Running head: AUTOMATED STRUCTURAL EQUATION MODELING	1
Automatic selection of robust individual-level structural equation models for time serie	es
data	
•	

Abstract

In order to analyze intensive longitudinal data collected across multiple individuals, researchers frequently have to decide between aggregating all individuals or analyzing each individual separately. This paper presents an R package, gimme, which allows for the automatic identification of individual-level structural equation models that combine group-, subgroup-, and individual-level information. This R package is a complement of the GIMME program currently available via a combination of MATLAB and LISREL. By capitalizing on the flexibility of R and the capabilities of the existing structural equation modeling package lavaan, gimme allows for the automated identification and estimation of group-, subgroup-, and individual-level relations in time series data from within a structural equation modeling framework. Potential applications include any data for which there are numerous observations taken across multiple samples, such as daily diary data and function magnetic resonance imaging data.

Automatic selection of robust individual-level structural equation models for time series data

Motivation for gimme

Across varied domains, researchers collect multivariate data for each individual unit of study across numerous measurement occasions. Frequently referred to as time series data (alternatively, intensive longitudinal data), examples include psychophysiological processes studied using neuroimaging (Beltz et al., 2013), daily diary studies (Sliwinski, Smyth, Hofer, & Stawski, 2006), and observational coding of social interactions among dyads (Anzman-Frasca et al., 2013). A primary goal in acquiring these data is to understand temporal processes. Within the neuroimaging community, the process of interest is brain functioning and connectivity, where relations among spatially disparate regions across time offer insight into this phenomenon. Similarly, in daily diary studies, the process of interest may be the dynamics of psychological processes, such as emotion, over time. Methods for analyzing these processes vary greatly, but most have the same underlying goal: identifying the temporal relations that best describe a process over time.

Using time series data affords researchers the ability to pose different questions than those which could be answered with cross-sectional designs. Indeed, analyzing data across time often identifies different patterns of relations than when looking at cross-sectional data (Molenaar, 2004). A key benefit of utilizing time series data is the ability to investigate potential individual differences in patterns of relations. Both theory (Lamiell, 1981; Molenaar, 2008) and emerging results (Anzman-Frasca et al., 2013; Fair, Bathula, Nikolas, & Nigg, 2012; Gates, Molenaar, Iyer, Nigg, & Fair, 2014) suggest that individuals differ in many processes of interest to social scientists. Taken together, understanding these temporal processes on the individual level may assist social science researchers in providing improved diagnostic tools; in turn, this understanding will aid in the development of individually-tailored prevention protocols and treatment programs.

Structural equation modeling (SEM) is a popular approach for analyzing time series

data, as it can be used to obtain information regarding both lagged and contemporaneous effects frequently found in time series data. Though SEM can be applied at the individual level, two primary concerns preclude researchers from doing so. The first is gathering a sufficient number of observations across time. Should a sufficient number be obtained, a secondary concern is that noise will drive the results in individual samples (MacCallum, Roznowski, & Necowitz, 1992). In an attempt to detect signal from noise, the current standard is to conduct group-level analysis by concatenating individual time series data; that is, each individual's data is pasted consecutively below the previous individual's data to arrive at one matrix. Here, the length of the matrix is total number of observations across time $(T_i$, for each individual i) times the number of individuals (sample size N), where the number of columns is equal to the number of variables, p. Analysis that enables insight into the relations of multiple variables, such as SEM, is then conducted on this aggregated data to arrive at a nomothetic, or group-level, model that can then be applied to the population.

At its best, aggregating across individuals in this way may aid the researcher in detecting signal from noise. However, combining data sets assumes homogeneity in the relations among variables that explain the processes across individuals. That is, it requires that the data satisfy a strong assumption that one process is sufficient to describe the individuals comprising the sample. However, this assumption likely does not hold in many areas of study within the social sciences. When data sets are heterogeneous in terms of their temporal processes, false positives and false negatives may occur (Gates & Molenaar, 2012; Molenaar, 2004). One reason for these false paths is that individuals with particularly strong (or weak) connections may drive the results. Additionally, in the case where not many paths exist for the majority of members in a group, any search procedure may erroneously identify paths in an attempt to fit a model to the data.

Thus, both individual-level and group-level approaches are associated with limitations, and it is a daunting task for the researcher to decide whether to analyze each

individual separately or aggregate the individuals prior to model selection. This issue motivated the original development of group iterative multiple model estimation (GIMME), a toolbox available in MATLAB which relies on two proprietary programs: MATLAB (The MathWorks, 2010) and LISREL (Jöreskog & Sörbom, 2006), where MATLAB facilitates the user interface and LISREL provides model estimation and optimization. By looking across individuals for patterns of relations among variables at both the group- and individual-level, GIMME has been found to provide among the most reliable approaches available (Mumford & Ramsey, 2014), particularly in the presence of processes which are heterogeneous across individuals (Gates & Molenaar, 2012).

Requiring the use of two proprietary programs impedes usability for a number of reasons. First, due to licensing restrictions, LISREL cannot be placed on a server. Thus, researchers are unable to utilize cluster computing resources while running GIMME. Second, LISREL is only supported on Windows systems; it is not supported on Linux-based systems. Additionally, for researchers who do not use MATLAB or LISREL in other contexts, purchasing these two programs for the use of GIMME may be cost-prohibitive. Finally, updates in LISREL often change the format and nature of the output, which requires constant updating of the MATLAB shell which reads in the output. Taken together, there exists a great need for one publicly available, stand-alone program for users that may be used on servers and on all platforms. We capitalize on previously shown equivalences in the lavaan and LISREL estimates for SEM (Rosseel, 2012) to arrive at an R version of GIMME that is flexible and does not require the user to purchase any programs. The present project developed, extensively tested, and packaged gimme (S. Lane, Gates, & Molenaar, 2014) for R. This package contains adaptations, improvements, and extensions to the original GIMME MATLAB toolbox, ensuring that the R package performs as well or better than the previously evaluated version.

Specifications of model for current program

gimme utilizes the structural equation modeling (SEM) framework to 1) identify the structure of relations among variables of interest and 2) estimate the weights of these relations. In order to accommodate the sequential dependence found in time series data, gimme estimates the unified SEM (uSEM; also referred to as structural vector autoregression, SVAR) to obtain relations among variables across time (Chen et al., 2011; Gates, Molenaar, Hillary, Ram, & Rovine, 2010; Kim, Zhu, Chang, Bentler, & Ernst, 2007). The uSEM estimates both lagged (up to a predefined order of Q) and contemporaneous relations (zero order) simultaneously as follows:

$$\eta_t = A\eta_t + \sum_{q=1}^{Q} \phi_q \eta_{t-q} + \zeta_t \tag{1}$$

where $\eta_t, t = 1, 2, ..., T$ contains the manifest p-variate time series (where t ranges across the time-ordered sequence of observations), A contains the (p, p)-dimension matrix of contemporaneous relations among variables (with zeros along the diagonal), ϕ_q contains the (p, p)-dimension matrix of the associations among variables at a lag of q, and ζ_t contains a $p \times 1$ vector white noise process. The parameters in A and ϕ are contained in the B matrix of standard SEM software packages (including LISREL, Mplus (Múthen & Múthen, 2012), and lavaan). GIMME and gimme currently offer the option to have a lag of q = 1. All paths where the current time point would predict the previous time point are set to zero; that is, all B paths which would predict η_{t-1} are constrained to zero (Gates et al., 2010).

Traditionally, these uSEM models are either applied separately for each individual's data or to data that have been aggregated across individuals. To circumvent the issues that arise from either approach, in a multi-step process, gimme obtains a group-level model using a process robust to outliers and heterogeneity. This structure is then used as a starting point for identifying relations that exist for the individual in an iterative model search procedure. Previous work has demonstrated that beginning model selection with

group-level relations greatly improves the recovery of individual-level paths, alleviating the concern that individual model selection will be driven by noise (Gates & Molenaar, 2012). The gimme package uses lavaan for the estimation of structural equation models.

gimme begins by estimating an empty model (i.e., no estimated relations in the A or ϕ submatrices of the B matrix) across each individual. At the beginning, the researcher may specify whether or not to begin estimation with the autoregressive (AR) paths freed for estimation. The estimates of AR effects indicate the degree to which a given variable at t-1 predicts itself at t; these effects are frequently found in time series data. In the gimme package, researchers may also specify additional paths they wish to have estimated. In this way, the model search can be considered a semi-confirmatory model.

Modification indices are then obtained for each individual's model. Modification indices indicate the extent to which the model would improve should the corresponding element of the B matrix be freely estimated. Because modification indices are asymptotically $\chi^2(1)$ distributed, we can conduct significance tests for each element. Modification indices corresponding to the diagonal of the A matrix are removed, as a variable cannot predict itself in contemporaneous time. Similarly, paths where a variable at t would predict a variable at t-1 are removed. Once the null model for each individual has been estimated, gimme proceeds by counting which element, if freed, would significantly (according to a Bonferonni-corrected alpha level) improve model fit for the greatest number of individuals. In the presence of a tie, the element with the highest average modification index across individuals is selected. If this path is significant for >=75% of individuals, gimme adds this path to every individual's model and continues searching until no path meets this criteria. The cutoff value of 75% is typically found in neuroimaging research (van den Heuvel & Sporns, 2011), and it provides an appropriate heuristic for what constitutes the "majority." However, this cutoff value may be modified by the user. Importantly, if no path exist that meets this criteria, then none will be chosen during the group-level search procedure. Thus, no group-level model will be forced onto data so

heterogeneous that a group-level path would fail to describe individuals comprising the sample (details of this procedure can be found in (Gates & Molenaar, 2012).

Once an appropriate group-level model is established, paths which are no longer significant for the majority are pruned in a manner similar to the iterative search procedure. Specifically, the t values associated with each path are evaluated, and if <=75% of paths are significant, that path will be pruned. In the case of a tie, the path with the lowest average t value will be pruned. Once no paths fit this criteria, the group-level model is established. In this manner, gimme arrives at a group-level model that contains only paths which are significant for the majority of individuals comprising the sample that cannot be swayed by outlier cases. Though all individuals have these paths, the weights are allowed to vary across individuals at all steps of the procedure.

It may be the case that a researcher anticipates not only group- and individual-level paths, but also subgroup level paths. In this case, gimme allows for the specification of subgroup = TRUE, which utilizes information following the group-level search using a robust community detection method known as Walktrap (Pons & Latapy, 2006). The similarity, or adjacency, matrix which is used to cluster individuals contains information regarding how similar each pair of individuals is in their temporal models. Specifically, each individual's group-level path and expected parameter change (EPC) estimates are used. EPCs are related to modification indices but can take both positive and negative values and are normally distributed. gimme obtains a count for each pair of individuals i and j that reflects the number of significant B and EPC estimates that they both have and are in the same direction (i.e., positive or negative). This $N \times N$ adjacency matrix contains counts that indicate the number of temporal effects that the individuals have in common. Walktrap then returns a vector indicating the subgroup (or community) membership of each individual. gimme then proceeds by searching for paths specific to each subgroup in a manner similar to the group-level search. Once subgroup-level paths are added, a similar pruning procedure is then conducted. Finally, once this search is done, a final search is

done to ensure that all group-level paths are still significant for the majority of individuals.

Finally, using any group-level and potentially subgroup-level paths as the starting model, individual-level models are then estimated. Modification indices are again obtained, and the element with the highest MI exceeding $\chi^2(1)_{,\alpha=.01}$ is freely estimated. The model search for the individual is terminated when an excellent fitting model is obtained as indexed by two of four fit indices: root mean square error of approximation (RMSEA; Steiger, 1990), non-normed fit index (NNFI; Bentler & Bonnett, 1980), comparative fit index (CFI; Bentler, 1990), and standardized root mean-square residual (SRMR; Bentler, 1995). For the RMSEA and SRMR, values less than .05 indicate an excellent fit; for the CFI and NNFI, values greater than .95 indicate an excellent fit (Brown, 2006). This approach is similar to the manner in which researchers identify the appropriate number of factors within the SEM framework, and it performed optimally in the original GIMME program.

Formally, the final model obtained by gimme can be written as follows:

$$\eta_{t,i} = (A_i + A_i^g + A_i^s)\eta_{t,i} + (\phi_{1,i} + \phi_{1,i}^g + \phi_{1,i}^s)\eta_{t-1,i} + \zeta_{t,i}$$
(2)

where, as before, η_t indicates the manifest p-variate time series, A contains the contemporaneous paths, ϕ_1 contains the lag-1 paths, and ζ_t contains the errors in prediction. The subscript i indicates that the parameters in the matrix are unique estimates for individual i for i...N individuals. Matrices with superscript g contain estimates for paths in the group-level structure; that is, for each open path in the g superscript matrices, a path estimate exists for each individual. Matrices with superscript g contain paths for the subgroup-level structure. Please note that the matrices with g superscripts are not included should the researcher specify subgroup = FALSE. The matrices without the superscript g or g contain estimates for paths that exist for that individual and are not contained in the group structure. In this way, it is clear that there

are two (or potentially three) sub-models: one group-level structure, one subgroup-level structure, and one individual-level structure, all of which are estimated at the individual level.

Program

The gimme package has one major function, gimmeSEM(), that provides many options to the researcher. This function is used to analyze data using the algorithm described above. The program begins by accessing data files stored in a directory created by the user, or by accessing data already stored in a list in the R environment.

Regardless of which option is used, there should exist a data file for each individual containing a $T_i \times p$ matrix, where the columns represent variables and the rows represent time. Here, we distinguish T_i because the number of time points can vary across individuals. The number of variables, p, however, cannot vary over individuals. Before analysis begins, the gimmeSEM() function accesses each data file and creates p additional variables to represent the variable at T-1.

Instructions for use

The user begins by installing the gimme package and loading the gimme library using the following code:

```
install.packages("gimme", dependencies = TRUE)
library(gimme)
```

In order to apply the gimme algorithm to a set of time series data across N individuals, a call to gimme could be structured as:

```
8 paths = NULL)
```

The arguments within this function include: data, the path to the directory of data files or the name of the list containing all data matrices; out, the path to the directory where results will be stored; sep, the spacing of the data files using standard R convention ("" for space-delimited, "\t" for tab-delimited, and "," for comma-delimited); header, a logical indicating whether the data files have a header row; ar, a logical indicating whether or not model search should begin with AR paths open; plot, a logical indicating whether the user desires automatically generated plots from qgraph (Epskamp, Cramer, Waldorp, Schmittmann, & Borsboom, 2012) depicting relations among variables; subgroup, a logical indicating whether the user would like the model search to include subgroup-level paths; and paths, an optional argument where the user can specify lavaan-style syntax with paths with which to begin model estimation. All logicals above indicate the default values.

where the raw data files are stored in the directory provided for data, the results will be stored in the directory specified by out, the files are comma delimited and contain no header row, and model estimation will begin with autoregressive paths open. By default, plots (plot = TRUE), autoregressive paths are estimated (ar = TRUE), subgroups are not obtained (subgroup = FALSE), and no additional paths are specified with which to begin model estimation (paths = NULL).

To clarify the structure of the data directory, we present an example of the contents using:

```
head(list.files("C:/example1", full.names = TRUE))
```

```
[1] "C:/example1/group_1_1.csv" "C:/example1/group_1_10.csv"
[3] "C:/example1/group_1_11.csv" "C:/example1/group_1_12.csv"
[5] "C:/example1/group_1_13.csv" "C:/example1/group_1_14.csv"
```

Here, we see the file path for the first six files in the data directory. All of these files contain comma separated values (.csv), though text files containing values

separated by spaces, tabs, or commas may also be provided. Each file contains an individual's time series data with length T_i and p variables.

We can view the structure of an individual's data file using:

```
head(read.csv("C:/example1/group_1_1.csv"))
```

```
٧2
                         ٧4
                                       ٧6
                                               ۷7
                                                     ٧8
   V 1
                  VЗ
                                ٧5
                                                             ٧9
                                                                  V10
                                    0.944
3.236
      -2.868
               0.434 -2.885 4.876
                                            0.743 3.473 -2.375 3.952
4.535
      -3.394
               1.160
                     -2.157 5.917
                                   -1.068
                                           0.903 3.962
                                                        -1.573
                     -5.336 7.042
                                  -0.652 -1.454 4.344 -2.789
6.229 -1.615
             -0.309
       0.520 -1.315 -4.488 5.366
                                    0.980 -0.707 4.517 -3.527 3.756
4.113
       2.599
             -1.834 -5.391 7.424
                                    1.918
                                            0.083 6.499 -2.716 1.757
4.295
       3.876
               0.651 -3.843 5.839
                                    3.710
                                            0.967 6.344 -1.378 0.000
```

From this demonstration, we see that there is a data file for each individual containing a $T_i \times p$ time series (only the first six time points are presented here for illustrative purposes). Alternatively, the user may bypass the need for the sep and header arguments by providing a list of $T \times p$ data matrices directly to the data argument. This use of the data argument may be useful for users who already have all individuals' time series contained in a single list.

If an output directory is specified by the user, multiple output files are produced. For each run of gimmeSEM, two subdirectories are produced, individual and subgroup (if subgroup = TRUE is selected). Within the individual directory, three output files exist for each individual data file: a matrix containing B values for both contemporaneous and lagged relations, a matrix containing standard errors, and a plot summarizing the individual-level paths (if plot = TRUE). In this graphic, blue represents negative B values, red represents positive B weights, and the thickness of the line represents the magnitude of the edge weight. All other files are placed in the main output directory. Table 1 describes the output files and location.

In this example, we see that there are ten variables in an individual's data set. We generally recommend between five and fifteen variables for analysis, as estimation becomes unwieldy after fifteen variables. Additionally, we recommend at least sixty time points for researchers interested in using gimme, though more may be beneficial with a large number of variables (Lane, Gates, Pike, Beltz & Wright, under review).

Models are estimated using full information maximum likelihood (FIML). Consequently, we take advantage of the ability of FIML to handle missing data. Although the assumption of row-wise independence is violated in this instance, previous research has indicated that these quasi-maximum likelihood estimates approximate maximum likelihood estimates for AR processes (Hamaker, Dolan, & Molenaar, 2002). The syntax for each individual is iteratively updated upon the addition and pruning of new paths using the aforementioned process, and gimmeSEM() proceeds by estimating group-, (potentially) subgroup-, and individual-level paths. Output is then directed to an (optional) directory specified by the user, and the user is notified upon the completion of a successful search.

Two complementary functions exist that enable the user to compare results from gimmeSEM to current standard approaches for arriving at individual-level models and group-level models. First, indSEM() identifies the model for each individual independently and does not utilize shared information across individuals to inform model selection. As noted above, one criticism of this approach is that results may be driven by noise (Gates & Molenaar, 2012). No group-level model is generated. An additional function, aggSEM(), concatenates all of the individual data files to arrive at one data set. It then runs the indSEM() procedure on this data set. This procedure results in a group model and no individual-level paths; thus, no individual-level output or graphs (if plot = TRUE) are provided. A summary of the available functions is provided in Table 2.

In the model search, the user may declare certain paths which are expected to exist that can be added at the start of estimation. For example, a paths argument for data containing no header row could be defined below, where V2 indicates the variable located at column 2 in the data file. These paths represent that V4 predicts V2 contemporaneously, V3 at t-1 predicts V6 at t, and that model estimation should begin with these paths open

for all individuals. Example code is shown below where two confirmatory paths are specified and data are read in from a list:

Alternatively, gimmeSEM() can be run by launching the graphical user interface provided with the gimme package. To launch the GUI, simply type gimmeInteractive() into the R console. The GUI can be viewed in Figure 2.

Simulated Data Example

Here, we simulate data to demonstrate the functionality of gimme. Using simple algebraic substitution, equation 1 may be rewritten in the following manner to generate data for one individual with a lag of one time point:

$$\eta_t = (I - A)^{-1} (\phi_{\eta_{t-1}} + \zeta_t) \tag{3}$$

where I is an identity matrix of order (p,p) and ζ_t is a vector of innovations with unit variance. Data of length T=200 were generated for 25 replications (i.e., individuals). All individual replications had the group-level paths are depicted in Figure 3(a). The group-level paths have a weight of .5 for all individuals unless otherwise dictated by their subgroup membership. There were two equally-sized subgroups comprising the sample. These subgroups differed from each other in that 1) one of the group-level paths was made negative for one subgroup and 2) each group had two additional subgroup-specific paths. These differences are depicted in Figure 3(b) and Figure 3(c). Finally, at the individual level, individuals had an extra path in the both the lagged and contemporaneous matrix at a probability of .01 (not depicted in Figure 3). These data replicate true data seen in the literature by having group, subgroup, and individual-level paths and weights that vary

systematically across these levels. These data are loaded with the gimme package, and may be analyzed with the following code:

```
fit <- gimmeSEM(data = sim_data,
subgroup = TRUE)
```

Upon successful completion of the model search, summary information prints to the console:

```
gimme finished running normally
Number of subgroups = 2
Modularity = 0.14043
```

Two main options exist for viewing and interacting with output. First, if the user specifies a file path in the out argument, a copy of all relevant output will be placed in the specified directory. If the directory at the specified file path does not exist, it will be created. The user may also direct the output from gimmeSEM to an object and use predefined functions to access individual-, subgroup-, and group-level output.

Group and subgroup-level output. In order to access group-level and subgroup-level information, we may use a series of functions to inspect the fit object. For example, in order to view a path diagram depicting relationships across the entire sample, we may use:

```
plot(fit)
```

This image is depicted in Figure 4(a). In order to view plots specific to each subgroup, we may specify

```
plot(fit, subgroup = 1)
plot(fit, subgroup = 2)
```

These images are depicted in Figure 4(b) and 4(c).

Similarly, to view a matrix containing the count of each relationship across all individuals, we may specify:

```
print(fit)
```

```
Please specify a file id for individual coefficient matrix.
   Otherwise, a summary count matrix and sample average matrix are presented
        below.
  Lagged Count Matrix for Sample
       V11ag V21ag V31ag V41ag V51ag V61ag V71ag V81ag V91ag V101ag
  V1
           25
                   1
                          0
                                  0
                                         0
                                                0
                                                        1
                                                               0
                                 0
                                                                               0
  ٧2
            1
                  25
                          0
                                         0
                                                0
                                                      13
                                                               0
                                                                      0
                   2
  VЗ
            1
                         25
                                 0
                                         0
                                                0
                                                       0
                                                               0
                                                                      0
                                                                               0
  ٧4
            0
                   0
                          1
                                25
                                         1
                                                0
                                                       0
                                                               0
                                                                      0
                                                                             25
  ٧5
            0
                   0
                                        25
                                                               0
                                                                     25
                          0
                                  0
                                                0
                                                       0
                                                                               0
10
  V6
            2
                   1
                         12
                                 0
                                         0
                                               25
                                                       0
                                                               0
                                                                               0
                                                                      1
11
  ٧7
            0
                   1
                          0
                                 1
                                         0
                                                0
                                                      25
                                                              1
                                                                               0
12
  ٧8
            1
                   2
                          0
                                12
                                        25
                                                       2
                                                              25
                                                                      0
                                                                               0
                                                0
13
  ٧9
           25
                   0
                                  0
                                         1
                                                        0
                                                              13
                                                                     25
                                                                               0
14
  V10
                   0
                                  0
                                         0
                                                       0
                                                               0
                                                                             25
            2
                          1
                                                                      1
15
16
  Contemporaneous Count Matrix for Sample
^{17}
       V1 V2 V3 V4
                     ٧5
                        V6
                            V7 V8
18
  V1
        0
            1 13
                   0
                      0
                          0
                              0 25
                                     0
                                         12
19
            0
               0
                   0
                              0
                                 0
  ٧2
       13
                      1 25
                                     0
20
               0 12
                                          2
  V3
        0
            0
                      1
                          0
                              0 25
                                     0
21
                          0 25
  ٧4
        0
            0
               0
                   0
                      0
                                  0 13
                                          0
22
  ٧5
        0
           0 25 13
                              0
                                  0
23
                      0
                          1
                                          0
  ٧6
        0
           1
               0
                   0
                      0
                          0
                              0
                                 0
                                     0
                                          0
24
       25
               1
                  0
                             0 12
  ٧7
           0
                      1
                          0
                                     0
25
  ٧8
        0
           0
              0
                   0
                      0
                              0
                                     0
                                          0
                          1
26
                                 0
  ۷9
        0
            0 13
                   0
                      1
                          0
                              0
                                     0
                                          0
27
  V10
        0
            1
               1
                   0
                      2
                          0 12
                                  0
                                          0
```

Similarly, we may use print(fit, subgroup = 1) to view the count matrix across individuals in subgroup 1.

Individual-level output. In order to access the fit indices, convergence status, and subgroup membership of a given individual, the summary() function may be used. With this function, the object containing the output as well as the file name should be specified. If data were read in from a physical directory, the file name should be the original name without the file extension. If data were provided in a list format, the file name should be the name of that individual's data matrix in the list. For example, to view the summary information for group_1_2 within the sim_data list, the following code may be

used:

```
summary(fit, file = "group_1_2")
```

which yields the information for a single individual:

```
Fit for file group_1_2 chisq df pval rmsea srmr nnfi cfi status subgroup 256.7882 117 0 0.0773 0.0169 0.9812 0.9695 converged normally 2
```

In order to view the coefficients for a single individual, the following code may be used:

```
coef(fit, file = "group_1_2")
```

```
Coefficients for group_1_2
        file
               dv
                       iv
                            beta
                                                          level
                                               z pval
                                     se
   group_1_2
               V 1
                   V1lag
                           0.563 0.051
                                         10.977
                                                          group
   group_1_2
               V1
                       8
                           0.757 0.033
                                         23.019
                                                    0
                                                          group
   group_1_2 V10 V10lag
                           0.561 0.032
                                         17.833
                                                          group
               ٧2
                   V2lag
                           0.581 0.029
                                         20.317
                                                    0
   group_1_2
                                                          group
   group_1_2
               ٧2
                       ٧6
                           0.579 0.029
                                         20.229
                                                          group
   group_1_2
               VЗ
                   V3lag
                           0.297 0.032
                                          9.415
                                                    0
                                                          group
               VЗ
                           0.841 0.038
                                         21.934
   group_1_2
                                                    0
                                                          group
   group_1_2
               V4 V10lag
                          -0.504 0.035
                                        -14.557
                                                          group
               ٧4
                   V4lag
                           0.526 0.035
                                         14.935
   group_1_2
                                                          group
11
   group_1_2
                       ٧7
                           0.356 0.033
                                         10.857
12
               ٧4
                                                    0
                                                          group
   group_1_2
               ۷5
                       VЗ
                           0.568 0.038
                                         14.995
                                                    0
                                                          group
13
                           0.529 0.039
               ٧5
                   V5lag
                                         13.603
                                                    0
   group_1_2
                                                          group
                   V9lag -0.389 0.035
   group_1_2
               ٧5
                                        -10.992
                                                    0
                                                          group
15
   group_1_2
                           0.604 0.030
               ٧6
                   V6lag
                                         19.969
                                                    0
                                                          group
16
   group_1_2
               ٧7
                       V1 -0.622 0.092
                                         -6.756
                                                    0
                                                          group
17
   group_1_2
               ٧7
                   V7lag
                          0.505 0.050
                                         10.008
18
                                                          group
   group_1_2
               87
                   V5lag -0.434 0.031
                                        -14.087
                                                    0
                                                          group
19
   group_1_2
               8
                   V8lag
                           0.623 0.033
                                         19.115
                                                    0
20
                                                          group
               ۷9
                   V1lag -0.547 0.035 -15.723
   group_1_2
                                                    0
                                                          group
21
   group_1_2
               ٧9
                   V9lag
                          0.630 0.034
                                         18.750
22
                                                          group
   group_1_2 V10
                   V1lag -0.482 0.029
                                        -16.725
                                                    0
                                                            ind
23
   group_1_2
               ٧7
                   V2lag
                          -0.888 0.052
                                        -17.041
                                                    0
                                                            ind
24
               V1
                      V10
                           0.471 0.047
                                          9.971
                                                    0 subgroup
   group_1_2
                           0.313 0.028
                                         11.311
                                                    0 subgroup
   group_1_2 V10
                       ٧7
26
   group_1_2
               VЗ
                      ٧4
                           0.153 0.033
                                          4.612
                                                    0 subgroup
27
               ٧6
                   V3lag -0.628 0.030 -20.890
                                                    0 subgroup
28
   group_1_2
                                                    0 subgroup
               ٧7
                       8
                           1.026 0.116
                                          8.858
   group_1_2
                   V4lag -0.310 0.024 -12.954
                                                    0 subgroup
   group_1_2
               8
```

Here, we see the coefficients for each path in the final model for individual group_1_2. The level column details whether the path was estimated across all individuals (group), across the individuals in the subgroup to which this individual belonged (subgroup), or within this specific individual (ind). Thus, we see the point estimate, standard error, p value, and z value associated with each path estimated for this individual.

Complementary information is available using the print() function, which displays the contemporaneous and lagged coefficient matrices for a given individual:

```
print(fit, file = "group_1_2")
```

```
Lagged Matrix for group_1_2
       V11ag V21ag V31ag V41ag V51ag V61ag V71ag V81ag V91ag V101ag
  V1
        0.56
               0.00
                      0.00
                            0.00
                                   0.00
                                            0.0
                                                 0.00
                                                        0.00
                                                               0.00
                                                                       0.00
        0.00
  ٧2
               0.58
                      0.00
                            0.00
                                   0.00
                                            0.0
                                                 0.00
                                                        0.00
                                                               0.00
                                                                       0.00
  ٧3
        0.00
               0.00
                      0.30
                            0.00
                                   0.00
                                            0.0
                                                 0.00
                                                        0.00
                                                               0.00
                                                                       0.00
  ٧4
        0.00
               0.00
                      0.00
                            0.53
                                   0.00
                                            0.0
                                                 0.00
                                                        0.00
                                                               0.00
                                                                      -0.50
        0.00
                     0.00
  ۷5
               0.00
                            0.00
                                   0.53
                                            0.0
                                                 0.00
                                                        0.00
                                                              -0.39
                                                                       0.00
  V6
        0.00
               0.00
                    -0.63
                            0.00
                                   0.00
                                            0.6
                                                 0.00
                                                        0.00
                                                               0.00
                                                                       0.00
  ۷7
        0.00 -0.89
                      0.00
                            0.00
                                   0.00
                                            0.0
                                                 0.51
                                                        0.00
                                                               0.00
                                                                       0.00
  ٧8
        0.00
               0.00
                      0.00
                           -0.31
                                  -0.43
                                                 0.00
                                                        0.62
                                                               0.00
                                                                       0.00
10
                                            0.0
                      0.00
11
  ٧9
       -0.55
               0.00
                            0.00
                                   0.00
                                            0.0
                                                 0.00
                                                        0.00
                                                               0.63
                                                                       0.00
  V10 -0.48
              0.00
                      0.00
                            0.00
                                   0.00
                                            0.0
                                                 0.00
                                                        0.00
                                                               0.00
                                                                       0.56
12
13
  Contemporaneous Matrix for group_1_2
14
                   VЗ
                         V4 V5
          V1 V2
                                  V6
                                              V8 V9
                                                      V10
15
                                        ٧7
16
  V 1
        0.00
              0 0.00 0.00
                              0 0.00 0.00 0.76
                                                  0 0.47
  ٧2
        0.00
               0 0.00 0.00
                              0 0.58 0.00 0.00
                                                  0 0.00
17
  VЗ
        0.00
              0 0.00 0.15
                              0 0.00 0.00 0.84
                                                  0 0.00
18
        0.00
               0 0.00 0.00
                              0 0.00 0.36 0.00
  ٧4
                                                  0 0.00
19
  ٧5
        0.00
              0 0.57 0.00
                              0 0.00 0.00 0.00
                                                  0 0.00
20
21
  V6
        0.00
              0 0.00 0.00
                              0
                                0.00
                                     0.00 0.00
                                                  0 0.00
                                                  0 0.00
  ۷7
       -0.62
              0 0.00 0.00
                              0 0.00 0.00 1.03
22
  ٧8
        0.00
              0 0.00 0.00
                              0
                               0.00 0.00 0.00
                                                  0 0.00
23
  ٧9
        0.00
              0 0.00 0.00
                              0 0.00 0.00 0.00
                                                  0 0.00
^{24}
  V10
        0.00
               0 0.00 0.00
                              0 0.00 0.31 0.00
                                                  0 0.00
```

Here, the rows contain the dependent (predicted) variables and the columns contain the independent variables. For instance, the value of 0.56 at the intersection of V1 and V11ag indicates that V11ag predicts V1 with a β of 0.56. An individual-level path diagram

depicting these relations may be obtained using plot(fit, file = "group_1_2"), where red paths indicate positive paths, blue paths indicate negative paths, and the width of the path represents its magnitude.

Importantly, the ability of gimmeSEM() to accurately recover group-, subgroup-, and individual-level paths in the presence of heterogenous data has been demonstrated previously (Gates & Molenaar, 2012; Gates, Lane, Varangis, Giovanello, and Guskiewicz, accepted). Our purpose here is simply to demonstrate the usage of the package and the navigation of the output.

Empirical Data Example

To illustrate the use and interpretation of the package, we use daily diary data collected by Borkenau and Ostendorf (1998). In this study, 22 individuals were asked for 90 consecutive days to respond to 30 self-report markers of the Big Five (Borkenau & Ostendorf, 1998). For illustrative purposes, we've selected six items pertaining to the neuroticism dimension of the Big Five. These items include irritable (irr), emotionally stable (emot), calm, bad-tempered (badtemp), resistant (res), and vulnerable (vul). Analyzing these data will allow for insight into the lagged and contemporaneous relationships characterizing intraindividual variation over time.

If all individuals' data matrices are contained within a list, a gimme run may be structured using:

```
fit <- gimmeSEM(data = borkenau)
```

Given that no output directory is specified, all relevant output will be directed to the fit object using the assignment operator (<-). We may view the summary matrix containing the count of paths across individuals using:

print(fit)

which displays:

```
Please specify a file id for individual coefficient matrix.
  Otherwise, summary count matrix is presented below.
4 Lagged Count Matrix for Sample
         irrlag emotlag calmlag badtemplag reslag vullag
5
              22
                      2
                                0
6 irr
                                           1
                      22
7
 emot
              1
                               0
                                           1
                                                  0
                                                          0
 calm
              0
                      0
                               22
                                           1
                                                  0
                                                          0
 badtemp
              0
                       0
                               0
                                          22
                                                  0
                                                          0
               0
                       0
                                                  22
                                                          0
10 res
                                           1
                                1
 vul
               0
                       1
                                0
                                                  0
                                                         22
11
12
13 Contemporaneous Count Matrix for Sample
          irr emot calm badtemp res vul
14
           0
15 irr
                      3
                               5
            4
              0
                      0
                               1
                                     22
16 emot
            0 12
                                   2
17 calm
                      0
                                       5
18 badtemp
            5
                7
                      0
                               0
                                   1
                                       3
19 res
           3
                 3
                      0
                               1
                                   0
                                      22
20 vul
           22
                 1
                      0
                               1
                                   4
                                       0
```

From these results, we see that three sample-level paths emerged contemporaneously: vulnerability predicting emotional stability, vulnerability predicting resistance, and irritability predicting vulnerability. This indicates that these relationships were significant for greater than 75% of the sample. We may view the average of the relationships across individuals using

```
print(fit, mean = TRUE)
```

```
Please specify a file id for individual coefficient matrix.
  Otherwise, a summary average matrix is presented below.
4 Lagged Average Matrix for Sample
          irrlag emotlag calmlag badtemplag reslag vullag
            0.11
                 0.00
                         0.00
                                      -0.01
                                                     0.00
6 irr
                                              0.00
           -0.01
                   0.08
                            0.00
                                      -0.01
                                              0.00
                                                     0.00
 emot
8 calm
            0.00
                   0.00
                            0.05
                                      0.01
                                              0.00
                                                     0.00
            0.00
                   0.00
                            0.00
                                       0.10
                                              0.00
                                                     0.00
 badtemp
            0.00
                   0.00
                         0.01
                                      -0.01
                                                     0.00
10 res
                                              0.05
           0.00
                   -0.01
                          0.00
                                      0.01
                                              0.00
                                                     0.05
 vul
11
12
13
 Contemporaneous Average Matrix for Sample
           irr emot calm badtemp
                                      res
                                            vul
14
15 irr
           0.00 -0.01 -0.11 0.11 -0.04
```

```
emot
           -0.10
                   0.00
                         0.00
                                  -0.02
                                          0.09 - 0.36
16
            0.00
                   0.31
                         0.00
                                  -0.04
                                          0.03 - 0.09
17
  calm
18 badtemp
            0.11 - 0.17
                          0.00
                                   0.00 - 0.01
                                                 0.07
           -0.09
                   0.05
                          0.00
                                  -0.01
                                          0.00 -0.33
19 res
            1.46
                   0.02
                          0.00
                                   0.01
                                          0.90
                                                 0.00
  vul
20
```

Similarly, the coefficients for a given individual may be accessed using their filename (without extension) or the name of their list. Here, the coefficient matrix for individual "BorkInd4" may be accessed using:

```
print(fit, file = "BorkInd4")
```

```
Lagged Matrix for BorkInd4
           irrlag emotlag calmlag badtemplag reslag vullag
2
  irr
             0.18
                      0.00
                               0.00
                                            0.00
                                                    0.00
                                                            0.00
3
                      0.11
             0.00
                               0.00
                                            0.00
                                                            0.00
  emot
                                                    0.00
             0.00
                      0.00
                               0.12
                                            0.00
                                                    0.00
                                                            0.00
  calm
             0.00
                      0.00
                               0.00
                                            0.24
                                                    0.00
                                                            0.00
  badtemp
7
  res
             0.00
                      0.00
                               0.23
                                            0.00
                                                    0.17
                                                            0.00
             0.00
                      0.00
                               0.00
                                            0.00
                                                    0.00
                                                            0.05
  vııl
  Contemporaneous Matrix for BorkInd4
             irr
                   emot calm badtemp res
                                              vul
11
            0.00
                   0.00
                            0
                                     0
                                             0.00
12
  irr
                                          0
  emot
           -0.29
                   0.00
                            0
                                     0
                                          0 - 0.32
13
            0.00
                   0.55
                            0
                                     0
                                          0
                                             0.00
  calm
                            0
  badtemp
            0.00 - 0.39
                                          0
                                             0.00
15
            0.00
                   0.00
                            0
                                     0
                                          0
                                             0.04
  res
16
  vul
            0.57
                   0.00
                                             0.00
17
```

Here, we may see an individual's coefficients for her final model, composed of group- and individual-level paths. For example, for the group-level path between irritability and vulnerability, we see $\beta=0.57$. Similarly, for the group-level path between vulnerability and emotional stability, we see $\beta=-0.32$. Interestingly, we see that all group-level paths surfaced contemporaneously. This may be due to a difference in the speed of the process under observation and the speed of the measurement occasion. That is, when processes occur faster than the rate of observation, effects may surface contemporaneously (Granger, 1969).

We may also view this using the pre-defined plot() function, where the plot for the same individual may be viewed using:

```
plot(fit, file = "BorkInd4")
```

This plot is displayed in Figure 6.

Discussion

The R package gimme described in this paper introduces an SEM-based method for identifying group-, subgroup-, and individual-level relations within time series data. This package promises to be useful for researchers analyzing a range of data, from establishing functional connectivity using fMRI data to investigating dynamic processes over time within daily diary data.

The gimme package is characterized by a number of strengths. It utilizes the popular and well-maintained lavaan package for estimation. Additionally, given the small number of commands required by the user, as well as the availability of a graphical user interface (GUI), gimme can be used by both inexperienced and experienced R users. The automatic identification and estimation of models greatly reduces user burden. Importantly, this implementation improves upon the original GIMME by offering a community detection based subgrouping procedure, automatically generated summary graphics using the qgraph package (Epskamp et al., 2012), and the ability to begin model estimation with semi-confirmatory paths. Additionally, this implementation of GIMME only requires R, not a combination of proprietary software like the original GIMME toolbox.

Multiple aspects of the gimme package are open to further development. For example, the current implementation slows considerably when trying to estimate relations among more than 20 variables; however, work is underway to expand the package to allow for the estimation of relations among more variables, including both a measurement and structural model, using an alternative estimation procedure. Another extension may allow for estimation of exogenous variables that have been convolved with a hemodynamic response

function for use fMRI data obtained during an event-related design. Additionally, the researcher may wish to implement a different definition of what constitutes the "majority" at the group- and subgroup-level, and we have made resources available to instruct users where they can modify code to achieve this purpose. We encourage users to contribute to our Github page at https://github.com/Author/gimme. In sum, gimme represents a flexible, user-friendly package to evaluate individual-level time-series data using an automated search procedure based in structural equation modeling.

References

- Anzman-Frasca, S., Liu, S., Gates, K. M., Paul, I. M., Rovine, M. J., & Birch, L. L. (2013). Infants' transitions out of a fussing/crying state are modifiable and are related to weight status. *Infancy*, 18(5), 662–686.
- Beltz, A. M., Gates, K. M., Engels, A. S., Molenaar, P. C., Pulido, C., Turrisi, R., Wilson, S. J. (2013). Changes in alcohol-related brain networks across the first year of college: A prospective pilot study using fmri effective connectivity mapping.
 Addictive Behaviors, 38(4), 2052–2059.
- Bentler, P. M. (1990). Comparative fit indexes in structural models. *Psychological Bulletin*, 107, 238–246.
- Bentler, P. M. (1995). Eqs structural equations program manual [Computer software manual]. Encino, CA: Multivariate Software.
- Bentler, P. M., & Bonnett, D. G. (1980). Significance tests and goodness of fit in the analysis of covariance structures. *Psychological Bulletin*, 88, 588-606.
- Borkenau, P., & Ostendorf, F. (1998). The big five as states: How useful is the five-factor model to describe intraindividual variations over time? *Journal of Research in Personality*, 32(2), 202–221.
- Brown, T. (2006). Confirmatory factor analysis for applied research. New York: Gilford Press.
- Chen, G., Glen, D. R., Saad, Z. S., Hamilton, J. P., Thompson, M. E., Gotlib, I. H., & Cox, R. W. (2011). Vector autoregression, structural equation modeling, and their synthesis in neuroimaging data analysis. *Computers in Biology and Medicine*, 41, 1142–1115.
- Epskamp, S., Cramer, A. O. J., Waldorp, L. J., Schmittmann, V. D., & Borsboom, D. (2012). qgraph: Network visualizations of relationships in psychometric data. *Journal of Statistical Software*, 48(4), 1–18. Retrieved from http://www.jstatsoft.org/v48/i04/

- Fair, D. A., Bathula, D., Nikolas, M. A., & Nigg, J. T. (2012). Distinct neuropsychological subgroups in typically developing youth inform heterogeneity in children with adhd. PNAS: Proceedings of the National Academy of the United States of America, 109, 6769–6774.
- Gates, K. M., Lane, S. T., Varangis, E., Giovanello, K., & Guskiewicz, K. (accepted).

 Unsupervised classification during time series model selection. *Multivariate*Behavioral Research.
- Gates, K. M., & Molenaar, P. C. (2012). Group search algorithm recovers effective connectivity maps for individuals in homogeneous and heterogeneous samples. *NeuroImage*, 63, 310–319.
- Gates, K. M., Molenaar, P. C., Hillary, F. G., Ram, N., & Rovine, M. J. (2010).

 Automatic search for fmri connectivity mapping: An alternative to granger causality testing using formal equivalences among sem path modeling, var, and unified sem.

 NeuroImage, 50, 1118–1125.
- Gates, K. M., Molenaar, P. C., Iyer, S. P., Nigg, J. T., & Fair, D. A. (2014). Organizing heterogeneous samples using community detection of gimme-derived resting state functional networks. *PLOS One*, 9(3), 1–11.
- Granger, C. W. J. (1969). Investigating causal relations by econometric models and cross-spectral methods. *Econometrica*, 37(3), 424-438.
- Hamaker, E., Dolan, C., & Molenaar, P. (2002). On the nature of SEM estimates of ARMA parameters. Structural Equation Modeling, 9, 347–368.
- Jöreskog, K., & Sörbom, D. (2006). Lisrel 8.8 for windows [Computer software manual]. Scientific Software International, Inc..
- Kim, J., Zhu, W., Chang, L., Bentler, P., & Ernst, T. (2007). Unified structural equation modeling approach for the analysis of multisubject, multivariate functional mri data. *Human Brain Mapping*, 28, 85–93.
- Lamiell, J. T. (1981). Toward an idiothetic psychology of personality. American

- Psychologist, 36(3), 276–289.
- Lane, S., Gates, K., & Molenaar, P. (2014). gimme: Group iterative multiple model estimation [Computer software manual]. Retrieved from https://CRAN.R-project.org/package=gimme (R package version 0.1-7)
- Lane, S. T., Gates, K., Pike, H., Beltz, A., & Wright, A. (under review). Uncovering general, shared, and unique temporal patterns in ambulatory assessment data.
- MacCallum, R. C., Roznowski, M., & Necowitz, L. B. (1992). Model modifications in covariance structure analysis: The problem of capitalization on chance. *Psychological Bulletin*, 111(3), 490–504.
- Molenaar, P. C. (2004). A manifesto on psychology as idiographic science: Bringing the person back into scientific psychology, this time forever. *Measurement*, 2, 201–218.
- Molenaar, P. C. (2008). On the implications of the classical ergodic theorems: Analysis of developmental processes has to focus on intra-individual variation. *Developmental Psychobiology*, 50, 60–69.
- Mumford, J., & Ramsey, J. (2014). Bayesian networks for fmri: A primer. *NeuroImage*, 86, 573–582.
- Múthen, L., & Múthen, B. (2012). Mplus user's guide, 7th edition [Computer software manual]. Múthen & Múthen, Los Angeles, CA.
- Pons, P., & Latapy, M. (2006). Computing communities in large networks using random walks. *Journal of Graph Algorithms and Applications*, 10, 191–218.
- Rosseel, Y. (2012). lavaan: An R package for structural equation modeling. *Journal of Statistical Software*, 48(2), 1–36. Retrieved from http://www.jstatsoft.org/v48/i02/
- Sliwinski, M. J., Smyth, J. M., Hofer, S. M., & Stawski, R. S. (2006). Intraindividual coupling of daily stress and cognition. *Psychological Aging*, 21(3), 545–557.
- Steiger, J. H. (1990). Structural model evaluation and modification: An interval estimation approach. *Multivariate Behavioral Research*, 25, 173–180.

The MathWorks, I. (2010). Matlab – the language of technical computing, version 7.10.0 [Computer software manual]. The MathWorks, Inc., Natick, Massachusetts. Retrieved from http://www.mathworks.com/products/matlab van den Heuvel, M. P., & Sporns, O. (2011). Rich-club organization of the human connectome. The Journal of Neuroscience, 31(44), 15775–15786.