RANDOM, FACTOR, OR NETWORK MODEL? PREDICTIONS FROM NEURAL NETWORKS

PSYARXIV PREPRINT

Alexander P. Christensen
Department of Neurology
University of Pennsylvania
Philadelphia, PA, 19104
alexpaulchristensen@gmail.com

Hudson Golino
Department of Psychology
University of Virginia
Charlottesville, VA, 22903
hfg9s@virginia.edu

September 29, 2020

ABSTRACT

The nature of associations between variables is important for constructing theory about psychological phenomena. In the last decade, this topic has received renewed interested with the introduction of psychometric network models. In psychology, these models are often contrasted with latent variable (e.g., factor) models. Recent research has shown that differences between the two tend to be more substantive than statistical. One recently developed algorithm called the *Loadings Comparison Test* (LCT) was developed to predict whether data were generated from a random, factor, or network model. A significant limitation of current LCT implementation is that it's based on heuristics that were derived from descriptive statistics. In the present study, we used artificial neural networks to replace these heuristics, and develop a more robust and generalizable algorithm. We performed a simulation study that compared neural networks to the original LCT algorithm as well as logistic regression models that were trained on the same data. We found that the neural networks performed as well as or better than both methods, demonstrating generalizablity across data generating models. We echo the call for more formal theories about the relations between variables and discuss the role of the LCT in this process.

***K*eywords** neural networks · machine learning · data generating mechanisms · factor model · network psychometrics

1 Introduction

The nature of associations between observable variables is one of the most critical considerations for constructing theory about psychological phenomena (Borsboom, van der Mass, Dalege, Kievet, & Haig, 2020; Haslbeck, Ryan, Robinaugh, Waldorp, & Borsboom, 2019). Whether variables are associated because they all have a common cause or because they reciprocally cause and effect one another is (ideally) theorized by the researcher and (often) implied by their choice of psychometric model (Borsboom, 2006; Haslbeck et al., 2019). Determining whether empirical data are generated by one of these mechanisms is therefore an important question. Although other possibilities exist (Kruis & Maris, 2016; Marsman et al., 2018), these two explanations are perhaps the most common perspectives in psychology and correspond to latent variable and network models, respectively. The debate over the plausibility of these mechanisms has sparked renewed interest in the ontology and epistemology of psychological phenomena (Borsboom, 2008; Guyon, Falissard, & Kop, 2017).

In the last few years, the apparent differences between these models have been shown to be more substantive than statistical (Guyon et al., 2017), with several studies demonstrating that they can produce statistically equivalent data structures (Hallquist, Wright, & Molenaar, 2019; Marsman et al., 2018; van Bork et al., 2019; Waldorp & Marsman, 2020). Indeed, recent simulation studies have demonstrated that network models can produce latent dimensions and loadings that are equivalent to their factor counterparts when the data are generated from a factor model (Christensen & Golino, 2020; Golino & Epskamp, 2017; Golino, Shi, et al., 2020). These findings suggest that if the statistical structure

of the data are similar to that of a factor model, then there will be little difference between the statistical representations of factor and network models. These equivalent statistical representations have led some to propose a "one-to-many" mapping of data structure to generating models (Marsman et al., 2018; van Bork et al., 2019).

Despite similar statistical structures, their substantive interpretations and representations imply different data generating mechanisms. For a common cause model, this is usually provided by latent variable (or factor) models where an unobservable variable is thought to cause the associations between observable variables (Edwards & Bagozzi, 2000). This model is statistically achieved by regressing the latent variable on the observable variables and depicted by arrows pointing from the latent variable to the observable variables. For a network model, observable variables are represented as nodes (circles) and their (unique) associations are represented as edges (lines) between the nodes. These models are statistically achieved by regressing the association between every pair of variables on all other variables (i.e., partial correlations), suggesting mutually reinforcing interactions (van der Maas et al., 2006). The implications of these different data generating mechanisms can be significant: Should clinicians treat an underlying psychopathological disorder or the symptoms that constitute the disorder (Borsboom, 2017)?

In the present research, we set out to develop a test to determine whether data were generated from a factor or network model. Such a test provides researchers with a tool to explore whether the data are structured more like their hypothesized data generating mechanism. Although data generated from either model can fit and be represented by the other (van Bork et al., 2019; van der Maas et al., 2006), researchers should attempt to design and use measures that align with their theoretical perspective (Christensen et al., 2020). One recent development called the *Loadings Comparison Test* (LCT) compares loadings from network and factor models with an equivalent number of dimensions to predict whether data were generated from a random, factor, or network model (Christensen & Golino, 2020). The use of loading structures serves as a summary of the overall data structure. In its current form, the LCT relies on descriptive heuristics, which are unlikely to generalize across many data conditions. To make the algorithm more robust, we used artificial neural networks from machine learning to improve the algorithm so that it generalizes to a broader set of conditions. We then performed a simulation study to evaluate whether these models outperform the original heuristic-based algorithm and a set of regularized logistic regression models.

2 Loadings Comparison Test

The LCT was inspired by van Bork et al. (2019) who demonstrated that unidimensional factor models and sparse network models provide subtle statistical differences that offer inference into whether empirical data are more likely to be generated from one or the other. In their paper, they identify two key differences: (1) the proportion of partial correlations that have a different sign than the corresponding zero-order correlations and (2) the proportion of partial correlations that are stronger than the corresponding zero-order correlations. The empirical value of these proportions are then compared against the distributions of data generated from factor and network models applied to simulated empirical covariance matrices. The model with the greater probability mass of the distribution is determined to be the most likely model. They referred to this test as the *Partial Correlation Likelihood Test*.

The Partial Correlation Likelihood Test is grounded in statistics and provides an explicit test for determining whether data were more likely to be generated from a factor or network model in unidimensional data structures. Although unidimensional structures are critical to psychology, the Partial Correlation Likelihood Test may not generalize to more complex models (e.g., multidimensional models; van Bork et al., 2019). The LCT was motivated by the need for such a test in multidimensional data. The development of the LCT was based on the descriptive differences between factor and network loadings when data were generated from a random, factor, or network model. Network loadings—the standardized sum of each node's connections to nodes in each dimension in the network—were demonstrated to be roughly equivalent to factor loadings when generated from a factor model, but different from factor loadings when data were generated from a random correlation matrix (i.e., random model) or small-world network model (Christensen & Golino, 2020).

The LCT was developed based on these differences, and heuristics were developed that were founded partly in theory and partly in simulated descriptive statistics. The algorithm works as follows: generate data from a multivariate normal distribution from the empirical covariance matrix, estimate the number of dimensions using exploratory graph analysis (EGA; a network psychometrics approach for dimension identification; see SI1 and Golino, Shi, et al., 2020 for a more detailed explanation), compute network and factor loadings using the same number of dimensions identified by EGA (see SI2 and Christensen & Golino, 2020 for a more detailed explanation of network loadings), and compute the proportion of loadings that are greater than or equal to small, moderate, and large effect sizes as well as dominant and cross-loadings that are greater than or equal to small effect sizes. Afterwards, compute several statistics that are used to determine the plausible data generating model: (1) the average number of moderate and large effect size factor loadings

that were equivalent, (2) the ratio of small effect size or larger network and factor loadings, and (3) the log ratio of dominant and cross-loadings that were a small effect size or larger for factor loadings.

The first statistic is used to determine whether data were generated from a random or non-random model. A proportion less than or equal to .20 (or 20% of the bootstrap samples) would suggest the data were generated from a random model; otherwise, it's suggested to be from a non-random model. If determined to be from a non-random model, then the second statistic is used to determine whether the data were generated from a network model: a ratio of small effect size or larger for network and factor loadings that was greater than 1.5 would suggest a network model; otherwise, check the third statistic. If the third statistic was greater than than 5, then suggest a factor model; otherwise, suggest a network model. Although relatively simple, these heuristics performed remarkably well in simulated samples: accuracies were 95.7% for random models, 77.9% to 100% for factor models, and 87.8% to 95.8% for network models (Christensen & Golino, 2020).

Despite high accuracy for all models, there were a few limitations in their simulation. First, the simulated models used novel data but with the same data structures that the descriptive statistics (and therefore heuristics) were derived from. Second, the simulated data conditions were limited to manipulating only a few parameters per model. The number of variables, for example, was held constant at fifteen, and factor models were always generated with three factors and five variables per factor. Finally, the sample sizes were all generated with 1000 cases, which is large relative to many samples used in psychology. These limitations are likely to result in overfitting and a lack of generalizability to other samples and data structures. These limitations motivated the current study where we sought to improve the LCT algorithm by replacing these descriptive heuristics with more sophisticated neural networks.

3 Artifical Neural Networks

Artificial neural networks are a commonly used technique in machine learning research (Dreiseitl & Ohno-Machado, 2002). They come in many forms but perhaps the most basic are feed-forward networks where data are input as nodes and are "fed through" as series of regressions in the network to output nodes (i.e., the prediction). The input and output nodes are known a priori and correspond to what we would like the neural network to "learn." In our study, the input corresponded to the network and factor loading proportions we've already described (i.e., small, moderate, large, dominant, and cross-loadings), which are derived from simulated data. Because the data are simulated, we also know the output, which corresponds to whether the data were generated from a random, factor, or network model. In between the input and output nodes are the *hidden layers* where the model learns the appropriate weighting scheme that optimizes the prediction of the output from the input nodes.

A neural network with no hidden layers can represent linear functions only and is equivalent to a standard regression model (e.g., an output node with a sigmoid activation function is a logistic regression model). With a single hidden layer, a neural network can approximate "any function that has a continuous mapping from one finite space to another" (Heaton, 2008). Two hidden layers can represent any arbitrary boundary (e.g., non-linear functions), approximating any mapping between the input and output (Hornik, 1991; Sontag, 1991). Because of this latter fact, it's been argued that more than two hidden layers is usually unnecessary (Heaton, 2008). A key question, however, is how *many* neurons (or nodes) should be in each of the hidden layers. The number of neurons will affect the amount of abstraction the hidden layers can afford: more neurons lead to more complex abstractions. Although two hidden layers may be all that are necessary, the number of neurons to approximate any arbitrary function may be numerous. This has led to the development of *deep neural networks* (Schmidhuber, 2015), which typically have three or more hidden layers. Just as with the number of neurons, the deeper the network, the more complex abstractions can be obtained. Importantly, deeper networks allow for fewer neurons to be in each layer to obtain similar levels of abstraction because the abstractions get increasingly more complex with each layer than when simply adding a few neurons to a previous layer.

One of the advantages of neural networks is that they can learn mappings between input and outcomes that are difficult for humans to immediately understand. In our case, going beyond simple descriptive heuristics to mapping loading structures to the data generating model. An important concept for neural network learning is *backpropogation*. Backpropogation refers to the adjustment of weights and biases in the network (starting from the output *back* to the input; Watt, Borhani, & Katsaggelos, 2016). In training, *batches* or a certain number of samples of the data are fed through the network's weights and predictions are made about the output. With each batch, the network updates its weights and biases by trying to minimize the loss of information between the predicted output and the actual output. The end goal is to minimize the loss of information between the predicted and actual output to maximize the accuracy of its predictions.

4 Simulation 1: Training Neural Networks

Our first simulation set out to build and train a set of neural networks to predict whether data were generated from a random, factor, or network model. Such a strategy is often referred to as an *ensemble* of networks (Zhou, Wu, & Tang, 2002) where each network is fine-tuned to a specific part of the problem to improve the overall prediction of a more complex problem. We parsed the complex problem of predicting the data generating model into four more specific problems: random vs. non-random model, factor model with low correlations between factors (.00 and .30) vs. network model, factor model with high correlations between factors (.50 and .70) with variables per factor greater than the number of factors vs. network model, and factor model with high correlations between factors with variables per factor less than or equal to the number of factors vs. network model. The random vs. non-random model is termed a "one-versus-all" classification; the factor vs. network models are termed "one-versus-one" classification (James, Witten, Hastie, & Tibshirani, 2013). The rationale for building several neural networks to predict different factor models from network models is that different information is likely to be more relevant for one set of factor models than another (primarily along the lines of the magnitude of correlations between factors). These separate models therefore allow different weighting schemes for each problem (even if they have the same *architecture* or number of hidden layers and nodes in those layers).

Correlations between factors are expected to be the most consequential parameter because they increase the extent to which there are cross-loadings and therefore the extent to which a factor model begins to have similar characteristics (e.g., loading structure) as a network model, especially in the case where there are high correlations between factors and variables are equal to or less than the number of factors. Because of this, we trained four neural networks with ten common inputs for all models and some additional inputs that were specific to each problem. Below, we describe how we generated the data to train the models and briefly describe important methodological aspects of building and training the neural networks. To determine whether a neural network was necessary, we compared their performance to their corresponding logistic regression models that were regularized using the least absolute shrinkage and selection operator (lasso; Tibshirani, 1996). Logistic regression is commonly used as a comparison method and is useful for determining the expected baseline performance of a neural network model (Dreiseitl & Ohno-Machado, 2002).

4.1 Data Generation

The training of our neural networks started with the generation of large amounts of data from random, factor, and network models. Our data generation for all models followed the approach described in Christensen and Golino (2020). We briefly detail how data for each model was generated here (for greater detail, we refer the reader to Christensen & Golino, 2020).

4.1.1 General parameters

All data were generated as continuous variables and sample sizes for all models were generated with 250, 500, and 1000 cases. For each model (random, factor, and network), a total of 240,000 samples were generated, resulting in 720,000 total samples. An equal number of samples was important to reliably train the neural networks so as to not bias them toward any one model.

4.1.2 Random model

Random variables, X_n, were generated from a normal distribution with a mean of zero and a standard deviation of five. The number of variables, n, were manipulated using 15, 20, 25, 30, and 35 variables. From these variables, a variance-covariance matrix was computed, decomposed using Cholesky decomposition, inversed, and pre-multiplied by the original data to obtain new (independent) variables. A separate $n \times n$ correlation matrix was generated from a random normal distribution with a mean of 0 and variance of 0.10. The diagonal of the correlation matrix was set to 1 and decomposed using Cholesky decomposition. This matrix was pre-multiplied by the independent variables to obtain the final data. For each condition (15 in total; sample size $\times$ number of variables), 16,000 samples were generated.

4.1.3 Factor model

Data generation for the factor models followed Golino, Shi, et al. (2020) where data were generated from a multivariate normal distribution by creating a reproduced population correlation from a factor loading matrix and correlation matrix. Cholesky decomposition was then performed on the reproduced population correlation matrix. If the population matrix was not positive definite, then data were re-generated following this procedure. The sample data was derived by post-multiplying data from a random multivariate distribution to the decomposed reproduced correlation matrix.

We manipulated number of variables per factor (3, 4, 5, 6, and 7), number of factors (3, 4, 5, and 6), and correlations between factors (.00, .30, .50, and .70). Importantly, as the magnitude of the correlations between factors increased, so too did the magnitude of the cross-loadings (following Christensen & Golino, 2020). Specifically, cross-loadings were drawn from a random normal distribution with a mean of 0 and standard deviation of .050, .075, .100, and .125, respectively. This allowed both positive and negative cross-loadings to be produced as well as larger loadings to appear when correlations between factors were large. Factor loadings on the dominant factors were randomly drawn from a uniform distribution with a minimum of .40 and maximum of .70. In total, there were 240 conditions (sample size $\times$ number of variables per factor $\times$ number of factors $\times$ correlations between factors). For each condition, 1,000 samples were generated.

4.1.4 Network model

In contrast to previous simulation studies on psychological networks which have generated data from random network models (e.g., Epskamp, Rhemtulla, & Borsboom, 2017; van Bork et al., 2019; Williams, Rhemtulla, Wysocki, & Rast, 2019), we generated all network models based on small-world networks. Despite being the most widely studied type of network, random network models are largely incongruous with most real-world networks (e.g., lack of clustering, no correlation between degrees of adjacent nodes, shape of degree distribution; Newman, 2010). Small-world networks, however, at least mirror some properties of real-world networks (e.g., clustering, shortcuts between nodes; Newman, 2010) and are commonly found in real-world networks (e.g., brain networks; Muldoon, Bridgeford, & Bassett, 2016). Therefore, small-world networks are more likely to represent many psychological phenomena (e.g., psychopathology; Borsboom, Cramer, Schmittmann, Epskamp, & Waldorp, 2011). Moreover, the structure of small-world networks (high clustering and low distances between nodes) are closer to structures produced by factor models than random networks. We generated small-world networks by adapting the `bdgraph.sim` algorithm in the *BDgraph* package (Mohammadi & Wit, 2015) in R (R Core Team, 2020) to incorporate the `sample_smallworld` function from the *igraph* package (Csardi & Nepusz, 2006).

The algorithm starts by generating a binary undirected small-world network that follows the Watts-Strogatz model (Watts & Strogatz, 1998). Next, following Williams et al. (2019), the weights are drawn from a *G*-Wishart distribution corresponding to 90% of partial correlations within $\pm$.40. As Williams et al. (2019) notes, large networks are more likely to have smaller partial correlations due to more variance being partialled out; however, given that many psychological assessment instruments have redundancies (Christensen et al., 2020), partial correlations as large as .40 may not be uncommon even when there are a large number of variables. Therefore, we allowed networks, regardless of the number of variables, to have weights $\pm$.40. The distribution of the absolute values of these weights were typically positively skewed.

Small-world networks have two parameters that can be manipulated: neighborhood and rewiring probability. The *neighborhood* of a small-world network refers to the number of nodes that each node is connected to in the initial lattice structure. Rather than using different neighborhood sizes, we used network density or the number of edges present divided by the total number of edges instead. To translate network density into neighborhood size, we computed the total number of edges given a certain number of variables ($\frac{n(n-1)}{2}$) and multiplied it by our desired density, producing the number of edges present in the network. The number of edges present in the network was then divided by the number of variables (i.e., n) and rounded to the nearest integer to obtain the neighborhood size. The *rewiring probability* refers to the probability that any one node's connection would be randomly connected to another node in the network (0 = lattice network, 0.01–0.10 = typical small-world network, and 1 = random network).

We manipulated number of variables (10, 20, 30, and 40), density (.20, .40, .60, and .80), and rewiring probability (.01, .05, .10, .25, and .50). In total, there were 240 conditions (sample size $\times$ number of variables $\times$ neighborhood $\times$ rewiring probability). For each condition, we generated 1,000 samples.

4.2 Neural Networks

4.2.1 Building neural networks

Formal articles on steps for how to train neural networks appropriately are sparse; however, there are several resources available. Our approach followed Andrej Karpathy's (Senior Director of Artificial Intelligence at Tesla) "recipe" for training neural networks (Karpathy, 2019). This recipe starts with thoroughly inspecting the data distributions and looking for patterns (which we used to develop additional inputs), developing a neural network skeleton by making a simplified model, overfitting a small portion of samples (e.g., 100) from the data, regularizing the model to prevent overfitting (e.g., early stopping), optimizing hyperparameters (e.g., number of nodes and hidden layers, learning rate, batch size), and using neural network ensembles (which we described earlier). To prevent overfitting the training data, we added *early stopping* criterion: when the validation loss plateaued (i.e., decreases in the loss function less than .001)

for ten epochs (or ten runs through the entire training dataset; Prechelt, 2012), then the best weights (highest training accuracy) were kept and used as our model.

4.2.2 Input nodes

Following Christensen and Golino's (2020) LCT algorithm, we submitted each dataset to EGA and EFA (using the same number of dimensions as estimated by EGA). For both the network and factor loadings, we computed the proportion of loadings that were greater than small (.15 and .40, respectively), moderate (.25 and .55, respectively), and large (.35 and .70, respectively) effect sizes as well as the proportion of loadings that were greater than small effect sizes for dominant and cross-loadings (Christensen & Golino, 2020; Comrey & Lee, 2013). For each dataset, this created 10 proportions in total (five proportions for each loading type) that were used as the base input nodes for all neural networks.

Additional input nodes were created by computing the ratio between the exponent of a base network loading (i.e., small, moderate, large, dominant, and cross) and the exponent of the corresponding base factor loading. To normalize these ratios to be between zero and one (the same range as the proportions), we used min-max normalization using the minimum and maximum possible ratio:

$$\frac{x - \frac{\exp(0)}{\exp(1)}}{\frac{\exp(1)}{\exp(0)} - \frac{\exp(0)}{\exp(1)}},$$

where x is the ratio between the exponent of a network loading (e.g., small) and the exponent of the corresponding factor loading.

Based on the descriptive statistics and distribution of these ratios, we decided to include or exclude these additional input based on whether there were substantial enough differences between the two models. When additional inputs were used, we mention them in their corresponding neural network descriptions.

4.2.3 Activation functions

Activation functions determine the output from a node given the input to the node, and therefore are influential in the performance of neural networks. All hidden layers for all neural networks used the *Parametric Rectified Linear Unit* (PReLu; He, Zhang, Ren, & Sun, 2015) activation function. The *Rectified Linear Unit* (ReLu; Nair & Hinton, 2010) is the contemporary choice for most applications of deep learning (as opposed to the historically and often still used sigmoid function; Nwankpa, Ijomah, Gachagan, & Marshall, 2018). The ReLu activation function is a non-linear function that returns the input of the function as the output unless the input is negative, which is instead set to zero (inspired by the action potential of biological neurons). One limitation of the ReLu function is that it can cause some neurons to never activate (no matter the input), always outputting zero (known as the "dying neuron problem"; He et al., 2015). PReLu overcomes this issue by allowing a trainable parameter α to be adjusted so that some small non-zero negative weights still activate neurons in the network. When α is zero for a node, then PReLu is equivalent to ReLu. This flexibility of PReLu allows it to perform at least as well as ReLu. For all output layers, we used the sigmoid function ($\frac{e^x}{e^x+1}$) to estimate the probability of a given sample belonging to the outcome model (i.e., the model designated as 1 in the output). A cut-off probability of .50 was used to determine what model the sample belonged to (e.g., random vs. non-random model, factor vs. network model).

4.2.4 Gradient descent optimizers

For all models, we used the *Nestorov Adaptive Moment Estimation* optimizer (NADAM; Dozat, 2016), which tends to be the contemporary choice of neural networks (Ruder, 2016). The details of gradient descent optimizers are beyond the scope of this paper; however, their purpose are to minimize their functions by iteratively moving towards the steepest part of the *gradient* or slope of the loss function (Watt et al., 2016). At each iteration, the algorithm takes certain sized steps on the gradient, which are called the *learning rate*. Higher learning rates lead to larger steps toward a loss minimum but can potentially over-step a more optimal minimum; lower learning rates are more likely to reach an optimal minimum but take more time to get there. NADAM is an adaptive algorithm that changes the learning rate over time in order to achieve appropriate descent. The foundation of this algorithm is based on the Adaptive Moment Estimation (ADAM) optimizer (Kingma & Ba, 2014), but uses an alternative momentum parameter called Nesterov's accelerated gradient momentum (NAG; Sutskever, Martens, Dahl, & Hinton, 2013). In NADAM, NAG moves toward an intermediate direction and then corrects toward the gradient, which allows the momentum to be shifted toward the minimum (even after moving past the minimum; for more details, see Dozat, 2016).

4.2.5 Loss and accuracy

Gradient descent optimizers aim to minimize a loss function or the error between the actual and predicted outcomes. In our neural networks, this was *binary cross entropy* or logarithmic loss. Binary cross entropy is defined as the distance between two probability distributions (e.g., actual and predicted outcomes) and mathematically represented as:

$$CE = -\big(y\log(p) + (1-y)\log(1-p)\big),$$

where y is the actual model and p is the predicted probability of the dataset belonging to the model. If $y = 1$, then CE; otherwise, if $y = 0$, then $1 - CE$.

Binary accuracy was our accuracy measure, which is the mean of correct identifications in the total sample. The accuracy typically corresponds to loss but not necessarily. This is because correct model identifications are part of the binary cross entropy equation. Their difference arises in the fact that binary cross entropy considers the probability in which a dataset belongs to the correct model. In the random vs. non-random model, for example, a probability $\geq .50$ would be considered a random model (1); otherwise, its considered a non-random model (0). A correct identification would be a 1 but its probability could be as low as .50. In terms of binary cross entropy, a correct identification could range from 0 ($p = 1$) to 0.693 ($p = .50$). Therefore, loss is informative about the decisiveness of the predictions and accuracy is informative about the correctness of the predictions.

4.2.6 Training neural networks

Models were set up with a certain number of samples, which were then split into the original training (80% of the overall sample) and validation (20% of the overall sample) samples. The original validation samples are then completely held out of the model training phase and were only seen after the model had been trained. The original training samples were used to train the model. During training, the original training samples are further split into a new training dataset (80% of the training samples) and validation dataset (20% of the training samples). This new training dataset is then randomly sampled without replacement with a specific number of *batch sizes* (number of training samples used in each update of the gradient and weights). After all of the new training dataset samples have been used once, the model is tested using the new validation dataset.

Loss and accuracy metrics are then provided with the training loss and accuracy representing the last model in the epoch and the validation loss and accuracy representing the performance of this last model on the validation dataset. The conclusion of a single run of this process is called an *epoch*. Each new epoch will randomly draw samples without replacement from the original training samples and form new training and validation datasets (a process known as *shuffling*). For all neural networks, we set the total number of epochs to 100 to allow training to proceed as necessary to settle into a minimum. Training was terminated when either the epochs reached 100 or our early stopping criterion was reached (i.e., decrease in validation loss less than .001 for ten consecutive epochs). After training was terminated, the final model was then tested on the original validation samples, which are considered to be novel because they had not been seen during the training of the model.

As a baseline comparison model, we trained the lasso regularized logistic regression models on the same original training data using the same input variables used in the neural networks. Regularized logistic regression models were chosen as a comparison for two reasons: (1) logistic regression models tend to perform better than other machine learning classification methods, such as support vector machines and decision trees, when there are overlapping classes, and (2) regularization reduces the flexibility of the model, which makes it less likely to overfit the underlying function in the training data and more likely to generalize to other data conditions (James et al., 2013). The use of logistic regression models provide inference into whether more complex neural networks are necessary. The coefficients of each trained logistic model were extracted and then solved for each case of the original validation dataset. Accuracy and loss were then computed for the original validation dataset.

4.2.7 Feature importance

In order to determine the importance of each input into each neural network, we computed a measure of feature importance on the original validation datasets that were held out of the original training datasets following Fisher, Rudin, and Dominici (2019). The approach works by permutating each input variable one-by-one and computing the loss. The loss is then divided by the original loss to obtain the relative decrease in performance for the permutated input. Because of the stochasticity of the permutations, we computed this analysis ten times and computed the mean of the values. Values greater than one suggest the input was important with larger values suggesting greater importance whereas values near one suggest that the input did not improve the model and less than one suggest that the input made the model worse.

4.3 Data Analysis

All analyses were performed in R. All neural networks were trained using the *keras* package (Allaire & Chollet, 2020) and all logistic regression models were fit with the *glmnet* package (Friedman, Hastie, & Tibshirani, 2010). All data, R code and scripts are available on the Open Science Framework (OSF). Each neural network is available on the OSF and can be further fine-tuned and improved with new data and examples (i.e., the models can be further trained with new models, data conditions, and methods of data generation).

5 Results

The mean proportions of the base network and factor loadings across each data generating models are presented in Figure 1.

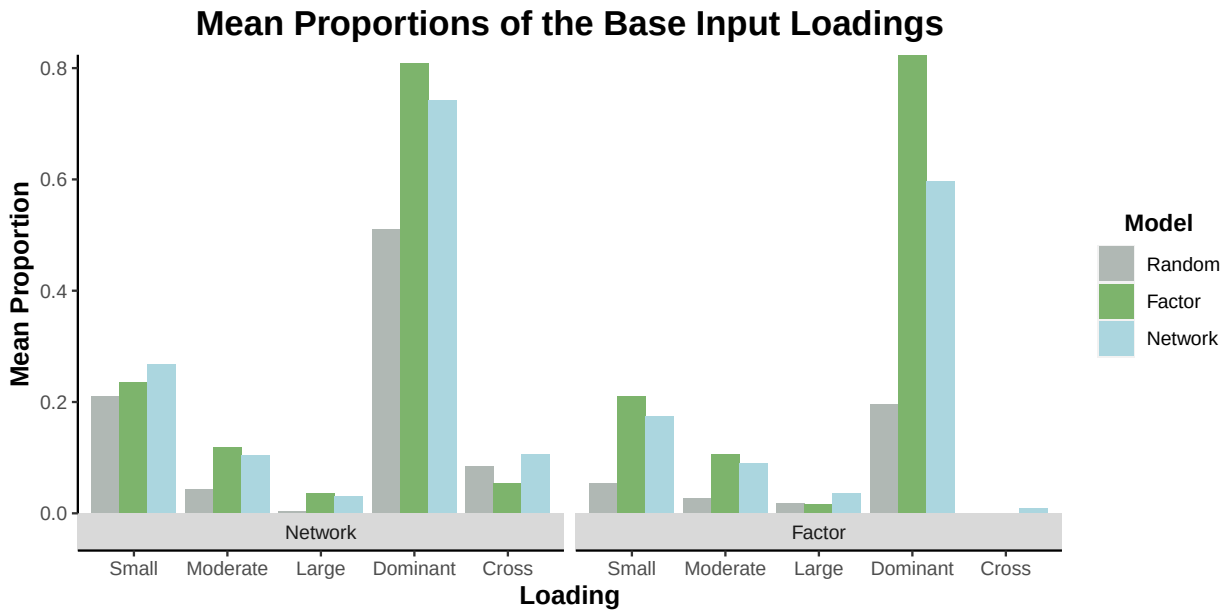

Figure 1: Mean proportions of the base input loadings for the neural network models.

The most glaring differences between models are proportion of dominant loadings that achieve a small effect size or larger for both network and factor loadings. Data generated from a random model had a substantially smaller mean especially for the factor loadings. This difference is smaller but also apparent for data generated from network models. Table 1 presents a summary of the architecture the neural networks including the parameters and validation estimates.

Table 1: Neural Network Architectures, Parameters, and Metrics

				Neural Network		Logistic Regression	
Model	Architecture	Batch Size	Learning Rate	Loss	Accuracy	Loss	Accuracy
1	$12 \times 3 \times 1$	192	.0001	0.038	0.986	0.034	0.988
2	$11 \times 9 \times 1$	64	.0003	0.180	0.928	0.286	0.890
3	$11 \times 9 \times 1$	32	.0005	0.159	0.937	0.257	0.908
4	$11 \times 9 \times 1$	32	.001	0.239	0.902	0.401	0.846

Note. Model: 1 = Random vs. non-random; 2 = low correlation vs. network; 3 = high correlation with variables greater than factors vs. network; 4 = high correlation with variables less than or equal to factors vs. network. Grey boxes denote best values of loss and accuracy for each model.

Across all neural networks, we found comparable or better performance than the logistic regression models, suggesting that the neural networks were reasonable and potentially necessary for optimal performance in the LCT algorithm.

5.1 Model 1: Random vs. Non-random

For the random vs. non-random model, we used the entire dataset and created a binary variable corresponding to random (1) and non-random (0) models (i.e., factor and network). The dataset was then split into a training dataset (576,000 samples or 80% of the sample) and validation dataset (144,000 samples or 20% of the sample). The input of this model consisted of our base input nodes with two additional nodes (small and dominant ratios) and one output node (our binary variable).

There was one hidden layer between the input and output layers containing three nodes. Our final model reached our early stopping criterion on epoch 39. We then evaluated the model on the validation dataset, which achieved a loss of 0.038 and accuracy of 98.6% (Table 1). The logistic regression model was slightly better than the neural network model in loss (0.034) and accuracy (98.8%) but only by narrow margins. The inputs that had the greatest importance were the dominant factor loading (17.80), dominant network loading (4.96), and small factor loading (2.57; Table 2).

5.2 Model 2: Low Correlation Factor vs. Network

For the low correlation factor vs. network model, we removed the datasets corresponding to the data generated from random models (240,000 samples) and factor models with correlations between factors of .50 and .70 (120,000 samples), leaving us with 120,000 samples of orthogonal and low correlations between factors (.00 and .30, respectively). To obtain an equivalent number of datasets generated from the network models, we randomly sampled 40,000 network datasets from each level of sample size (i.e., 250, 500, and 1000), resulting in 120,000 total network datasets. In total, we used 240,000 datasets.

As with Model 1, we created a single binary output variable with 1 corresponding to a factor model and 0 corresponding to not a low correlation factor model. Importantly, it's possible that the learned weights of the low correlation factor model could still correspond to other factor models even though they weren't observed in the trained model. This potential for overlap was on purpose and allowed multiple checks of factor models to be learned against network models in the LCT algorithm (as we describe later in Simulation 2).

The input of this model consisted of our base input nodes along with an additional input: dominant ratio. This made for eleven input nodes in total. There was one hidden layer with nine nodes. Our final model did not reach our early stopping criterion and was terminated after the 100th epoch. We then evaluated the model on the validation dataset, which achieved a loss of 0.180 and accuracy of 92.8%. The neural network model outperformed the regularized logistic regression model by a full tenth in loss and over three percent in accuracy (Table 1). The inputs that had the greatest importance were the cross factor loading (2.57), dominant factor loading (2.55), and large factor loading (2.12).

Table 2: Importance of Input for Each Model

	Network					Factor					Ratio	
Model	Small	Moderate	Large	Dominant	Cross	Small	Moderate	Large	Dominant	Cross	Small	Dominant
1	1.03	2.09	1.90	4.96	1.00	2.57	1.32	1.05	17.80	1.04	1.51	1.80
2	2.09	1.53	1.16	1.59	1.68	1.66	1.21	2.12	2.55	2.57	—	1.09
3	2.20	2.27	1.23	1.28	1.27	3.07	1.30	2.44	1.54	3.28	—	1.93
4	6.65	1.81	1.35	2.05	1.88	1.67	1.18	1.84	2.22	2.45	—	1.37

Note. Model: 1 = Random vs. non-random; 2 = low correlation vs. network; 3 = high correlation with variables greater than factors vs. network; 4 = high correlation with variables less than or equal to factors vs. network. Grey boxes denote top three most important features for each model.

5.3 Model 3: High Correlation with Variables per Factor Greater than Factors vs. Network

The set up of the high correlation with variables greater than factors vs. network model was identical to Model 2 except the samples retained were the high correlation between factors (i.e., .50 and .70; 120,000 samples) rather than the low correlation between factors. From these samples, we extracted samples that were generated with the number of variables per factor that were greater than the number of factors (e.g., 4 variables per factor and 3 factors). This resulted in 60,000 samples used in training. Just as Model 2, we randomly sampled an equal number of network samples across the same sample size levels, resulting in a total of 120,000 samples.

The exact same input and hidden layers were used as Model 2. Similarly, our final model did not meet our early stopping criterion and was terminated after the 100th epoch. We then evaluated the model on the validation dataset, which achieved a loss of 0.159 and accuracy of 93.7%. This neural network outperformed the logistic regression model in loss and accuracy (Table 1). The inputs that had the greatest importance were the cross factor loading (3.28), small factor loading (3.07), and large factor loading (2.44).

5.4 Model 4: High Correlation with Variables per Factor Less than or Equal to Factors vs. Network

The set up of the high correlation with variables less than or equal to factors vs. network model was the same as Model 3 except models with the samples retained were the moderate and high correlation between factors (i.e., .50 and .70) with variables per factor than were equal to or less than the number of factors (60,000 samples; e.g., 3 variables per factor and 5 factors). Similarly, an equivalent number of network models were randomly drawn from the 240,000 network models (across the same sample size levels), resulting in a total of 120,000 samples. The inputs and hidden layers were the same as Model 2 and 3. Our final model reached our threshold of early stopping on epoch 88. We then evaluated the model on the validation dataset, which achieved a loss of 0.239 and accuracy of 90.2%. Relative to the other models, the neural network substantially outperformed the logistic regression model on both loss and accuracy (differences of .162 and 5.6%, respectively). The inputs that had the greatest importance were the small network loading (6.65), cross factor loading (2.45), and dominant factor loading (2.22).

6 Simulation 2: Validating the Neural Networks

Our second simulation set out to validate the neural networks against Christensen and Golino's (2020) original LCT heuristics and the logistic regression models that were trained alongside the neural networks. Although the neural network (and logistic regression) models were already validated on novel samples held out from their training samples, we sought to further test their generalizeability by generating data using different conditions than the ones they were trained on—that is, manipulating the parameters of the random, factor, and network models such that they are completely novel. Moreover, our goal was to combine these models into a single algorithm in order to predict whether the data were generated from a random, factor, or network model. The purpose of this algorithm was to improve on the original LCT algorithm proposed by Christensen and Golino (2020) by replacing their descriptive heuristics with more sophisticated neural networks.

The updated LCT algorithm makes predictions following a similar procedure as the original such that the data are first tested for whether they were generated from a random or non-random model. Thus, the data are passed through the random vs. non-random neural network and a prediction is made. If the data are predicted to be from a random model (i.e., probability $\geq$ .50), then the algorithm stops and outputs a prediction of a random model. If the data are predicted to be from a non-random model, then they are passed through the other three neural networks. This ensemble of neural networks produce probabilities for whether the data were generated from a factor model. If any of these probabilities are greater than .50, then the data are predicted to be from a factor model; otherwise, the data are predicted to be from a network model. In this sense, this ensemble of neural networks behave as a "winner-takes-all" model where only one positive prediction of a factor model is necessary to declare the model a factor model. The algorithm is thus biased towards the detection of factor models, making the prediction of a network model more conservative.

The use of the neural networks further allows for different types of predictions to be made (in contrast to the original algorithm's necessity of using bootstrap). First, the neural networks could make a prediction based on the empirical data, which would be in line with how the neural networks were trained (i.e., on single, isolated samples). Second, because bootstrapping has the potential to improve the accuracy of the prediction, the empirical data could be bootstrapped for a certain number of iterations (e.g., 100) and the means of the proportions could be computed and used to make a prediction (identical to the original LCT algorithm). Finally, because the neural networks can make predictions on individual datasets, a prediction could be made for the empirical dataset as well as the bootstrap datasets to provide the proportion of times each model was predicted from the data. In this simulation, we test each type of prediction (hereafter referred to as *empirical*, *bootstrap*, and *proportion*, respectively). As comparisons, we computed these predictions for the trained logistic regression models as well as used the original LCT algorithm.

6.1 Data Generation

We simulated data for random, factor, and network models following the procedure found in Simulation 1. The only difference was that we manipulated the parameters to have mostly novel conditions (i.e., data conditions that the neural networks were not trained on).

6.1.1 General parameters

As in Simulation 1, all data were generated as continuous variables. For each model, a total of 7,200 samples were generated. An equal number of samples was important to ensure that adequate statistical comparisons (e.g., confusion matrix metrics) could be estimated. The sample sizes for all models were 400 and 750.

6.1.2 Random model

For the random models, we were only able to manipulate the number of variables. We generated 12, 18, 21, 24, 27, and 33 variables from random models. For each condition (sample size $\times$ number of variables), 600 samples were generated.

6.1.3 Factor model

For the factor models, number of factors (2, 4, and 6) and variables per factor (4, 6, and 8) were manipulated. The correlations between factors remained the same (i.e., .00, .30, .50, and .70). It's important to note that some conditions were identical to the samples the neural network and logistic regression models were trained on, but the conditions were generated with different sample sizes. For each condition (sample size $\times$ number of factors $\times$ variables per factor $\times$ correlations between factors), 100 samples were generated.

6.1.4 Network model

For the small-world network models, number of variables (12, 24, 36, and 48), rewiring probabilities (.075, .15, and .30), and densities (.30, .50, and .70) were manipulated. The rewiring probabilities were chosen on the basis of typical small-world network models where the standard Watts-Strogatz small-world model is around .10 (± 5) and typical psychological small-world networks, which are likely somewhere between .01 and .50. Importantly, the number of variables tended to be within the same range as the factor models (which ranged from 8–48) to allow for closer comparisons of the two models, which had a similar number of variables. For each condition (sample size $\times$ number of variables $\times$ rewiring probabilities $\times$ densities), 100 samples were generated.

6.2 Confusion Matrix Metrics

We computed confusion matrix metrics for the models using the empirical, bootstrap, and proportion predictions of the algorithm. To provide an example of these metrics, we use the random model as the model under consideration. A true positive (TP) was when the predicted and true generating model matched the model under consideration (e.g., random). A true negative (TN) was when the predicted and true generating model (e.g., factor or network) were not the model under consideration (e.g., random). A false positive (FP) was when the predicted generating model matched the model under consideration (e.g., random) but not the true generating model (e.g., factor or network). A false negative (FN) was when the predicted generating model (e.g., factor or network) did not match the model true generating model and model under consideration (e.g., random).

Using this confusion matrix, we computed sensitivity ($\frac{TP}{TP+FN}$), specificity ($\frac{TN}{TN+FP}$), false discovery rate (FDR; $\frac{FP}{FP+TP}$), accuracy ($\frac{TP+TN}{TP+FP+TN+FN}$), and Matthews correlation coefficient (MCC; $\frac{(TP\times TN)-(FP\times FN)}{\sqrt{(TP+FP)\times(TP+FN)\times(TN+FP)\times(TN+FN)}}$). Sensitivity is the proportion of positives that are correctly identified as TPs, while specificity is the proportion of negatives that are correctly identified as TNs. The FDR is the proportion of FPs that are found relative to the total positives that are predicted by the algorithm. Accuracy is the proportion of correct predictions (TPs and TNs) of the algorithm, representing an overall summary of sensitivity and specificity. Finally, the MCC is considered to the best overall metric for classification evaluation because it is an unbiased measure that uses all aspects of the confusion matrix, representing a special case of the phi coefficient between the predicted and true model (Chicco & Jurman, 2020).

7 Results

Starting with general accuracy, the neural network predictions had the highest percent correct: proportion (97.4%), bootstrap (96.2%), and empirical (91.7%). These were followed by the logistic regression predictions: bootstrap (85.4%), proportion (84.7%), and empirical (82.5%). The original LCT algorithm performed the worst with 81.6% correct. More nuanced accuracy metrics for the neural networks are provided in the confusion matrix results reported in Table 3 (other methods can be found in SI3).

Table 3: Confusion Matrix of Neural Network Predictions

	Random			Factor			Network		
	Empirical	Bootstrap	Proportion	Empirical	Bootstrap	Proportion	Empirical	Bootstrap	Proportion
Sensitivity	0.962	0.955	0.974	0.977	0.986	0.993	0.810	0.946	0.954
Specificity	0.989	0.999	0.998	0.908	0.972	0.978	0.977	0.973	0.984
False Discovery Rate	0.022	0.003	0.004	0.158	0.054	0.042	0.053	0.053	0.032
Accuracy	0.980	0.984	0.990	0.931	0.976	0.983	0.922	0.964	0.974
MCC	0.955	0.964	0.977	0.857	0.948	0.963	0.822	0.920	0.942

Note. Grey boxes indicate best metric value for each model. MCC = Matthews Correlation Coefficient.

Across all metrics, the bootstrap and proportion predictions were superior to the single-shot empirical predictions. It's important to note that these improvements were incremental and that the empirical predictions still performed very well (and better than the original LCT algorithm; compare Table 3 with SI3). The LCT algorithm using the neural networks had high sensitivity and specificity. This suggests that even in novel conditions that the neural networks were not trained on they were highly accurate at correctly identifying whether a data were (or were not) generated from the true population model. Furthermore, false discovery rate remained small (≤ 0.054) except for the empirical estimates of factor models (0.158). Relative to the other predictions, the empirical factor prediction was around three times more likely to produce a false positive relative to the number of true positives. Accuracy and MCC were very high for all predictions and particularly for the proportion prediction: random (0.977), factor (0.963), and network (0.942). In sum, the LCT using the neural networks demonstrated that they could generalize beyond their training samples and conditions. Furthermore, they did so better than logistic regression and the original LCT heuristics (compare Table 3 with SI3). A more nuanced perspective was revealed, however, when breaking down percent correct by each model, method, type of prediction, and their respective conditions.

7.1 Random Model Percent Correct

The random model had exceedingly high percent correct ($\geq 95\%$) for all predictions for the neural network and logistic regression methods (Figure 2) except for when there were twelve variables. The original LCT algorithm decreased in performance (i.e., percent correct) as the number of variables increased. The predictions were worst when there were few variables (12) but were near perfect when there were 18 or more variables for the neural network and logistic regression methods.

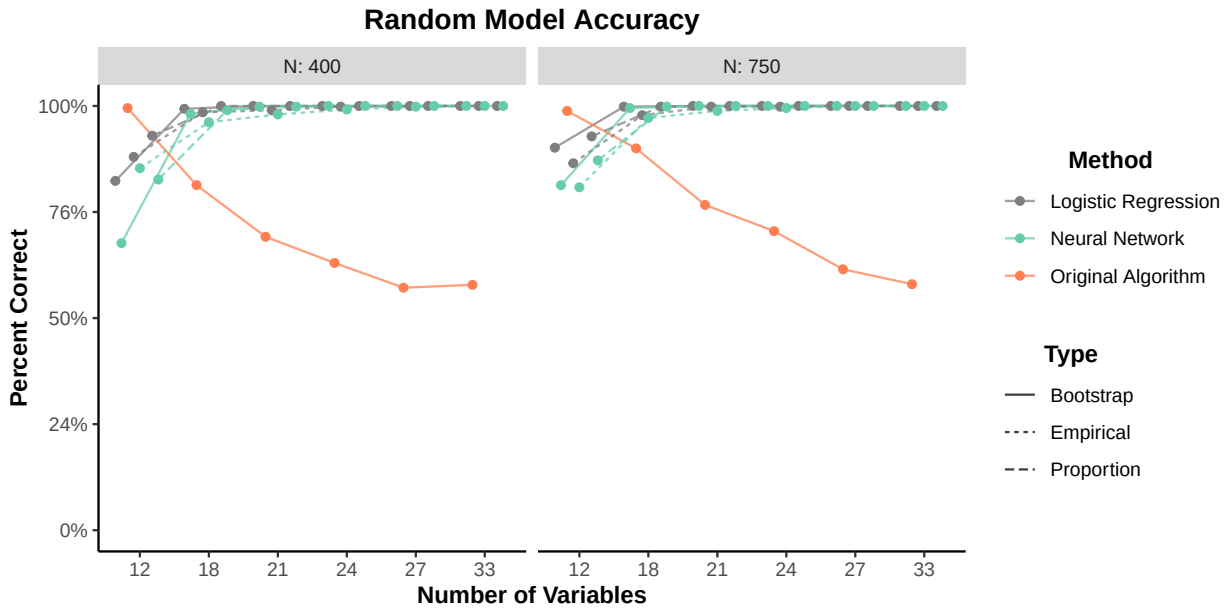

Figure 2: Percent correct for random models in each condition. N = sample size.

It's noteworthy that the neural network and logistic regression methods were trained on number of variables equal to or greater than fifteen and that their performance was poorer when there were fewer variables. In contrast, the original

algorithm was based on fifteen variables only, which is likely why it demonstrates poor generalizability as the number of variables increase. The logistic regression predictions performed the best across all conditions (97.4–98.8%) followed by the neural networks (95.5–97.4%) and original algorithm (73.6%).

7.2 Factor Model Percent Correct

In general, predictions for the factor model were highly accurate ($\geq$ 75%) across all conditions for the neural network and logistic regression methods (Figure 3). Lower accuracy for all methods tended to occur when correlations between factors were large (.70). This is unsurprising as factor models begin to appear more like network models as the cross-loadings increase in magnitude.

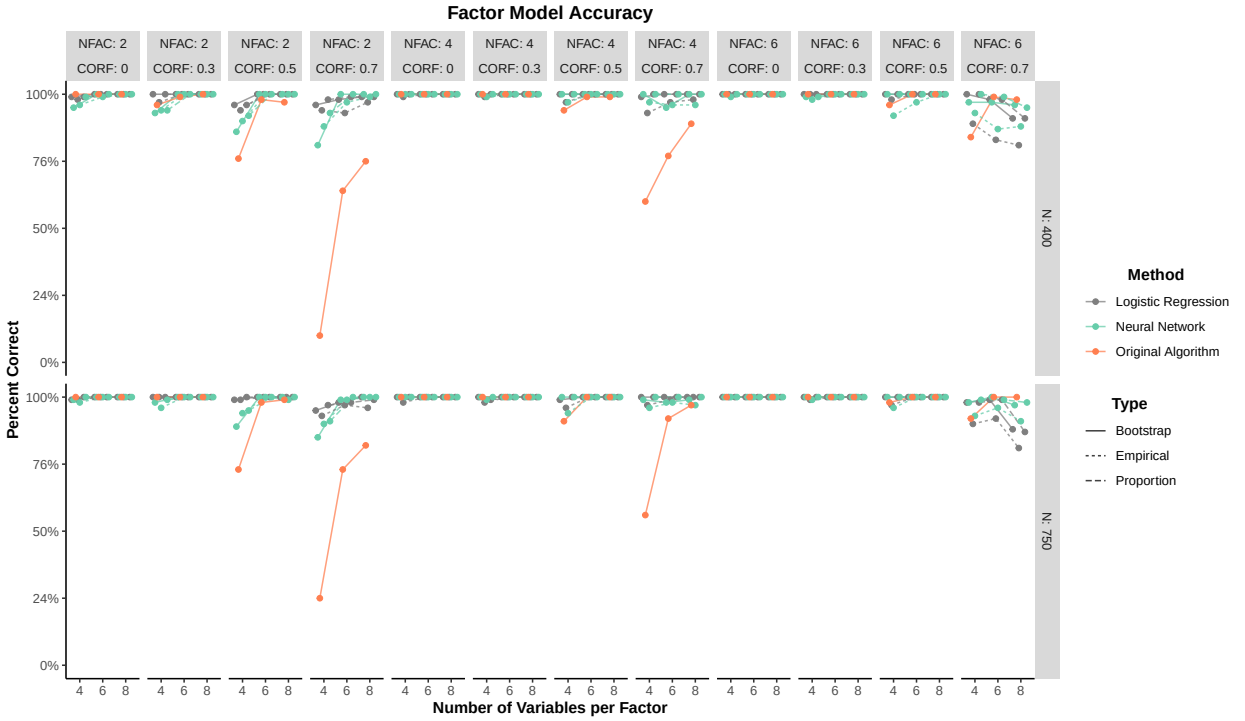

Figure 3: Percent correct for factor models in each condition. NFAC = number of factors, CORF = correlations between factors, and N = sample size.

Across all conditions except for one (6 factors, 8 variables per factor, and .70 correlations between factors), the neural network and logistic regression methods were comparable to or better than the original LCT algorithm. The neural network method was comparable to logistic regression method on all three prediction types: empirical (97.7% and 97.8%), bootstrap (98.6% and 99.3%, respectively), and proportion (99.3% and 98.4%). The logistic regression method performed slightly better when their were 2 factors, especially in the smaller sample size (n = 400). The original algorithm was the worst overall (92.9%) despite superior performance in specific conditions.

7.3 Network Model Percent Correct

As a general trend, all methods tended to improve in percent correct as the network models became more dense (Figure 4). The neural network method by far outperformed the logistic regression and original algorithm methods when the networks were sparse (0.30). Across all conditions, the neural networks performed as well as or better than the logistic regression and original algorithm predictions, with the proportion predictions achieving at least 75% correct or greater. The number of variables had a substantial effect on the logistic regression predictions ranging from moderate ($\eta_p^2 = 0.07$) for the empirical prediction to large ($\eta_p^2 = 0.22$) for the bootstrap prediction. The original algorithm was substantially affected by the density of the networks ($\eta_p^2 = 0.31$). In contrast, the neural networks only had a small effect for density ($\eta_p^2 = 0.01$) across its predictions.

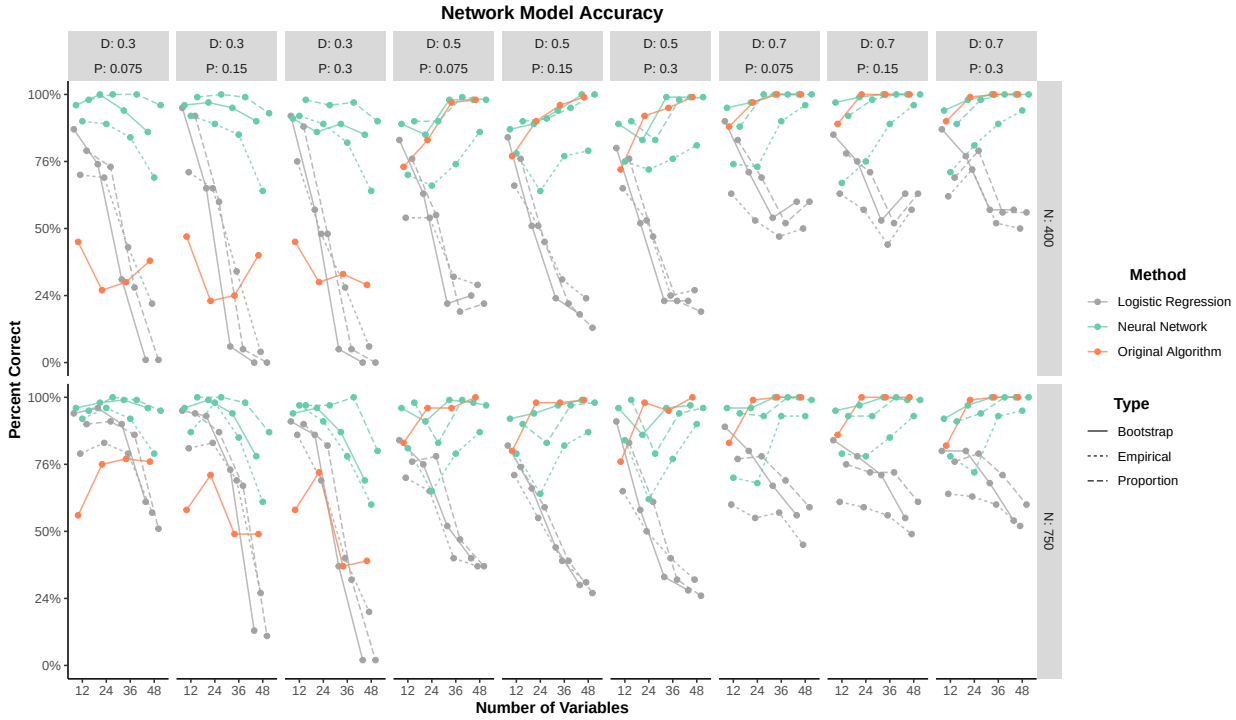

Figure 4: Percent correct for network models in each condition. P = rewiring probability, D = density, and N = sample size.

Relative to the neural network method, the logistic regression and original algorithm did not perform as well. The logistic regression's performance was likely hindered by its tendency to prefer factor models—its false discovery rate for factor models was twice as much (or more) than the false discovery rate of the neural network predictions (ranging from 0.289 to 0.322; compare Table 3 with SI3). In contrast, the original algorithm had a tendency to prefer network models relative to factor models, which is noted by its nearly twofold false discovery rate of network models (0.298) over factor models (0.156; SI 3). Taken together, the neural networks were robust across the network models but were also the most balanced in terms of their bias for predicting any one model (Table 3).

8 Real-world Examples

The results of Simulation 2 provide evidence that the LCT algorithm paired with neural networks can be a powerful predictive tool for identifying whether data are generated from a specific model. It's important, however, to demonstrate that the LCT works in practice. To illustrate this, we examine two different datasets that are assumed to be generated from a factor and network model.

8.1 International Personality Item Pool Big Five Inventory

The first example dataset consisted of 2800 observations on items from the International Personality Item Pool's (Goldberg, 1999) Big Five Inventory (BFI; John, Donahue, & Kentle, 1991), which is available in the *psych* package (Revelle, 2017) in R. The BFI traditionally has five factors, each with five items, corresponding to the Big Five factor model: openness to experience, conscientiousness, extraversion, agreeableness, and neuroticism. The robustness of this factor structure has been demonstrated across a variety of samples (e.g., Donnellan, Oswald, Baird, & Lucas, 2006). Although there is no way to determine that the BFI is actually generated from a factor model, its robust factor structure suggests that the data structure should follow a factor model.

We applied the LCT to the full dataset as well as sub-samples that were randomly split into 400 cases each (seven sub-samples in total; see SI4 for code to replicate this analysis). For the full dataset, all predictions—empirical, bootstrap, and proportion—were for a factor model. Across the sub-samples, the results varied slightly by prediction: empirical (6 factor and 1 network), bootstrap (7 factor), and proportion (7 factor).

8.2 Resting State Default Mode Network

The second example dataset consisted of mean blood oxygen level-dependent (BOLD) activation levels of twenty regions of interest (ROIs) in the brain that corresponded to the default mode network (DMN) during five minute resting state scans in 144 participants from Beaty et al. (2018). The DMN corresponds to a set of cortical midline, medial temporal, and posterior inferior parietal regions that often co-activate together. Recent research has demonstrated that the DMN can be broken down into several distinct sub-networks (Andrews-Hanna, Smallwood, & Spreng, 2014; Gordon et al., 2020). Brain networks are a well-known real-world example of networks, which make them an appropriate test of whether the LCT performs as expected.

We applied the LCT to the correlation matrices of the 20 ROIs based on the DMN structure identified in the Shen brain atlas (Shen, Tokoglu, Papademetris, & Constable, 2013; see SI5 for code to replicate this analysis). The correlation matrices were derived from time series with the length of 150, which was used as the sample size input for the LCT. For the bootstrap and proportion predictions, all participants DMN were suggested to be generated from a network model. The empirical prediction suggested that most 140 (97.2%) were generated from network models with the other four being predicted as factor models.

8.3 Summary

Taken together, these examples demonstrate the validity of the LCT on real-world datasets with data that were expected to be generated from factor and network models. Given the robustness of the proportion prediction of the LCT in Simulation 2 and our examples here, we suggest that researchers should place the most weight on this prediction. A consensus across predictions is most likely to be robust but when they conflict researchers should give priority to the proportion prediction followed by the bootstrap and empirical predictions. One benefit of the proportion prediction is that it provides some inference into the certainty of the data generating model by offering the proportion of samples that were predicted to be from each given model.

9 Discussion

The present study sought to use artificial neural networks to improve the LCT algorithm, which was designed to determine whether data are generated from a random, factor, or network model based network and factor loading structures. We briefly reviewed some of the methodological basics and described some of the parameters that are necessary to understand and train feed-forward neural networks. Our results demonstrate how artificial neural networks can be a powerful tool for developing highly predictive models. In the context of our study, we demonstrated that neural networks (specifically with proportion predictions) outperform human identified heuristics (i.e., the original LCT algorithm) and logistic regression models for predicting the data generating model.

The significance of this problem has grown increasingly relevant as recent studies have been demonstrated the equivalence between latent variable and network models (Hallquist et al., 2019; Marsman et al., 2018; van Bork et al., 2019; Waldorp & Marsman, 2020). This has shifted the focus of the differences between these models from statistical to theoretical (Guyon et al., 2017; Kruis & Maris, 2016). Indeed, when the data generating mechanism is a factor model, then the statistical representations (e.g., loadings) can be shown to be identical (Christensen & Golino, 2020; Kruis & Maris, 2016). These representations start to differ, however, when the data generating mechanism is not a factor model. This raises an important question: What is the difference between the structure of factor and network models?

Unfortunately, neural networks are (typically) a black box of linear and nonlinear transformations of the input to the output and therefore make our predictions accurate but not necessarily explanatory (but see Buhrmester, Münch, & Arens, 2019; Yarkoni & Westfall, 2017). Although some hints are provided by our feature importance analysis, the exact mapping of between the loading structures and predicted model is likely multifaceted (as demonstrated by the better performance in training and validation of the neural networks over logistic regression). In unidimensional models, there appears to be some statistical differences that can be exploited but this may not generalize to more complex models (van Bork et al., 2019). We show that at the very least summaries of the data's structure (proportions of small, dominant, and cross-loadings) are important for differentiating data generated from these models.

When considering statistical assumptions and the feature importance analysis, our results point to the interconnectedness of the variables: factor models tend to have few interconnections whereas network models typically have many (Christensen & Golino, 2020). Indeed, cross-loadings of the factor models were either the first or second most important input for the neural networks predicting whether the data were generated from a factor or network model. Another difference is the extent to which there is clustering due to a common cause: factor models explicitly assume this whereas network models do not. This does not mean that common causes cannot or do not exist in network models but rather it is not an explicit statistical assumption. This is made evident by the importance of the dominant factor loading across

the models. For the random models, the dominant factor loadings were around four times more important (relatively) than the next most important input (dominant network loadings). This strongly suggests that the lack of identifiable common causes in random and network models are a substantial contributor for differentiating them from factor models.

Although our findings may not be able to provide an exact statistical answer about the differences between these models (e.g., van Bork et al., 2019), they do provide a predictive tool for whether data are structured as a random, factor, or network model. Specifically, the proportion predictions of the neural network following the LCT algorithm had high sensitivity, specificity, and overall accuracy (MCC) for all models. Importantly, we do not suggest that the LCT can inform the researcher about whether their data was *actually* generated from a specific model. This is a critical distinction: The LCT can accurately predict whether the data are *structured* as a specific model rather than actually being generated by it. Indeed, our simulated data were generated from specific models but this does not mean that data structured like a factor model could not be generated from a network model (and vice versa; Fried, 2020; van Bork et al., 2019; van der Maas et al., 2006).

The issue of statistical equivalence has been discussed at length in the literature (Christensen & Golino, 2020; Fried, 2020; Marsman et al., 2018; van Bork et al., 2019; Waldorp & Marsman, 2020), so we do not review it here; however, this issue has led to recent calls for researchers to develop formal (i.e., computational and mathematical) theories about their psychological phenomena of interest (Borsboom et al., 2020; Fried, 2020; Haslbeck et al., 2019). Theories and hypotheses about the relations between components of the phenomena should be developed a priori to test their relations and whether a latent variable (e.g., factor) or network model is a more appropriate statistical model for the representation of those relations. We view the LCT as a test for whether the components are structured like a factor or network model, which can inform the researcher as to whether the relations between components are behaving as expected. Said differently, we do not advise that the LCT supplant theory about the relations between variables but suggest that it can serve as a tool for reasoning about the hypothesized structure of psychological phenomena.

In this respect, scale developers can structure their scales to align more with the structure of a factor or network model—that is, the data structure can be manipulated to produce data that appear to be generated from one model or the other. In fact, contemporary psychometric practice has been doing exactly this for many years now: items or variables that have substantial cross-loadings are usually removed from potential scales (DeVellis, 2017). This approach is often justified to ensure that the phenomena of interest are being cleanly measured (i.e., unidimensional), yet most researchers rarely discuss whether the theory about the relations between the variables actually dictate such distinctions. Therefore, it again comes down to theory as to whether the data are actually generated from said model.

For more practical terms, researchers must consider the data generating model when estimating scores from these psychometric models (network scores can be computed as a weighted composite; see for example Golino et al., 2020). As shown in Figure 1 and Christensen and Golino (2020), the loading structures for factor and network loadings are roughly equivalent, which suggests there is little consequence in whether a factor or network model is used to estimate scores (Golino et al., 2020). When the data are generated (or even structured) as a network model, then there is divergence between the loading structures with variables (e.g., dominant loadings; see Figure 1). Indeed, this consequence has been noted with sum scores and factor scores where differences can be observed when a τ-equivalent latent variable model (i.e., sum scores) is applied to data generated from a congeneric latent variable model (i.e., factor scores; McNeish & Wolf, 2020). Such differences can have substantial consequences for the reliability and validity of measurement. Moreover, these consequences further underscore the importance for researchers to consider that "scoring scales—by any method—is a statistical procedure that requires evidence and justification" (McNeish & Wolf, 2020, p. 2). Our study demonstrates that the LCT can be used as one method to provide such evidence and justification.

Importantly, we also echo recent calls by researchers who have stated that there is no need to pit these models against each other but rather develop hybrid models that include components that are from common causes and causal systems (Christensen et al., 2020; Epskamp et al., 2017; Fried, 2020; Guyon et al., 2017). In this way, researchers should consider the level of organization at which each phenomena is being measured. Factor models, for example, may be more appropriate when measuring a specific phenomenon with highly similar variables like a single characteristic of personality whereas network models may be more appropriate for understanding how these specific characteristics coalesce into more complex systems like a personality trait (Christensen et al., 2020; Mõttus & Allerhand, 2017). Even still, individual personality traits may then appear as a factor model when examined together (as shown in our example). This suggests that the level of organization may influence the data structure and the relationships between the psychological components, which highlights the point that hybrid models may be the most optimal stance (Fried, 2020; Guyon et al., 2017). The LCT can help researchers explore and verify these hypothesized structures to better determine how hybridization should occur.

There are several limitations that researchers must consider when using the LCT. First, the LCT was trained on small-world network models and therefore carries the assumption that most psychological networks will be generated from small-world network models. We think this assumption is reasonable because many real-world networks show

small-world structure (e.g., brain networks; Muldoon et al., 2016) and many psychological phenomena exhibit properties that align with these assumptions such as psychopathological disorders (Borsboom et al., 2011): clustering of symptoms within a disorder (high clustering coefficient) yet bridges between symptoms to other disorders (low average shortest path lengths; Cramer, Waldrop, van der Maas, & Borsboom, 2010). More random networks may, however, be more appropriate when the network consists of unique variables that have independent causes like a network comprised of individual latent variables that represent independent phenomena. Although we suggest this as a limitation of the current implementation of the LCT's neural networks, it's important to emphasize that researchers can continue to train them to improve their predictive power by using different data conditions or methods (see our R code on the OSF).

This leads us to a second, influential limitation: the predictions of the neural networks are only as good as the data they are trained on. Therefore, we must be critical of our own data generating methods and question whether they resemble real-world data. We believe that we have provided reasonably realistic datasets that include factor models with dominant loadings between .40 and .70 and a varying degree of cross-loadings. The range of loadings represent what are considered to be acceptable to very high (Comrey & Lee, 2013) with .40 being considered a rule of thumb for appropriate measurement of a latent variable (DeVellis, 2017). Still, not all datasets will have loadings on the dominant factor that are within this range. Moreover, there are few standards for the characteristics and topology of what can be considered a "typical" psychological network. Our data generating assumptions were based on previous evidence that most real-world networks tend to be small-world (including psychological networks; Borsboom et al., 2011), but the extent to which psychological networks are represented by small-world networks and whether the parameters used in the study mimic real-world psychological networks lacks empirical validation. In large part, this is because few psychological network studies have examined the topological features of psychological networks such as their degree distribution, which is a critical characteristic for determining the type of network (e.g., random, small-world, scale-free, exponential random graph; Newman, 2010). In practice, this task is difficult because network estimation methods differ in their preference for sparsity, which affects the estimated degree distribution. Better data generation follows from more studies examining and reporting the topology of psychological networks (e.g., Battiston et al., 2020), which can in turn be used to train better neural networks to make more valid predictions.

Finally, in light of our discussion on theory, the LCT is focused on cross-sectional datasets when most phenomena are likely to be dynamical systems (e.g., Haslbeck et al., 2019). This is a limitation of the current implementation of the LCT but we suspect that the LCT can be generalized to time series data by using dynamic factor analysis and dynamic EGA (Golino et al., 2020). Another possibility is to use other types of neural networks such as a multi-scale convolutional neural network, which can accommodate time series data structures into classification neural networks (Cui, Chen, & Chen, 2016), and recently developed temporal graph networks, which can learn directly from a graph (e.g., a psychometric network; Rossi et al., 2020). Such an approach could determine whether some people represent a phenomena of interest as a common cause or causal system. This in turn could offer inferences into individualized psychopathological intervention (Wright & Woods, 2020), providing more specific answers to the question about whether it would be more effective for a clinician to treat an underlying disorder or specific symptoms.

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Supplementary Information

Random, Factor, or Network Model? Predictions from Neural Networks

SI1. Exploratory Graph Analysis

Exploratory graph analysis (EGA; Golino & Epskamp, 2017; Golino, Shi, et al., 2020) is a network psychometrics dimension identification method. The approach begins by estimating a network from the empirical data and applying a community detection algorithm to identify *communities* (or dimensions) in the network. The traditional EGA method estimates a Gaussian graphical model (GGM; Lauritzen, 1996) where nodes are variables and edges are the partial correlations between nodes after being conditioned on all other nodes. In psychological networks, the most common way of estimating a GGM is to use the graphical least absolute shrinkage and selection operator (glasso; Friedman, Hastie, & Tibshirani, 2008, 2014) with extended Bayesian information criterion (EBICglasso; Chen & Chen, 2008; Epskamp & Fried, 2018). Once the EBICglasso is applied, the *Walktrap* (Pons & Latapy, 2006) community detection algorithm is applied. The Walktrap algorithm uses random walks or stochastic steps from one node over an edge to another to determine the distance and similarity between two nodes. These random walks tend to stay within subsets of related nodes because they tend to be closer and more similar to one another. The algorithm merges the results, based on an agglomerative clustering approach (Ward, 1963), of the random walks to separate the communities. *Modularity* or the extent to which nodes maximize the proportion of connections within their community relative to connections to other communities (Newman, 2006) is then used as criterion for selecting the optimal clustering (or community) organization.

SI2. Network Loadings

The development of network loadings were based on the simulation studies performed by Hallquist, Wright, and Molenaar (2019), which showed that the network measure *node strength* (or the sum of a node's connections) was roughly redundant with confirmatory factor analysis (CFA) loadings. Their simulations demonstrated that although node strength was roughly redundant with CFA loadings, the measure was confounded by different latent causes. To circumvent this limitation, Christensen and Golino (2020) derived an alternative measure of node strength which accounted for different latent causes by dividing each node's strength between the dimensions in a network. In their simulations, they demonstrated that this alternative measure, network loadings, could overcome the limitation of latent confounding and that network loadings were equivalent to exploratory factor analysis loadings when the data generating model was a factor model. One difference between the factor and network loadings was their magnitude—network loadings tended to be smaller than their factor counterpart because they were based on partial correlations rather than zero-order correlations. Importantly, they determined the correspondence between factor and network loading effect sizes: small (.40 and .15, respectively), moderate (.55 and .25, respectively), and large (.70 and .55, respectively; Comrey & Lee, 2013). Mathematically, network loadings are defined as:

$$S_i = \sum_{j=1}^{n} |w_{ij}|,$$

$$L_{if} = \sum_{j \in f}^{F} |w_{ij}|,$$

where $|w_{ij}|$ is the absolute weight (e.g., partial correlation) between node i and j, S_i is the sum of the edge weights connected to node i across all nodes (n; i.e., node strength for node i), L_{if} is the sum of edge weights in factor f that are connected to node i (i.e., node i's loading for factor f), and F is the number of factors (in the network). This measure can be

standardized using the following formula:

$$z_{L_{if}} = \frac{L_{if}}{\sqrt{\sum L_{.f}}},$$

where the denominator is equal to the square root of the sum of all the weights for nodes in factor f. Notably, the standardized loadings are absolute weights with the signs being added after the loadings have been computed (following the same procedure as factor loadings; Comrey & Lee, 2013). In contrast to factor loadings, the network loadings are computed after the number of factors have been extracted with the variables being assigned to specific factors by the community detection algorithm.

SI3. Confusion Matrix of Logistic Regression and Original Algorithm Predictions

	Random				Factor				Network			
	Empirical	Bootstrap	Proportion	Original	Empirical	Bootstrap	Proportion	Original	Empirical	Bootstrap	Proportion	Original
Sensitivity	0.974	0.976	0.988	0.736	0.978	0.993	0.994	0.929	0.523	0.593	0.560	0.782
Specificity	0.983	0.996	0.994	0.975	0.768	0.798	0.784	0.914	0.986	0.987	0.993	0.834
False Discovery Rate	0.034	0.008	0.011	0.063	0.322	0.289	0.303	0.156	0.049	0.042	0.024	0.298
Accuracy	0.980	0.989	0.992	0.896	0.838	0.863	0.854	0.919	0.832	0.855	0.849	0.817
MCC	0.955	0.976	0.983	0.763	0.704	0.748	0.734	0.825	0.621	0.675	0.663	0.601

Note. Original refers to the original algorithm and the Empirical, Bootstrap, and Proportion are prediction types of the Logistic Regression method. Grey boxes indicate best metric value for each model. MCC = Matthews Correlation Coefficient.

SI4. Reproducible Code for the Loadings Comparison Test with Big Five Inventory

```r
# Set seed
set.seed(3532)

# Install latest EGAnet package
devtools::install_github("hfgolino/EGAnet")

# Load packages
library(psych)
library(EGAnet)

# Get BFI data
bfi.data <- bfi[,1:25]

# LCT of the full dataset
LCT(bfi.data)

# Randomly sample from BFI data
samps <- sample(1:nrow(bfi), nrow(bfi))

# Split samples into sizes of 400
start <- seq(1, nrow(bfi), 400)
end <- seq(400, nrow(bfi), 400)
```

```r
# New samples
new.samps <- list()

for(i in 1:length(start))
{new.samps[[i]] <- bfi.data[samps[start[i]:end[i]],]}



# Apply LCT to new BFI samples
res.bfi <- lapply(new.samps, LCT)

## Empirical
mean(lapply(res.bfi, function(x){x$empirical}) == "Factor")

## Bootstrap
mean(lapply(res.bfi, function(x){x$bootstrap}) == "Factor")

## Proportion
mean(lapply(res.bfi, function(x){
  names(x$proportion)[which.max(x$proportion)]
}) == "Factor")
```

SI5. Reproducible Code for the Loadings Comparison Test with Default Mode Networks

```
# Install latest EGAnet package
devtools::install_github("hfgolino/EGAnet")

# Load packages
library(googledrive)
library(EGAnet)

# Create path to temporary file
temp <- tempfile()

# Download to temporary file
drive_download(
  paste("https://drive.google.com/file/d/",
        "1T7_mComB6HPxJxZZwwsLLSYHXsOuvOBt",
        "/view?usp=sharing", sep = ""),
  path = temp
)

# Load resting state brain data
load(temp)
```

```
# Get default mode network from Shen atlas (from NetworkToolbox)
atlasNet <- c(2,4,3,2,3,3,2,2,2,1,4,1,3,2,4,1,2,4,2,4,2,
              2,5,5,5,5,5,4,4,2,2,4,5,5,5,4,5,5,5,5,8,6,
              8,4,5,5,2,2,3,3,5,1,1,1,2,1,1,5,8,5,5,5,5,
              1,1,8,8,6,8,2,8,6,8,8,6,7,6,7,6,6,7,6,4,5,
              3,3,6,4,5,3,4,5,4,4,4,3,5,6,4,7,4,7,4,4,4,
              4,4,4,5,4,2,2,4,4,3,2,4,4,4,4,4,4,4,4,4,4,
              4,4,4,4,4,4,4,3,4,4,1,3,2,1,3,2,2,4,1,4,2,
              1,1,1,1,4,1,2,4,1,2,5,5,5,5,1,5,2,1,5,5,5,
              4,5,5,5,5,5,8,6,8,4,5,5,5,2,1,2,1,1,1,5,5,
              1,5,1,2,1,5,2,5,6,2,8,8,5,3,8,6,8,6,6,8,8,
              6,7,7,7,6,6,4,5,1,4,4,3,3,4,3,4,3,5,4,4,4,
              4,4,4,5,4,4,4,3,8,7,2,4,4,4,2,2,4,4,4,4,4,
              4,4,4,4,4,4,4,4,4,4,4,4,4,4,4,4)

dmn <- which(atlasNet == 3)

# Grab only default mode networks
rest.dmn <- restOpen[dmn,dmn,]

# Convert array to list
dmn.list <- list()
```

```r
## Make diagonals 1
for(i in 1:dim(rest.dmn)[3])
{
  net <- rest.dmn[,,i]
  diag(net) <- 1

  dmn.list[[i]] <- net
}

# Apply LCT to DMN list
## 150 = length of original time series
res.dmn <- lapply(dmn.list, LCT, n = 150)

## Empirical
mean(lapply(res.dmn, function(x){x$empirical}) == "Network")

## Bootstrap
mean(lapply(res.dmn, function(x){x$bootstrap}) == "Network")

## Proportion
mean(lapply(res.dmn, function(x){
  names(x$proportion)[which.max(x$proportion)]
}) == "Network")
```

SI6. Session Information for SI4 and SI5

```
R version 4.0.2 (2020-06-22)
Platform: x86_64-w64-mingw32/x64 (64-bit)
Running under: Windows 10 x64 (build 19041)

Matrix products: default

locale:
[1] LC_COLLATE=English_United States.1252
[2] LC_CTYPE=English_United States.1252
[3] LC_MONETARY=English_United States.1252
[4] LC_NUMERIC=C
[5] LC_TIME=English_United States.1252

attached base packages:
[1] stats     graphics  grDevices utils     datasets  methods   base

other attached packages:
[1] psych_2.0.8       EGAnet_0.9.7      googledrive_1.0.1 ggplot2_3.3.2
[5] papaja_0.1.0.9997

loaded via a namespace (and not attached):
 [1] splines_4.0.2       tmvnsim_1.0-2       gtools_3.8.2
 [4] Formula_1.2-3       BDgraph_2.62        stats4_4.0.2
 [7] latticeExtra_0.6-29 yaml_2.2.1          d3Network_0.5.2.1
[10] pbivnorm_0.6.0      pillar_1.4.6        backports_1.1.10
[13] lattice_0.20-41     glue_1.4.2          digest_0.6.25
```

```
[16] RColorBrewer_1.1-2  checkmate_2.0.0     colorspace_1.4-1
[19] htmltools_0.5.0     Matrix_1.2-18       plyr_1.8.6
[22] pkgconfig_2.0.3     bookdown_0.20       purrr_0.3.4
[25] corpcor_1.6.9       scales_1.1.1        whisker_0.4
[28] glasso_1.11         jpeg_0.1-8.1        fdrtool_1.2.15
[31] huge_1.3.4.1        htmlTable_2.1.0     tibble_3.0.3
[34] generics_0.0.2      farver_2.0.3        ellipsis_0.3.1
[37] withr_2.3.0         pbapply_1.4-3       nnet_7.3-14
[40] mnormt_2.0.2        survival_3.2-3      magrittr_1.5
[43] crayon_1.3.4.9000   evaluate_0.14       nlme_3.1-149
[46] MASS_7.3-53         foreign_0.8-80      tools_4.0.2
[49] data.table_1.13.0   lifecycle_0.2.0     stringr_1.4.0
[52] munsell_0.5.0       cluster_2.1.0       compiler_4.0.2
[55] rlang_0.4.7         grid_4.0.2          rstudioapi_0.11
[58] rjson_0.2.20        htmlwidgets_1.5.1   igraph_1.2.5
[61] lavaan_0.6-7        base64enc_0.1-3     labeling_0.3
[64] rmarkdown_2.3       gtable_0.3.0        abind_1.4-5
[67] reshape2_1.4.4      qgraph_1.6.5        R6_2.4.1
[70] gridExtra_2.3       knitr_1.30          dplyr_1.0.2
[73] Hmisc_4.4-1         stringi_1.5.3       parallel_4.0.2
[76] Rcpp_1.0.5          vctrs_0.3.4         rpart_4.1-15
[79] png_0.1-7           tidyselect_1.1.0    xfun_0.17
```

SI7. Example of Data Generating Model Manipulation

To demonstrate how the structure of data can be manipulated toward a certain model, we used a dataset that consisted of 2,832 observations on items from the Broad Autism Phenotype Questionnaire (BAPQ; Hurley, Losh, Parlier, Reznick, & Piven, 2007) that was a collected as a part of the Simons Foundation Autism Research Initiative's Simplex Collection (https://www.sfari.org/). The BAPQ was completed by the mothers and fathers of children on the Autism spectrum. The BAPQ consists of three sub-scales—aloof personality, pragmatic language problems, and rigid personality—that are based on direct assessment interviews with parents of autistic people that correspond to defining behavioral domains of autism: social, communication deficits, and stereotyped-repetitive behaviors (Hurley et al., 2007). The BAPQ has demonstrated a robust three-factor structure (Ingersoll, Hopwood, Wainer, & Donnellan, 2011) with each sub-scale containing twelve items that are rated on a 6-point Likert scale. Correlations between the means of the sub-scales tend to be highly correlated in clinical samples (r's from .50 to .70; Hurley et al., 2007) but smaller when using factor analysis in non-clinical samples (r's from .10 to .30; Ingersoll et al., 2011).

Because we have data for both mothers and fathers, we applied the LCT to each parent's datasets. We split the datasets into training (n = 1,699) and testing (n = 1,133) sets to validate the LCT's results. Below we present a table for the predictions of the LCT.

		Predictions		
Parent	**Dataset**	Empirical	Bootstrap	Proportion
Mother	Training	Factor	Network	Network (0.59) Factor (0.41)
	Testing	Factor	Network	Network (0.71) Factor (0.29)
Father	Training	Factor	Factor	Factor (0.72) Network (0.28)
	Testing	Network	Network	Network (0.55) Factor (0.45)

The results demonstrate that the BAPQ in mothers is a factor model based on the empirical prediction and network model based on the bootstrap and proportion prediction. For the fathers, the training data were predicted to be a factor model across all predictions while the testing data were predicted to be a network model across all predictions. In short, the results are mixed but lean towards a network model with three out of for datasets having network predictions for the proportion prediction. Based on this result, we would conclude that the data for mothers and fathers are most likely generated from a network model. Notably, the fathers datasets were leaning towards a factor model relative to the mothers datasets (including the training data being a factor model across predictions).

If, for example, we thought that the data generating mechanism was a factor model, then we should try to adjust the data's structure toward a factor model. To do so, we could analyze the structure of the data to see which items are multidimensional or leading to larger cross-loadings between dimensions. One approach for achieving these results is called *bootstrap exploratory graph analysis* (bootEGA; Christensen & Golino, 2019).

bootEGA applies a parametric bootstrap approach where N number of replicate samples are generated from a multivariate normal distribution based on the empirical correlation matrix. Each replicate sample is then analyzed using EGA (see SI1 for a description), forming a distribution of factors and item placement within those factors. Taking advantage of the deterministic allocation of items into factors, we can determine how often items are replicating in their empirical dimension as well as other dimensions. That is, we can determine how stable the factors are with respect to how items are placed into them (Christensen et al., 2020). Items that are not replicating well in their empirically-derived factor (e.g., EGA identified factor) indicate that these items are likely to be multidimensional, have larger cross-loadings, and are likely leading the data structure to be more like a network model.

When performing such an analysis, we found that there were four factors with identical item placement for the mothers and fathers datasets' empirically-derived structure (using

EGA). Using this factor structure and item placement, we applied bootEGA ($n = 500$) to the training and testing datasets for both mothers and fathers. The item stability analysis found one factor containing items that were relative unstable. These items and their stability (number of times replicating in their empirically-derived structure) are presented below:

	Replication Proportion			
	Mother		Father	
Item Description	Training	Testing	Training	Testing
7. I am "in-tune" with the other person during conversation	0.41	0.59	0.18	0.11
12. People find it easy to approach me	0.33	0.10	0.03	0.02
21. I can tell when someone is not interested in what I am saying	0.42	0.62	0.18	0.11
23. I am good at making small talk	0.33	0.10	0.03	0.02
25. I feel like I am really connecting with other people	0.33	0.10	0.03	0.02
28. I am warm and friendly in my interactions with others	0.34	0.10	0.03	0.02
34. I can tell when it is time to change topics in conversation	0.42	0.62	0.18	0.11

When removing these items, the data structure for all datasets moved closer to a factor model structure:

		Predictions		
Parent	**Dataset**	Empirical	Bootstrap	Proportion
Mother	Training	Factor	Factor	Factor (0.73) Network (0.27)
	Testing	Network	Network	Network (0.58) Factor (0.42)
Father	Training	Factor	Factor	Factor (1.00) Network (0.00)
	Testing	Factor	Factor	Factor (0.72) Network (0.28)

Indeed, three out of four datasets now suggest a factor model relative to a network

model. For those three models suggesting a factor model (mothers training and both fathers), all predictions were for a factor model. The testing mothers dataset was a network across all predictions but notably the proportions prediction suggested that the model moved away from a network model and closer to a factor model (from 0.71 to 0.58 for a network model and 0.29 to 0.42 for a factor model).