



Utrecht University

FACULTY OF SCIENCE

APPLIED DATA SCIENCE

Supervisor: Dr. David Goretzko

IANTHI ATHANASIA TSIMEKI

Automated specification search using meta-heuristics

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Abstract

This thesis investigates the integration of Particle Swarm Optimization (PSO) with Structural Equation Modeling (SEM) to enhance model identification and hyperparameter adjustment. The objective function in the PSO-SEM algorithm combines various fit measures and considers the trade-off between model complexity and fit. For this analysis two datasets that provide different model complexity are employed. These datasets undergo similar preprocessing steps, including handling missing data and partitioning into training and validation sets. The PSO-SEM algorithm is applied to optimize the model fit, and the performance of the final models is evaluated using the validation sets. Through the exploration of different hyperparameter combinations and values, valuable insights are obtained regarding their relative importance and optimal settings. Additionally, the transferability of the selected hyperparameters across different datasets is assessed, and further testing and refinement are conducted to ensure their applicability in diverse contexts. The integration of PSO with SEM offers a flexible and efficient approach for addressing complex problems and uncovering latent relationships in data, while the computational time can be adjusted in each problem, by appropriately tuning parameters such as the number of iterations while sacrificing a certain degree of the accuracy. Generally, this research contributes to the fields of metaheuristics and structural equation modeling by exploring the integration of PSO with SEM for enhanced model identification and hyperparameter adjustment. The findings offer valuable insights and practical implications for researchers engaged in solving complex problems and uncovering latent relationships in data. Furthermore, the results encourage additional investigations, including different metaheuristic algorithms, a variety of datasets and the application of more hyperparameter combinations.

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1. Introduction

1.1 *Motivation and context*

In today's rapidly evolving technological landscape, the ability to efficiently solve complex problems has become increasingly significant. Many real-world challenges require the exploration of a vast solution space to find optimal or near-optimal solutions. As the size and complexity of these problems continue to grow, traditional search algorithms often fall short in providing effective solutions within a reasonable timeframe. Metaheuristics, as a branch of optimization in computer science and applied mathematics, are offering good solutions on challenging problem instances characterized by large search spaces, while they exhibit a high degree of flexibility, allowing them to be tailored and adapted to suit different problem domains and requirements (Talbi, 2009). The use of metaheuristics is becoming more and more popular in different research areas and industries ranging from optimization tasks in engineering (Bozorg-Haddad, 2017) and logistics (Çakmak, 2021) to decision-making problems in finance (Doering *et al.*, 2019) and healthcare (Tongur, 2020).

Nature has been a source of inspiration for a plethora of metaheuristic optimization algorithms, which has been continuously growing in recent years (Tzanetos and Dounias, 2021). Among the most well-known algorithms in this category is the Particle Swarm Optimization (PSO) algorithm, which is based on the movement of swarms, herds, and flocks of animals, birds, or other living organisms in general. The main characteristic of their movement is the influence of collective behavior and member interactions. It was proposed by Eberhart and Kennedy (1995) to solve continuous space optimization problems, and subsequently, hundreds of other algorithms have been developed based on it, covering a broader range of problem-solving domains.

In the field of data analysis, Structural Equation Modeling (SEM) has emerged as a powerful tool for uncovering latent relationships and understanding complex systems, by providing a framework for examining the underlying structures and causal pathways among observed and latent variables in a dataset. By incorporating latent variables, SEM allows researchers to explore unobservable concepts such as attitudes, traits, and psychological constructs. Its application extends beyond traditional statistical methods, as it not only measures the direct relationships between variables but also captures the indirect effects and interdependencies among them. This approach enables researchers to test and refine theoretical models, evaluate hypotheses, and gain insights into complex phenomena. Also, SEM has proven particularly useful in examining the intricate dynamics of human behavior, where latent variables often play a critical role in shaping outcomes.

In the context of this thesis, the integration of PSO with SEM presents an innovative approach for model identification with hyperparameter adjustment. Since every model and every dataset are different, there might be a set of hyperparameters that, in combination with PSO, produce acceptable and fast results for different datasets and models, providing a useful tool for the researchers.

1.2 Literature review

1.2.1 Structural Equation Modeling

According to Ullman (2006), Structural Equation Modeling (SEM) is a statistical approach used to analyze relationships between independent variables (IVs) and dependent variables (DVs), which can be either observed or unobserved (latent). SEM enables the examination of both measured variables and underlying constructs that may not be directly observed. It is also known as causal modeling, causal analysis, simultaneous equation modeling, analysis of covariance structures, path analysis, and Confirmatory Factor Analysis (CFA). More specifically, CFA and path analysis are special types of SEM. Generally, SEM provides a comprehensive framework for exploring complex relationships, testing hypotheses, and understanding the underlying mechanisms. In SEM the measured variables, also called observed variables or indicators, and factors that have at least two indicators are called latent variables, constructs, or unobserved variables.

CFA, as a type of SEM, has the characteristic that is a statistical technique used to validate or confirm a pre-defined theoretical structure or model (Ullman, 2006). Firstly, the researcher specifies a hypothesized model with predetermined factors and their relationships. Then CFA tries to assess whether the observed data supports the proposed structure and tests the fit of the model to the data, by evaluating the adequacy of the hypothesized model and making inferences about the relationships between latent variables and observed indicators.

1.2.2 Particle Swarm Optimization

Eberhart and Kennedy (1995) were the first to study and algorithmically simulate the behavior of bird flocks and fish schools during their movement. According to this behavior, each member of the flock or school is redirected based on the movement of the nearest member. Particle Swarm Optimization (PSO) is based on the interaction among the members of the swarm.

PSO is inspired by the movement of a flock of birds (population) consisting of individuals (particles) that move in a space (search space) towards the bird with the best position (best solution of the objective function). During the search, each particle identifies the best position of the search space (best solution) among all the particles. In general, each position in the search space represents a solution to the problem. This position is described by the values taken by the decision variables, which, when input into the objective function of the problem, yield the value of the solution based on the objective function, which is called fitness. In maximization problems, the best fitness is considered the highest, while in minimization problems, the aim is to find the lowest possible fitness. After the particles compute the fitness of their current positions, they tend to move towards the best position found among all the searchers, i.e., towards the particle with the best fitness. At the same time, they also consider their own best position, i.e., the position with the best fitness they have found so far. Therefore, the next position they will explore is directly dependent on the best position of the population and their personal best position. This relationship can be expressed mathematically as:

$$v_i^{t+1} = v_i^t + \omega_1(xBest_i^t - x_i^t) + \omega_2(gBest^t - x_i^t)$$

where v_i^{t+1} is the new velocity of the particle i , v_i^t is the current velocity of particle i at iteration t , $xBest_i^t$ represents the best position found by particle i (personal best position), while $gBest^t$ denotes the best solution among all particles. The parameters ω_1 and ω_2 represent learning factors, that are uniform

random values in the range [0,1]. They also determine the contribution rate that the personal and the global best solutions at iteration t influence the velocity value at iteration $t + 1$.

1.2.3 Descriptive Measures

Measures of overall model fit provide insights into the extent to which a structural equation model aligns with the empirical data. These measures are obtained by evaluating the concordance between the sample covariance matrix, denoted as S , and the model's expected covariance matrix, denoted as $\Sigma(\hat{\theta})$. In this research the different indices that evaluate the model fit, include Root Mean Square Error of Approximation (RMSEA) and Standardized Root Mean Square Residual (SRMR). Another method to evaluate a model fit is by comparing the indices fit with to the fit of a baseline model (Schermelleh-Engel, 2003). Comparative Fit Index (CFI) is one of these methods, which evaluate the fitness of a model, by typically comparing it to the null model. The CFI ranges between 0 and 1, with values closer to 1 indicating a better fit, while values above 0.90 are generally considered indicative of an acceptable fit.

RMSEA was proposed by Steiger and Lind in 1980, and is a statistical measure used to assess the approximate fit of a model in the population. In practical situations, it is often unrealistic to expect an exact fit between the model and the data, especially with large sample sizes. Instead, the focus is on evaluating whether the model fits closely enough to the population. The traditional null hypothesis of exact fit is replaced with a null hypothesis of "close fit". A "close fit" To calculate RMSEA the discrepancy due to approximation by estimating the square root of the estimated discrepancy per degree of freedom, as:

$$\hat{\epsilon}_\alpha = \sqrt{\max \left\{ \left(\frac{F(S, \Sigma(\hat{\theta}))}{df} - \frac{1}{N-1} \right), 0 \right\}}$$

where, $F(S, \Sigma(\hat{\theta}))$ is the minimum fit function, N is the sample size and df denotes the degrees of freedom and is calculated as $df = s - t$. A lower $\hat{\epsilon}_\alpha$ value indicates a better approximate fit, and more specifically, values smaller than 0.05 are typically considered to indicate good fit, values ranging from 0.05 to 0.08 as fair model fit, and values greater than 0.10 as poor fit (Schubert *et al.*, 2017).

On the other hand, SRMR equation is constructed as a standardized version of the Root Mean Square Residual (RMR), which measures the average discrepancy between the observed and predicted covariances. This way, it allows for easier interpretation and comparison across different models. So, starting with calculating the RMR as:

$$RMR = \sqrt{\frac{\sum_{i=1}^p \sum_{j=1}^i (s_{ij} - \hat{\sigma}_{ij})^2}{\frac{p(p+1)}{2}}}$$

where s_{ij} is an element of the empirical covariance matrix, $\hat{\sigma}_{ij}$ is an element of the model-implied covariance matrix and p is the total number of the observed variables. To proceed to the calculation of SRMR, the part $s_{ij} - \hat{\sigma}_{ij}$ is divided by $s_i = \sqrt{s_{ii}}$ and $s_j = \sqrt{s_{jj}}$, leading to a standardized residual matrix. Similarly, to RMSEA, results close to zero represent a good fit.

Finally, CFI was proposed by Bentler (1990) and is defined as the improvement in fit of the proposed model compared to the null model, which assumes no relationships between the observed variables. It is calculated as follows:

$$CFI = 1 - \frac{\max[(\chi_t^2 - df_t), 0]}{\max[(\chi_t^2 - df_t, \chi_i^2 - df_i), 0]}$$

where χ_t^2 is the chi-square score of the model, χ_i^2 is the chi-square score of the target model and df represents the total number of degrees of freedom.

1.3 Research question

The aim of this research is to utilize the particle swarm optimization metaheuristics algorithm to perform automated specification search and identify the best model for a given dataset. The focus is on models involving latent variables and other relevant factors. The goal is also to explore how this approach can effectively identify the most suitable model that accurately represents the underlying structure of the data. By combining the descriptive measures to search for a good model in a short amount of time, the research seeks to address the following question:

“How does the automated specification search using the particle swarm optimization metaheuristics algorithm can contribute to identify the optimal model that captures the latent variables and factors within a dataset?”

2 Data

2.1 Description

The datasets of this research are obtained from the “Open Science Framework” (OSF), an online platform for sharing and accessing data and material. The first dataset is the “Validation of a German Short Version of the Short Dark Triad Scale” (Wehner, 2021). This dataset is based on the German version of the Short Dark Triad, which includes three subscales designed to measure narcissism, psychopathy, and Machiavellianism. Participants rated the 27 items using a 6-point rating scale, where 1 = “strongly disagree” to 6 = “strongly agree”. The dataset consists of 341 variables (columns) and contains a total of 1100 entries (rows).

The second dataset is the “IPIP120” from Johnson's IPIP-NEO data repository, which is a shorter version, containing the results of International Personality Item Pool Representation of the NEO PI-R questionnaire. Participants were asked to complete this 300-question questionnaire, which aimed to measure personality traits based on the Five Factor Model (Neuroticism, Extraversion, Conscientiousness, Agreeableness, and Openness to Experience) framework (Johnson, 2014). The total entries of the specific dataset are 619150 and there are 130 variables. The 10 first variables of the dataset are related with the participants background, like age, sex, and country, while each of the last 120 variables represent the answer given on a specific question of the questionnaire, and take values the values 1 to 5, where 1 = “very inaccurate”, 2 = “moderately inaccurate”, 3 = “neither accurate nor inaccurate”, 4 = “moderately accurate”, and 5 = “very accurate”. The missing values were coded as 0.

2.2 Preparation of Data

2.2.1 Validation of a German Short Version of the Short Dark Triad Scale

A total of 27 variables, which are associated with the answers of the participants, were chosen to specify the best model to calculate more accurately the traits. Each of these traits represent a latent variable and 9 indicators. Some of the questions were formulated using negations and to maintain consistency in the scoring, a value of 7 was subtracted from these answers. Furthermore, any entries that contain missing values, were removed.

2.2.2 IPIP120

The data were given in SPSS format (.por) and were loaded in RStudio through “haven::read_spss” function. Since the primary goal in this research is calculating the “Extraversion” of each person, only 24 questions related with this trait are kept. Since 0 values represent the missing values, each entry containing 0 is removed. Reverse-scored items in the dataset have already been recoded during the respondent's completion of the inventory. The recoding involved swapping the values of 1 and 5, 2 and 4, and keeping 3 unchanged, without further recoding needed.

3 Method Description

3.1 Method Selection

In the field of structural equation modeling (SEM), the exploration of the search space to improve models, fitted in “lavaan” functions, is often accomplished using metaheuristic algorithms. These algorithms provide a powerful means to solve optimization problems by utilizing a binary indicator vector to represent the model's identified parameters. PSO is chosen as the metaheuristic algorithm for exploring the search space and improving fitted lavaan models. As it was mentioned before, it is a population-based optimization algorithm that draws inspiration from the social behavior of bird flocking or fish schooling. It simulates the movement of particles in a multi-dimensional space, where each particle represents a potential solution or model specification. The particles iteratively adjust their positions and velocities based on their own best-known solution (personal best) and the best-known solution of the entire swarm (global best).

The PSO-SEM method begins with an initial fitted lavaan model and a search table that lists candidate parameters and their possible modifications. The objective criterion for the search is typically based on fit indices such as the standardized root mean square residual (SRMR), comparative fit index (CFI), and root mean square error of approximation (RMSEA). The method aims to find a model specification that maximizes the goodness of fit while considering model parsimony. The algorithm operates in iterations called generations. In each generation, the particles in the swarm update their velocities and positions based on mathematical formulas that incorporate the personal best and global best solutions. The number of particles is specified with the algorithm parameters, and it is called population. The velocities guide the particles towards potentially better model specifications in the search space. The binary indicator vector, representing the identified parameters, is modified based on the particle's

position. To ensure the search process explores the solution space effectively, a logistic transformation is applied to the velocities, converting them into the range of probabilities. This transformation allows a transition between including and excluding parameters in the model specification. Additionally, a penalization factor (λ) is introduced to balance the importance of goodness of fit and model parsimony in the objective function. The assessment of the solution that was provided from each particle is evaluated with fitness values, that is determined by the objective function. Each time the particles find a new personal best or global best solution, there is an update on these values. This process continues for a predefined number of generations in which the algorithm didn't update the solutions, allowing for potential improvement.

PSO-SEM Pseudocode

1. Initialize population size, number of generations and objective function parameters
 2. Define objective function
 3. Initialize the velocity and position of each particle in the population
 4. Evaluate the fitness of each particle
 5. Set the personal best and global best values to the initial fitness values of the particles
 6. Set generation = 1
 7. **While** the generation \leq number of generations, do:
 8. Update the velocity and position of each particle using the PSO equations and the current pbest and gbest values.
 9. Evaluate the fitness of each particle.
 10. Update the pbest and gbest values if a particle's fitness is better than its previous best.
 11. **If** the gbest value has improved compared to the previous generation
 12. Set generation = 1
 13. **Else** generation = generation + 1
 14. Select the best particle as the final solution
 15. Return personal bests, fitness values, the final model, final parameters index and the best fitness
-

At the end, the algorithm provides a list of personal best solutions, fitness values for each particle, the final model specification, the binary indicator vector that represent the best-found model and the best fitness. This model represents an improved version of the initially proposed lavaan model.

3.2 Data Simulation and Models

The implementation of PSO was conducted using RStudio (version 4.2.1; Gromping, 2015) with the use of “lavaan” package (version 0.6-12; Rosseel, 2012) and “pso_sem_revised.R” from the “MetaSS” package which is available through <https://gitlab.lrz.de/KarikSiemund/MetaSSGitLab>, with a

few modifications in order to fit the datasets correctly. It also requires functions from Carl F. Falk and Katerina M. Marcoulides (2018). For the presentation of the results, the used packages were “ggplot2” (version 3.4.0; Gómez-Rubio, 2017) and “plot3D” (version 3.4; C and Greenacre, 2007). Also, the packages “semPlot” (version 1.1.6; Epskamp, 2022) and “lavaanPlot” (version 0.6.2; Lishinski, 2021) were used for plotting the models path diagrams. The coding used to provide the results is available through <https://gitlab.com/IanthiTsim/model-search-with-pso-sem>.

The starting model for the “Dark Triad” is represented in Figure 1, where M, N and P stand for Machiavellianism, Narcissism and Psychopathy respectively, and they are the factors (oval shape). In the graph there are lines with only one arrow (edge) and lines with pointing arrows in both directions. The variable, with the arrow pointing to it, is the dependent variable. while a line with an arrow at both ends indicates a covariance between the two variables. The rectangles below the factors indicate the observed values.

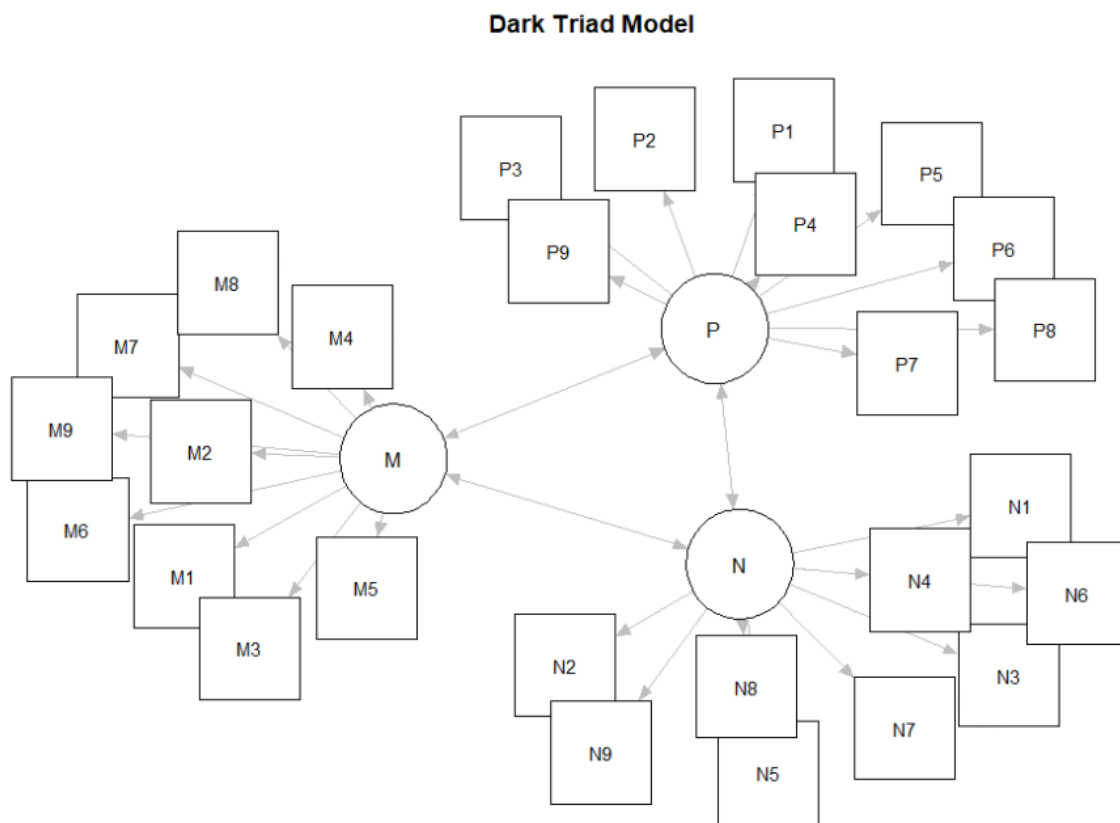


Figure 1. Dark Triad Model

More generally, the mathematical representation that expresses the Dark Triad model is:

$$\text{Machiavellianism} = M1 + M2 + M3 + M4 + M5 + M6 + M7 + M8 + M9$$

$$\text{Narcissism} = N1 + N2 + N3 + N4 + N5 + N6 + N7 + N8 + N9$$

$$\text{Psychopathy} = P1 + P2 + P3 + P4 + P5 + P6 + P7 + P8 + P9$$

Similarly, for the “IPIP120” dataset, the initial model is shown in Figure 2. In this case also, F, A, G, AL, ES and C are the latent variables and stand for Friendliness, Gregariousness, Assertiveness, Activity Level, Excitement Seeking and Cheerfulness. These are the main variables that could calculate the “Extraversion” of a person, based on their answers on the questions mentioned as observed variables (e.g. I2 is the second question on the IPIP120 questionnaire).

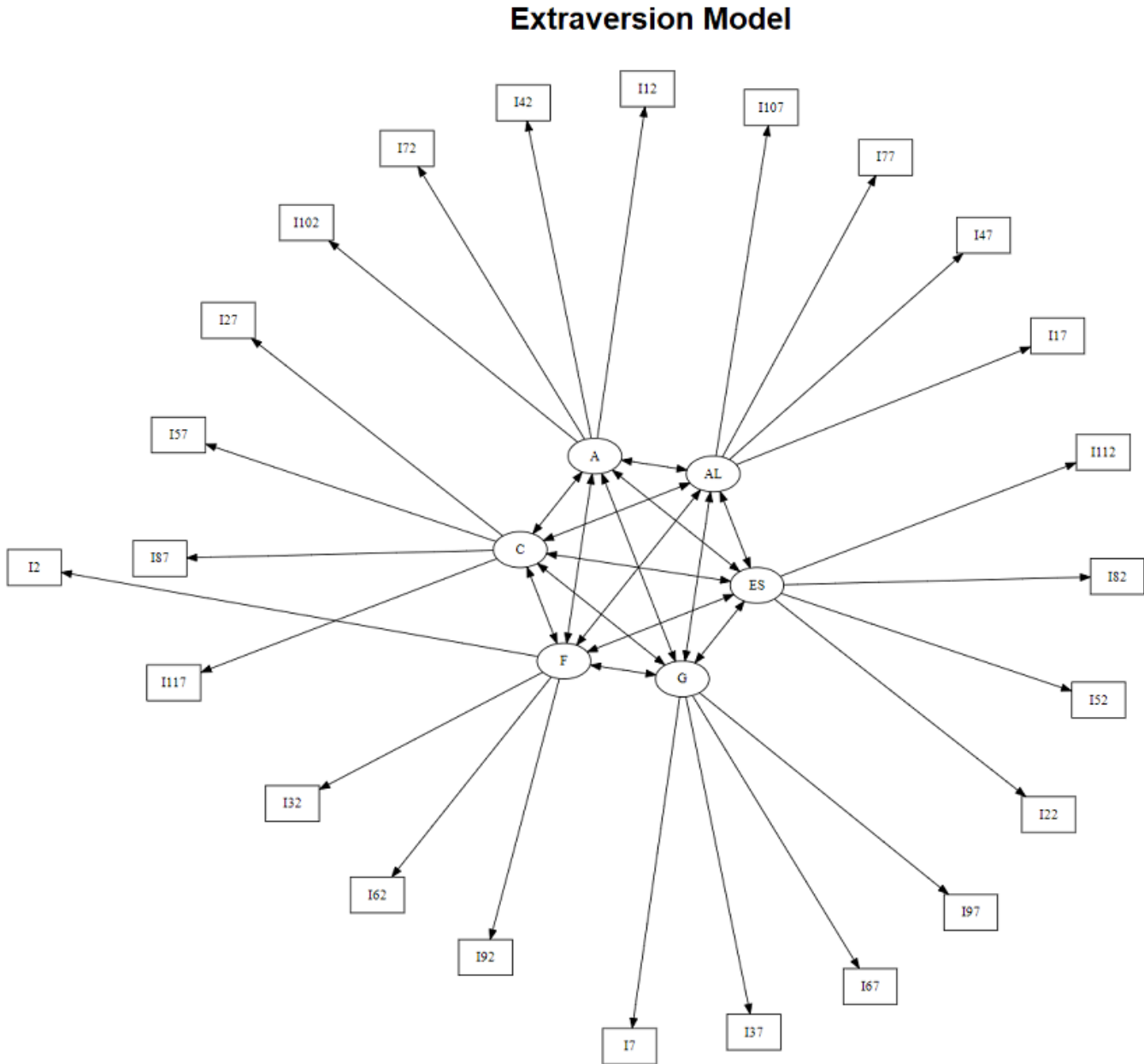


Figure 2. Extraversion Model from IPIP120 dataset

The mathematical representation that expresses the Extraversion model is:

$$\text{Friendliness} = I2 + I32 + I62 + I92$$

$$\text{Gregariousness} = I7 + I37 + I67 + I97$$

$$\text{Assertiveness} = I12 + I42 + I72 + I102$$

$$\text{Activity Level} = I17 + I47 + I77 + I107$$

$$\text{Excitement Seeking} = I22 + I52 + I82 + I112$$

$$\text{Cheerfulness} = I27 + I57 + I87 + I117$$

3.3 Objective Function and Hyperparameter Adjustment

The objective function aims to assess the overall fit of a structural equation model by combining different fit measures and considering the trade-off between model complexity and fit. It consists of two main components. The first component evaluates the fit of the model based on three fit measures: SRMR, CFI and RMSEA. Each fit measure is transformed using the logistic function and a slope parameter. The transformed values are then combined using a weighted average, where λ or *lambda* determines the weight given to the model fit measures. The objective is to minimize this component, indicating better fit when the values of SRMR, CFI, and RMSEA approach desired thresholds. The second component considers the model complexity by incorporating the ratio of the total number of free parameters (*total_free*) to the total number of parameters in the model (*total*). This component penalizes more complex models, as higher values of *total_free* relative to *total* indicate greater complexity, aiming to promote simpler models.

More specifically the objective function used with the PSO method is:

$$\text{Obj} = \frac{(1 - \lambda)}{3} * \left(1 - \left(\frac{1}{1 + \exp(\text{slope} * (p_1 - \text{SRMR}))} \right) + \left(\frac{1}{1 + \exp(\text{slope} * (p_2 - \text{CFI}))} \right) \right) + \left(1 - \frac{1}{1 + \exp(\text{slope} * (p_3 - \text{RMSEA}))} \right) + \lambda * \frac{\text{total_free}}{\text{total}}$$

where, the *slope* parameter determines the steepness of the function, determining how quickly the fitness score decreases as the fit indices deviate from the specified thresholds. A larger negative slope implies a steeper decline in fitness as the fit indices move away from the desired values. The p_1 , p_2 and p_3 are parameters that represent the thresholds or cutoff values for the SRMR, CFI, and RMSEA fit measures respectively (Hu and Bentler, 1999). These thresholds are used to determine the level of acceptability for each fit measure, and by specifying these values, the objective function assigns different weights to the fit indices based on their relative importance in model evaluation.

The initial hyperparameters values selected are:

p_1	p_2	p_3	<i>slope</i>	λ
0.08	0.95	0.06	-55	0.5

The p_1 , p_2 and p_3 values were chosen based on the work of Hu and Bentler (1999). The λ value is set to 0.5 and *slope* to -55 but will be adjusted according to the needs of each model.

Both datasets prepared and preprocessed with similar procedures. This involved selecting the appropriate variables, handling missing data by keeping only complete entries, and partitioning the data into training and testing sets. The Dark Triad dataset was split into training and validation (test) sets using a 60:40 ratio, while the IPIP120 dataset was further divided into a training set consisting of 1000 cases and a validation set consisting of 1000 cases, keeping a 50:50 ratio. Bigger sets in the IPIP120 would increase the complexity of the model.

After identifying the training set, the examined model is specified, and was then fitted to the training data using the “cfa” lavaan function. Then the PSO-SEM algorithm was employed to explore the search space and optimize the fit of the model. The `pso.sem.revised` function was utilized, which takes the fitted model, an initial search space configuration and the hyperparameter values as input. Finally CFI value was computed to assess the model fit for each combination of hyperparameters. Additionally, the final model resulting from the PSO-SEM algorithm with the best fit was evaluated using the validation set to test its performance on unseen data.

The selection of hyperparameters involved exploring different combinations as well as testing a range of values for specific parameters while keeping the remaining parameters constant. Specifically in the Dark Triad dataset, the search started with investigating the significance of different combinations of p_1 , p_2 , and p_3 in calculating the CFI, while keeping *lambda* and *slope* steady. By systematically varying these parameters, the aim was to identify the impact of individual parameters on the CFI and understand their relative importance in the model evaluation process. In addition, a similar analysis was conducted for the *slope* and *lambda* parameters, while using the initial values of p_1 , p_2 , and p_3 . The objective was to investigate whether increasing or decreasing these parameter values would lead to improved results in terms of model fit. After obtaining a general idea of the effects of individual hyperparameters, a more extensive testing phase was initiated to identify the optimal values for all parameters. The optimal model was chosen by training the model in different seeds, since it’s a stochastic algorithm and the search for the best solution can be influenced by the initial conditions, ensuring that the model’s performance is not biased by a specific seed and that the selected solution was robust and consistent across different initializations (e.g., splitting the dataset into training and validation sets).

The approach to determining the hyperparameters for the IPIP120 dataset started by leveraging the optimal combination of hyperparameters found in the Dark Triad dataset. This initial combination, which demonstrated promising results in the Dark Triad analysis, was used as a starting point for the IPIP120 dataset. By adopting this approach, the aim was to assess the transferability and generalizability of the selected hyperparameters across different datasets. However, recognizing that each dataset may have unique characteristics and requirements, further testing and refinement were conducted. The initial

combination of hyperparameters was systematically adjusted and evaluated by exploring a range of values for specific parameters while keeping the rest constant.

4 Results

4.1 Dark Triad Results

All the Dark Triad model runs, employed a fixed population size of 30 and a generation count of 50, due to model simplicity. Figure 3 shows a 3D representation of the CFI values, among the combinations of $p_1 = \{0.05, 0.08, 0.1\}$, $p_2 = \{0.93, 0.95, 0.98\}$ and $p_3 = \{0.03, 0.06, 0.09\}$, while $\lambda = 0.5$ and $\text{slope} = -55$. Among the parameters, p_1 showed a noteworthy influence on the model's fit, since higher values of consistently yielded better CFI results. Similarly, p_2 demonstrated a strong positive relationship with CFI. In contrast, the specific values of p_3 had relatively less impact on CFI. More precisely, the nodes that are diamond shaped in the figure are the combinations that provided the best 5 results, where the final model CFI value was ~ 0.79 , indicating that there is still potential for further improvement.

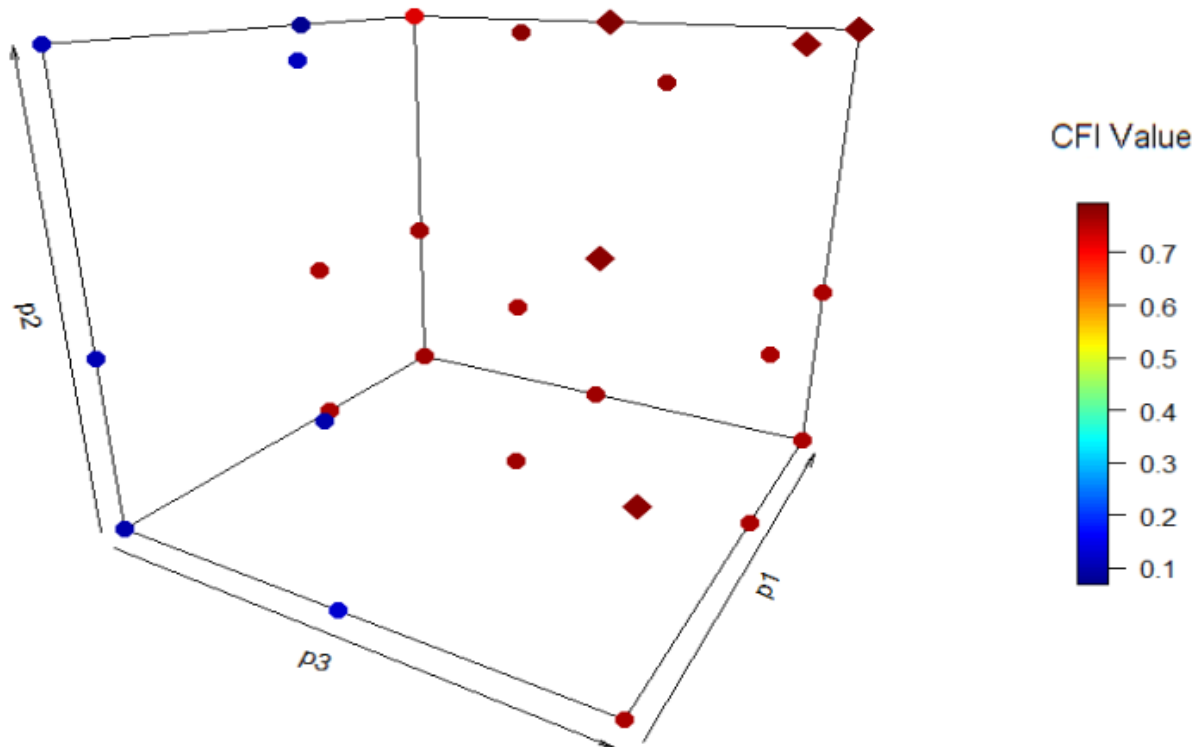


Figure 3. 3D result representation for different p_1, p_2 and p_3 parameter combination

To further explore the influence of different combinations of slope and lambda on CFI, there was some extra analysis where the combinations of $slope = \{-30, -55, -70\}$ and $lambda = \{0.1, 0.25, 0.5\}$ were tested, while the rest parameters are equal to the initial. Figure 4 visualizes the relationship between these different settings.

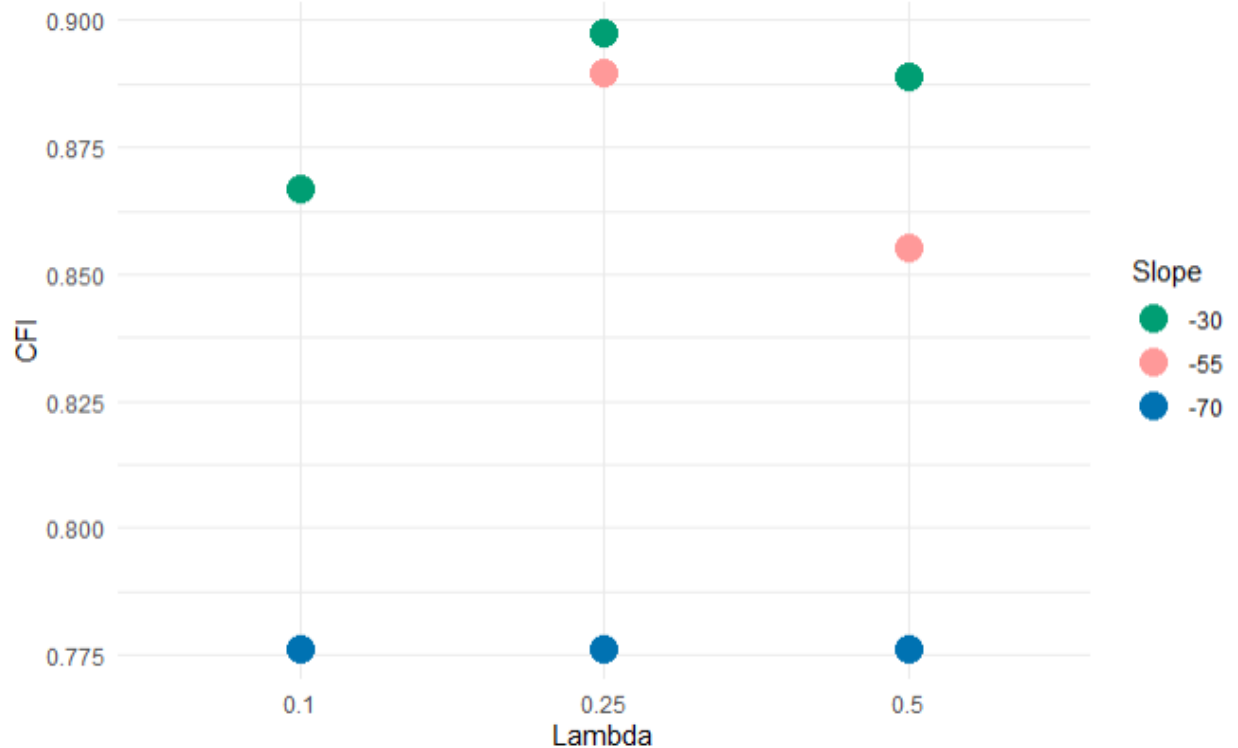


Figure 4. Result representation for different combinations of Lambda and Slope

When further decreasing the $slope$ from its initial -55 value, the CFI worsens, suggesting that the optimal slope is higher. Additionally, the impact of lambda appeared to be less pronounced, with similar CFI values observed across different lambda levels.

Keeping in mind that both p_1 and $slope$ parameters exhibited strong associations with CFI values, further investigations were conducted by exploring combinations involving these parameters. In this run turn, the constant parameters are $p_2 = 0.98$, $p_3 = 0.09$ and $lambda = 0.25$, while $p_1 = \{0.1, 0.12, 0.15\}$ and $slope = \{-30, -25, -20\}$. This range of values could assist in finding the right place to search for the most suitable parameters for this model. The representation of the results is shown in Figure 5, the influence of p_1 and $slope$ on the model's fit, is highlighted. According to the plot, higher values of p_1 and a less negative slope seem to have a positive impact on the CFI scores. More specifically, it can be observed that when $p_1 = 0.15$, the CFI gets the lower scores regardless the $slope$ value, but 0.1 and 0.12 present similar scores, indicating a good value for this parameter. The impact of the $slope$ parameter indicates that exploring less negative values, may lead to improved model, since the CFI keeps increasing when increasing this parameter.

After obtaining an overview of the parameters effect, in the final model, it is noticed that a further search is needed for $lambda$ and $slope$ values. For this analysis, $p_1 = 0.1$, $p_2 = 0.98$ and $p_3 = 0.09$,

which are the values that presented the best results. Since *slope* seems to have bigger impact in the model, the analysis starts by keeping constant $\lambda = 0.25$.

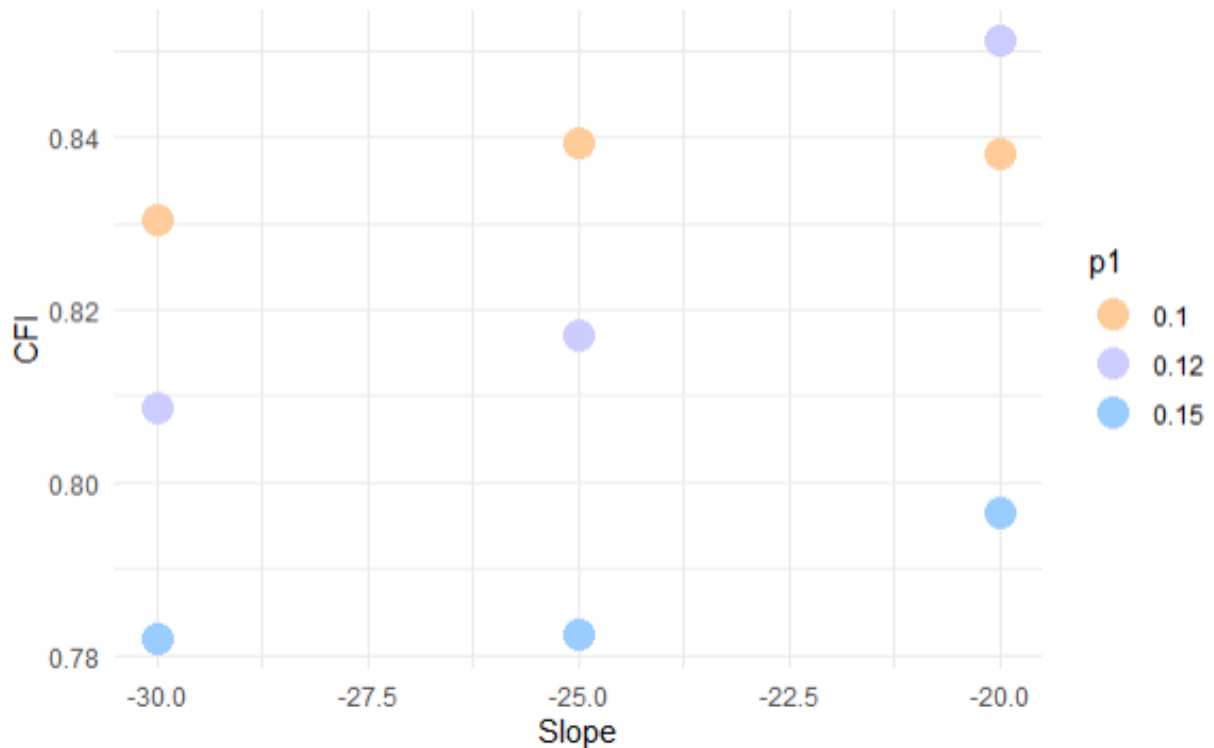


Figure 5. Result representation for different combinations of p_1 and Slope

In Figure 6, the measurement results for *slope* values that ranging from -25 to -15 are presented. The SRMR and RMSEA values hover around 0.06, indicating relatively similar fit across the slope range. Consequently, it is difficult to discern which *slope* value fits better, based on these measures alone. In the other hand, there are notable variations when considering the CFI scores, and more specifically when $\text{slope} = \{-20, -19, -18\}$. Despite that the presence when $\text{slope} = -19$, it is important to note that the CFI score at -20 is relatively close and significantly higher compared to -18. While the difference between -19 and -20 may not be substantial, the larger discrepancy between -20 and -18 further supports the notion that -20 is the optimal *slope* value for the model.

The next step is to identify the value of λ that gives the best model fit. In Figure 7, the results are presented for λ values ranging from 0.15 to 0.28, since in previous analysis the higher CFI appeared close to 0.25. In this graph, SRMR and RMSEA are also overlapping, while they take values around 0.06. Based on the CFI values, it must be noted that even though it appears that smaller values tend to give better fit measures, there were issues with model convergence for λ values of 0.17 and 0.19, requiring manual intervention to force the model to converge. As a result, the reliability of the measurement results for these λ values may be compromised.

Furthermore, while a λ value of 0.18 also produced a relatively low fit measure, it is near the subsequent λ value of 0.20, which performed significantly better. Considering this, the λ

value of 0.20 can be regarded as the optimal choice, as it balances both a good fit and a more stable model convergence. The analytical results are available in A.1 appendix, where any values marked in red indicate a forced convergence, hence an unreliable result.

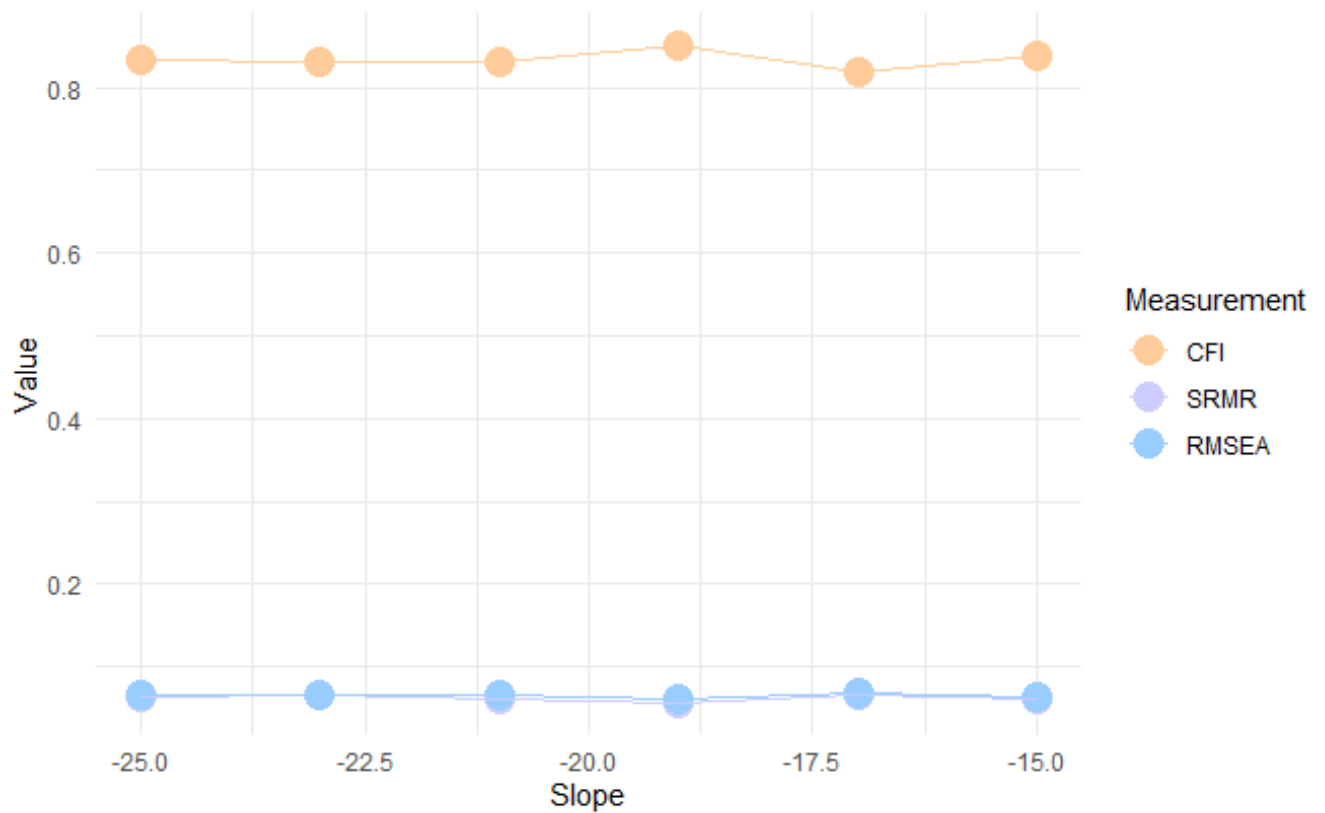


Figure 6. Measurements based on different Slope values

To account for the stochastic nature of the PSO-SEM algorithm, a robust approach was adopted to ensure the reliability of the results. The top three models, based on their CFI values, were selected for further evaluation.

Model	p_1	p_2	p_3	λ	slope	Average CFI
Model 1	0.1	0.98	0.09	0.2	-20	0.862636
Model 2	0.08	0.95	0.06	0.25	-30	0.869909
Model 3	0.08	0.95	0.06	0.25	-55	0.852182

Table 1. Average of models in different seeds

To assess their performance across different random seeds, each of the top models was executed multiple times. The average of their results was calculated to determine the most suitable parameter selection.

Table 1 presents the results of the procedure where Model 1 and Model 2 give the highest average CFI values, but Model 2 is slightly better.

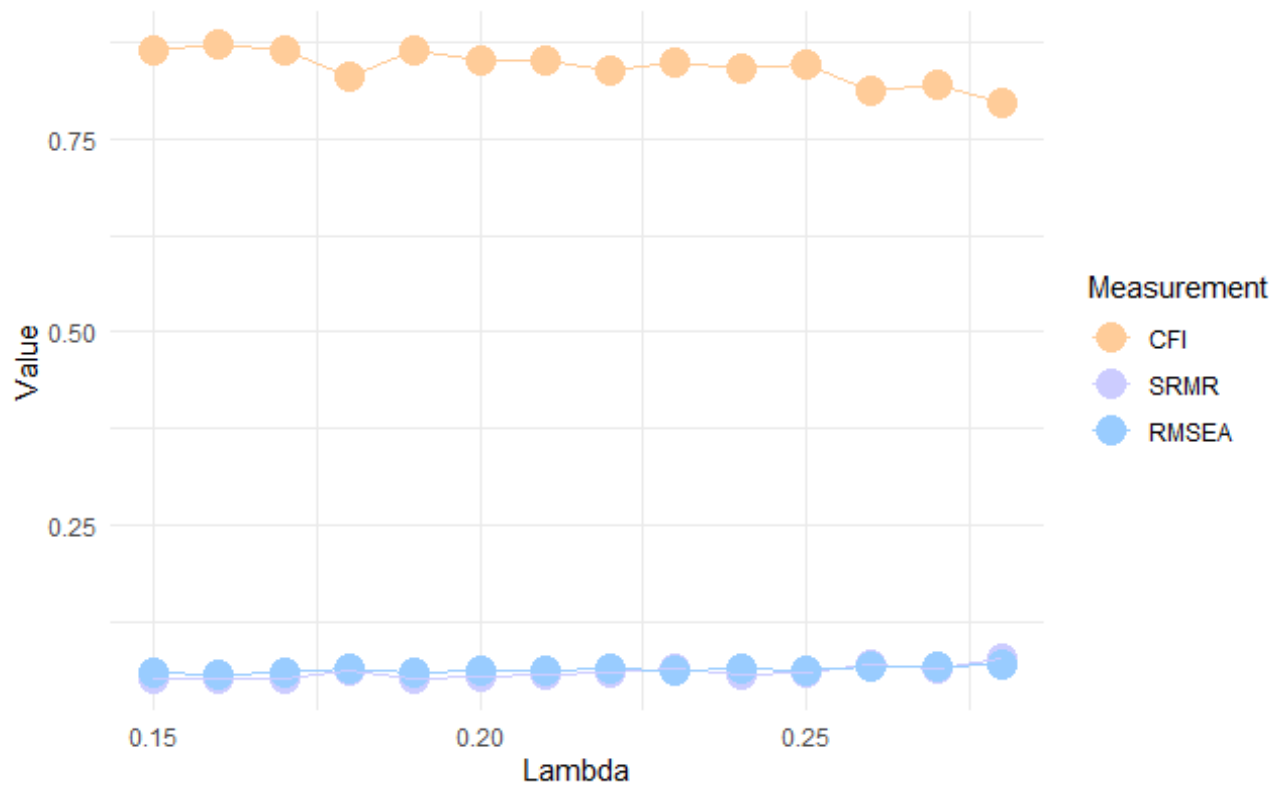


Figure 7. Measurements based on different lambda values

4.2 Extraversion Model Results

The Extraversion Model is more complex than the Dark Triad model, resulting to way higher computational time. For these reason, alternative population sizes and generation counts were considered.

Population	Generation	CFI	Time
30	10	0.899	> 6 hours
15	25	0.953	> 12 hours
15	10	0.899	~ 40 minutes

Table 2. Computational Time for population and generation combinations

Table 2 provides an overview of the computational time required for different combinations of population size and generation count with the initial hyperparameters. Although a higher population size of 15 and a generation count of 25 provide a higher CFI value, the computational time associated with

this configuration is significantly longer, exceeding 12 hours. Given the practical constraints of the research, conducting an extensive analysis with such computational demands is not feasible. To address this limitation, a population size of 15 and a generation count of 10 were chosen as a more efficient alternative. Despite the reduced computational time, this configuration produces comparable results to a population size of 30 and a generation count of 10, as indicated by the similar CFI values.

When $slope = \{-55, -40, -30, -20\}$ combined with the initial values, the CFI results remains the same and equal to 0.9, meaning that this parameter doesn't affect the training of this specific dataset. The same results were given when trying $p_1 = [0.03, 0.09]$ or $p_2 = [0.93, 0.99]$ or $p_3 = [0.03, 0.09]$, while keeping the rest of the parameters steady.

On the other hand, Figure 8 illustrates the impact of changing the $lambda$ parameter on the fit measures (CFI, SRMR, and RMSEA). As $lambda$ values increase beyond 0.4, there is a noticeable deterioration in the fit of the model, as indicated by lower CFI values and higher SRMR and RMSEA values.

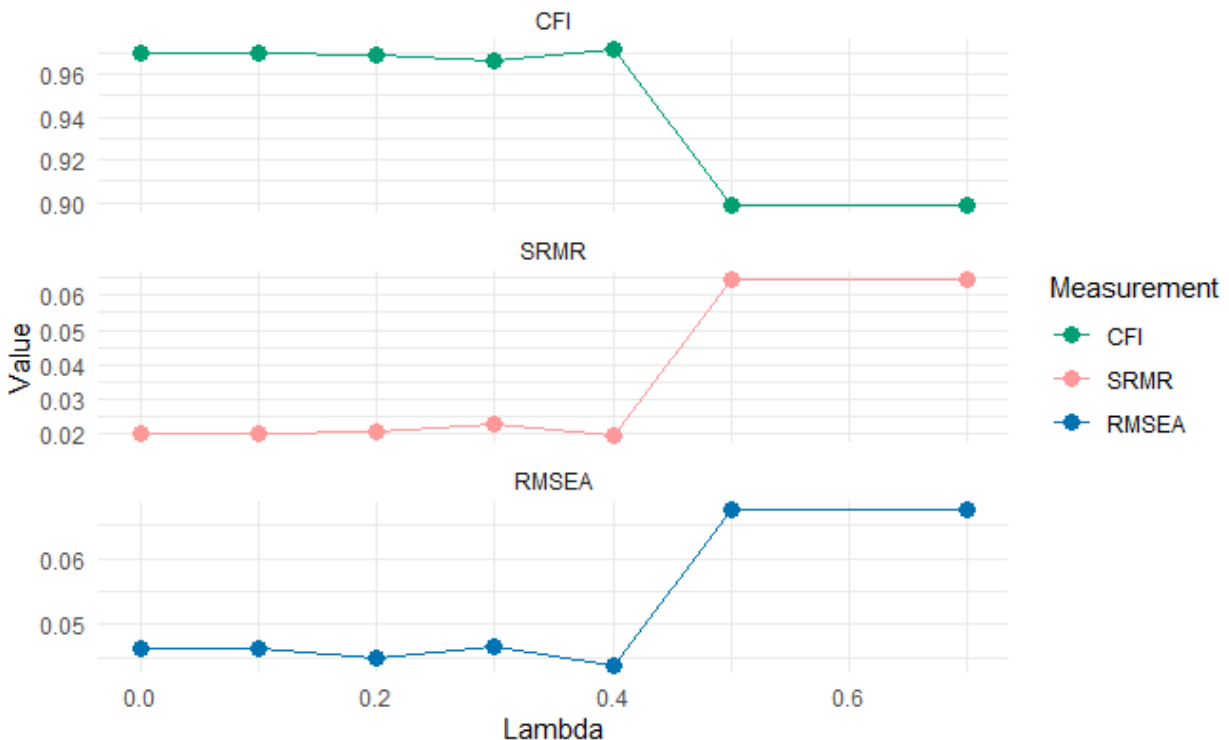


Figure 8. Measurements based on different lambda values

It is noticed that for $lambda = 0.4$ the measurements achieve the best values, but the result was an output of a forced convergence, therefore it is not reliable. Beside this value, both $lambda = 0$ and $lambda = 0.1$ give the best results among the rest values, suggesting lower values for this parameter. The extensive list can be found on A.4. appendix. After identifying the top 3 models, their performance was evaluated on various training and test splits to assess their generalization capabilities. Table 3 presents the model parameters and their final CFI, where Model 1 has the highest average CFI value, which also was the one with the less convergence errors.

Model	p_1	p_2	p_3	λ	slope	Average CFI
Model 1	0.08	0.95	0.06	0.1	-55	0.964364
Model 2	0.1	0.98	0.09	0.2	-20	0.963
Model 3	0.08	0.95	0.06	0.3	-20	0.9202

Table 3. Average of models in different seeds

4.3 More Models

The parameters that yielded the best results for the Extraversion Model were also used for analyzing other aspects of the IPIP120 dataset. The chosen parameters are:

p_1	p_2	p_3	slope	λ
0.08	0.95	0.06	-55	0.1

and were employed in examining four models that can be formed with the rest of the IPIP120 questions. The new models are, the Neuroticism model, which explores neurotic tendencies based on the corresponding questions:

$Anxiety = I1 + I31 + I61 + I91$
$Anger = I6 + I36 + I66 + I96$
$Depression = I11 + I41 + I71 + I101$
$Self\ Consciousness = I16 + I46 + I76 + I106$
$Immoderation = I21 + I51 + I81 + I111$
$Vulnerability = I26 + I56 + I86 + I116$

achieved a CFI of 0.969.

The Openness to Experience model:

$Imagination = I3 + I33 + I63 + I93$
$Artistic\ Interests = I8 + I38 + I68 + I98$
$Emotionality = I13 + I43 + I73 + I103$
$Adventurousness = I18 + I48 + I78 + I108$
$Intellect = I23 + I53 + I83 + I113$
$Liberalism = I28 + I58 + I88 + I118$

which achieved a CFI of 0.955. The specific model needed several reruns on different seeds, because on the first tries it didn't converge, hence the estimates would be unreliable.

The Agreeableness model:

$$\begin{aligned} \text{Trust} &= I4 + I34 + I64 + I94 \\ \text{Morality} &= I9 + I39 + I69 + I99 \\ \text{Altruism} &= I14 + I44 + I74 + I104 \\ \text{Cooperation} &= I19 + I49 + I79 + I109 \\ \text{Modesty} &= I24 + I54 + I84 + I114 \\ \text{Sympathy} &= I29 + I59 + I89 + I119 \end{aligned}$$

which resulted in a CFI of 0.979.

And finally, the Conscientiousness model:

$$\begin{aligned} \text{Self Efficiency} &= I5 + I35 + I65 + I95 \\ \text{Orderliness} &= I10 + I40 + I70 + I100 \\ \text{Dutifulness} &= I15 + I45 + I75 + I105 \\ \text{Achievement Striving} &= I20 + I50 + I80 + I110 \\ \text{Self Discipline} &= I25 + I55 + I85 + I115 \\ \text{Cautiousness} &= I30 + I60 + I90 + I120 \end{aligned}$$

with a CFI value equal to 0.98, which is the highest among the rest of IPIP120 models.

Overall and based on the CFI values, the models have relatively good fit, with values greater than 0.95, indicating that the specified models capture a substantial proportion of the covariance patterns between the observed variables.

5 Conclusion

The automated specification search using the PSO provides a valuable contribution to effectively identifying a good model, which captures the latent variables relationships within a dataset. It efficiently explores the solution space and finds near-optimal models. The search process is guided by fit measures that evaluate the model fit, such as SRMR, CFI, and RMSEA. By integrating these fit measures into the objective function, the algorithm aims to find models that best align with the observed data while considering the trade-off between model complexity and fit, through the *lambda* hyperparameter.

The PSO algorithm optimizes the hyperparameters, including the cut off values for each fit measure, the steepness of the function and the penalty parameter, which play crucial roles in capturing the latent variables and factors within the dataset. By exploring different combinations and values of these

hyperparameters, the algorithm identifies the settings that result in a model fit. The contribution of the automated specification search lies in its ability to efficiently search the solution space and identify the optimal model that best captures the underlying relationships and structures in the data. Overall, the automated specification search using the PSO metaheuristics algorithm provides a powerful tool to uncover latent variables within a dataset, given that there is the appropriate hyperparameter tuning.

6 Discussion

6.1 Findings and Insights

The integration of PSO with SEM provides a novel approach for model identification with hyperparameter adjustment. By combining the strengths of these two methodologies, exploration of complex relationships and discovery of latent variables in data, can be efficient. The use of PSO allows for effective optimization of the model's fit, while SEM provides a comprehensive framework for examining underlying structures and causal pathways. The findings from the analysis of the Dark Triad and IPIP120 datasets revealed the impact of specific hyperparameters and their combinations on the examined dataset. It was highlighted that *lambda*, *slope* and in some cases the SRMR cut off value (c_1), influence the CFI performance the most. The transferability of the selected hyperparameters, was examined across different datasets using the optimal values from the Dark Triad analysis as a starting point for the IPIP120 dataset. While the initial combination showed promising results, further testing and refinement were conducted to ensure the applicability of the hyperparameters to different contexts. This approach demonstrated the need for dataset-specific exploration and adjustment to achieve optimal model fit.

6.2 Limitations

There are several limitations that should be considered in this research. Due to time constraints, it was not possible to exhaustively explore all possible hyperparameter combinations. This limitation restricts the comprehensive evaluation of different settings and may have limited the identification of the optimal configuration for the models. Additionally, it should be noted that in some cases, the lavaan package required the use of the "optim.force.converged = TRUE" parameter to obtain convergence and view the results, indicating potential issues with model convergence, and forcing the result, that could be inaccurate. Also, more complex models, that could potentially provide deeper insights into the underlying relationships, require at least 12 hours for a single run.

APPENDIX A

A.1. Dark Triad Results

p_1	p_2	p_3	$slope$	λ	CFI	p_1	p_2	p_3	$slope$	λ	CFI
0.08	0.95	0.06	-30	0.25	0.8975447	0.1	0.98	0.09	-20	0.27	0.81965
0.08	0.95	0.06	-55	0.25	0.8898366	0.1	0.98	0.09	-17	0.25	0.81842
0.08	0.95	0.06	-30	0.5	0.8888708	0.1	0.98	0.09	-20	0.26	0.81172
0.08	0.95	0.06	-30	0.1	0.8669237	0.1	0.98	0.06	-55	0.5	0.79357
0.1	0.98	0.09	-20	0.17	0.864	0.1	0.98	0.09	-55	0.5	0.79357
0.1	0.98	0.09	-20	0.19	0.864	0.05	0.95	0.09	-55	0.5	0.79288
0.08	0.95	0.06	-55	0.5	0.8550302	0.08	0.98	0.09	-55	0.5	0.78731
0.12	0.98	0.09	-20	0.25	0.8512312	0.1	0.95	0.06	-55	0.5	0.78665
0.1	0.98	0.09	-25	0.25	0.8393729	0.08	0.98	0.06	-55	0.5	0.78638
0.1	0.98	0.09	-20	0.25	0.8379451	0.1	0.93	0.03	-55	0.5	0.77626
0.1	0.98	0.09	-30	0.25	0.8303871	0.1	0.95	0.03	-55	0.5	0.77626
0.12	0.98	0.09	-25	0.25	0.8171378	0.1	0.93	0.06	-55	0.5	0.77552
0.12	0.98	0.09	-30	0.25	0.8086524	0.08	0.93	0.06	-55	0.5	0.77513
0.15	0.98	0.09	-20	0.25	0.7965048	0.08	0.95	0.03	-55	0.5	0.76988
0.08	0.95	0.06	-55	0.1	0.7762625	0.1	0.93	0.09	-55	0.5	0.76988
0.08	0.95	0.06	-70	0.1	0.7762625	0.1	0.95	0.09	-55	0.5	0.76988
0.08	0.95	0.06	-70	0.25	0.7762625	0.08	0.95	0.09	-55	0.5	0.76744
0.08	0.95	0.06	-70	0.5	0.7762625	0.1	0.98	0.03	-55	0.5	0.73254
0.15	0.98	0.09	-25	0.25	0.782408	0.05	0.93	0.06	-55	0.5	0.12746
0.15	0.98	0.09	-30	0.25	0.781902	0.05	0.98	0.06	-55	0.5	0.11025
0.1	0.98	0.09	-20	0.16	0.87334	0.05	0.98	0.03	-55	0.5	0.10464
0.1	0.98	0.09	-20	0.15	0.86508	0.05	0.95	0.03	-55	0.5	0.10397
0.1	0.98	0.09	-20	0.21	0.85231	0.05	0.93	0.03	-55	0.5	0.09654
0.1	0.98	0.09	-19	0.25	0.85045	0.05	0.95	0.06	-55	0.5	0.09654
0.1	0.98	0.09	-20	0.2	0.85042	0.1	0.98	0.09	-20	0.24	0.8415
0.1	0.98	0.09	-20	0.23	0.84914	0.1	0.98	0.09	-20	0.28	0.7965
0.1	0.98	0.09	-20	0.25	0.84485	0.05	0.98	0.09	-55	0.5	0.7819
0.1	0.98	0.09	-20	0.22	0.83781	0.08	0.98	0.03	-55	0.5	0.06891
0.1	0.98	0.09	-15	0.25	0.83732	0.08	0.93	0.03	-55	0.5	0.77
0.1	0.98	0.09	-25	0.25	0.83407	0.08	0.95	0.06	-55	0.5	0.77
0.1	0.98	0.09	-21	0.25	0.83039	0.05	0.93	0.09	-55	0.5	0.77
0.1	0.98	0.09	-23	0.25	0.83039	0.08	0.93	0.09	-55	0.5	0.77
0.1	0.98	0.09	-20	0.18	0.83025						

A.2. Different Seeds Dark Triad

Try	Model 1	Try	Model 2	Try	Model 3
1	0.874	1	0.866	1	0.851
2	0.862	2	0.877	2	0.872
3	0.853	3	0.879	3	0.857
4	0.869	4	0.888	4	0.806
5	0.884	5	0.877	5	0.854
6	0.862	6	0.86	6	0.835
7	0.836	7	0.849	7	0.87
8	0.86	8	0.898	8	0.866
9	0.901	9	0.866	9	0.87
10	0.837	10	0.863	10	0.858
11	0.851	11	0.846	11	0.835

A.3. Extraversion Model Results

p_1	p_2	p_3	λ	slope	gen	pop	CFI	p_1	p_2	p_3	λ	slope	gen	pop	CFI
0.1	0.98	0.09	0.2	-20	10	15	0.972	0.08	0.95	0.06	0.5	-40	10	15	0.899
0.08	0.95	0.06	0.4	-55	10	15	0.972	0.08	0.95	0.06	0.7	-55	10	15	0.899
0.08	0.95	0.06	0.4	-55	10	15	0.972	0.08	0.95	0.06	0.5	-55	10	15	0.899
0.1	0.98	0.09	0.2	-20	10	30	0.969	0.08	0.95	0.06	0	-55	10	15	0.97
0.08	0.98	0.08	0.2	-20	10	15	0.969	0.08	0.95	0.06	0.1	-55	10	15	0.97
0.08	0.98	0.08	0.2	-30	10	15	0.969	0.08	0.95	0.03	0.1	-55	10	15	0.97
0.08	0.99	0.06	0.2	-55	10	15	0.969	0.08	0.95	0.04	0.1	-55	10	15	0.97
0.08	0.95	0.06	0.2	-55	10	15	0.968	0.08	0.95	0.05	0.1	-55	10	15	0.97
0.08	0.96	0.06	0.2	-55	10	15	0.968	0.08	0.95	0.06	0.1	-55	10	15	0.97
0.08	0.97	0.06	0.2	-55	10	15	0.968	0.08	0.95	0.07	0.1	-55	10	15	0.97
0.08	0.98	0.06	0.2	-55	10	15	0.968	0.08	0.95	0.08	0.1	-55	10	15	0.97
0.08	0.95	0.06	0.2	-55	10	15	0.968	0.08	0.95	0.09	0.1	-55	10	15	0.97
0.08	0.93	0.06	0.1	-55	10	15	0.968	0.03	0.95	0.06	0.1	-55	10	15	0.97
0.1	0.98	0.09	0.2	-20	25	30	0.965	0.04	0.95	0.06	0.1	-55	10	15	0.97
0.1	0.98	0.09	0.2	-20	25	15	0.963	0.05	0.95	0.06	0.1	-55	10	15	0.97
0.08	0.95	0.06	0.3	-55	10	15	0.963	0.06	0.95	0.06	0.1	-55	10	15	0.97
0.08	0.95	0.06	0.5	-55	50	30	0.956	0.07	0.95	0.06	0.1	-55	10	15	0.97
0.08	0.95	0.06	0.5	-55	50	30	0.956	0.08	0.95	0.06	0.1	-55	10	15	0.97
0.08	0.95	0.06	0.5	-55	25	30	0.956	0.09	0.95	0.06	0.1	-55	10	15	0.97
0.08	0.95	0.06	0.5	-55	25	15	0.953	0.08	0.94	0.06	0.1	-55	10	15	0.97
0.08	0.95	0.06	0.5	-55	15	30	0.899	0.08	0.95	0.06	0.1	-55	10	15	0.97
0.08	0.95	0.06	0.5	-55	10	30	0.899	0.08	0.96	0.06	0.1	-55	10	15	0.97
0.08	0.95	0.06	0.5	-55	10	15	0.899	0.08	0.97	0.06	0.1	-55	10	15	0.97
0.08	0.95	0.06	0.5	-20	10	15	0.899	0.08	0.98	0.06	0.1	-55	10	15	0.97
0.08	0.95	0.06	0.5	-30	10	15	0.899	0.08	0.99	0.06	0.1	-55	10	15	0.97

A.4. Different Seeds Extraversion Model

<i>Try</i>	<i>E1</i>	<i>Try</i>	<i>E2</i>	<i>Try</i>	<i>E3</i>
1	0.956	1	0.964	1	0.939
2	0.966	2	0.966	2	0.896
3	0.969	3	0.956	3	0.964
4	0.963	4	0.969	4	0.878
5	0.97	5	0.966	5	0.9
6	0.961	6	0.967	6	0.944
7	0.963	7	0.949	7	0.88
8	0.972	8	0.974	8	0.963
9	0.957	9	0.959	9	0.95
10	0.969	10	0.963	10	0.888
11	0.962	11	0.969	11	0.957

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