate inter-
349 actions does not undermine the utility of SEM trees in suggesting potential interactions.
350 Especially when intersectionality is of interest to applied researchers but substantive
351 theories or knowledge regarding the form of interactions are lacking, SEM trees offers a
352 data-driven and exploratory approach that can be adopted to identify possible interaction
353 effects that explain latent classes in FMM. As demonstrated in the paper, an uncondi-
354 tional FMM can be conducted first to identify latent classes and the level of equality
355 constraints on parameters across classes. Next, the SEM trees can be conducted with a
356 comparable level of constraints to FMM (e.g., loadings are equal across classes) and the
357 suggested covariate interactions could be added to the multinomial logistic regression on

358 top of the main effects via the three-step approach. Alternatively, if hypothesis regarding
359 interaction effects is available, the two modeling approaches can be used concurrently
360 and SEM trees at least offer an alternative perspective into how heterogeneity is shaped
361 by covariates.

362 While we highlight the utility of SEM trees in suggesting covariate interactions, a few
363 caveats are worth mentioning. First, future Monte Carlo simulation studies are needed to
364 systematically evaluate the efficacy of this approach of integrating SEM trees with FMM.
365 For example, multiple splitting methods and options to control the growth of the tree
366 are available in the implementation of the SEM trees approach, and simulation studies
367 are needed to examine which method and option would be optimal under which data
368 conditions (Jacobucci et al., 2017). Additional factors that can be considered in simulation
369 studies include numbers of latent classes, degrees of class separation, number of covari-
370 ates, forms of interactions (e.g., two-way or higher-order interactions), etc. Second, the
371 SEM trees approach should not be considered as a replacement of substantive theories
372 or knowledge in identifying covariate interactions (Brandmaier et al., 2013). Covariate
373 interactions suggested by the SEM trees should be meaningful and interpretable through
374 a retrospective check with theories or knowledge of researchers, prior to the addition
375 of interactions into the multinomial logistic regression. Third, this study demonstrated
376 the utility of the SEM trees for FMM and future research is needed to examine the
377 potential of this approach for other mixture models (e.g., growth mixture model, latent
378 class analysis) via demonstrations and Monte Carlo simulations. Despite these caveats,
379 we encourage FMM users to tap into the advantage of the SEM trees in identifying
380 potential covariate interactions that advance their understanding of intersectionality and
381 heterogeneity.

382 **Funding:** This research was supported by the American Educational Research Association Division D
383 (00000000035095); the Eunice Kennedy Shriver National Institute of Child Health and Human Development of the
384 National Institutes of Health (R01HD093814). The content is solely the responsibility of the authors and does not
385 necessarily represent the official views of the American Educational Research Association Division D or the National
386 Institutes of Health.

387 **Acknowledgments:** The Traumatic Brain Injury (TBI) Model Systems National Database is a multicenter study of
388 the TBI Model Systems Centers Program, and is supported by the National Institute on Disability, Independent Living
389 and Rehabilitation Research (NIDILRR), a center within the Administration for Community Living (ACL),
390 Department of Health and Human Services (HHS). However, these contents do not necessarily reflect the opinions or
391 views of the TBI Model Systems Centers, NIDILRR, ACL or HHS.

392 **Competing Interests:** The authors have declared that no competing interests exist.

393 **Data Availability:** The sample data for the demonstration above can be requested by researchers from the National
394 Data and Statistical Center, NDSC (<https://www.tbindsc.org>).

Supplementary Materials

395

396 The supplementary materials provided are the annotated codes for unconditional FMM analyses,
397 annotated codes for SEM Trees, and the annotated codes for the three-step approach to estimate
398 covariate and covariate interaction effect on latent class membership (see Wang et al., 2023).

399 Index of Supplementary Materials

400 Wang, Y., Xu, T., & Shen, J. (2023). *Supplementary materials to "Incorporating machine learning into*
401 *factor mixture modeling: Identification of covariate interactions to explain population*
402 *heterogeneity"* [Model systems program, Annotated codes]. PsychOpen GOLD.
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