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Estimating Both Directed and Undirected Contemporaneous Relations in Time Series Data Using Hybrid-Group Iterative Multiple Model Estimation

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Abstract

Researchers across varied fields increasingly are collecting and analyzing intensive longitudinal data (ILD) to examine processes across time at the individual level. Two types of relations are typically examined: lagged and contemporaneous. Lagged relations capture how variables at a prior time point can be used to explain variance in variables at a later time point. These are always modeled using auto- and cross-regressions by means of vector autoregression (VAR). By contrast, there are two types of relations commonly used to model the contemporaneous relations, which model how variables relate instantaneously. Until now, researchers must opt to either model contemporaneous relations as undirected relations among residuals (e.g., partial or full correlations) or as directed relations among the variables (e.g., paths or regressions). The choice for how to model contemporaneous relations has implications for inferences as well as the potential to introduce bias in the VAR lagged relations if the wrong type of relation is used. This article introduces a novel data-driven method, hybrid-group iterative multiple model estimation (GIMME), that provides a solution to the problem of having to choose one or the other type of contemporaneous relation to model. The modeling framework utilized in hybrid-GIMME allows for both types of contemporaneous relations in addition to the standard VAR relations. Both simulated and empirical data were used to test the performance of hybrid-GIMME. Results suggest this is a robust method for recovering contemporaneous relations in an exploratory manner, particularly with an ample number of time points per person.

Translational Abstract

This paper describes the development of a new statistical method for examining processes for individuals across time. There are two main types of contemporaneous relations: directed and undirected. A directed relation is typically interpreted as one variable (e.g., sleep quality) explains variability (or changes) in another variable (e.g., mood next day), while an undirected relation is commonly understood as two variables' variability being explained by a third one (e.g., mood the day before). Unlike most existing statistical methods that only allow for one of these two types of contemporaneous relations to be estimated, this new algorithm (hybrid-GIMME) allows for them both to be estimated simultaneously. And it thus allows for new questions to be explored. Both our simulation and empirical examples show promising results of this new method.

Keywords: structural equation modeling, time series analysis, vector autoregression, exploratory factor analysis

Increasingly researchers are looking to intensive longitudinal data (ILD) to answer questions about processes across time at the individual level. In the social and behavioral sciences ILD typically takes the form of multivariate time series data, or a time-ordered sequence of observations (Wei, 2012). Interest in time series data has been growing in recent years due to technological advances in data collection and the increasing appreciation of variability in the structures of dynamic processes between individuals. Examples of research studying time series data include daily diary studies (Sliwinski et al., 2006; Wright & Simms, 2016) and functional MRI experiments (fMRIrid; Beltz, Gates, et al., 2013), to name a few.

With ILD, researchers and clinicians can understand and describe individuals' temporal processes via their lagged and contemporaneous relations. Lagged relations refer to any relation

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where variability at a given time point t for a given variable is explained by prior time points (e.g., t-1, t-2) of itself or other variables, whereas contemporaneous relations refer to the relationship of a given variable at t with another variable also at t. Lagged relations are usually modeled using directed auto- and cross-regressions. However, for contemporaneous relations there are more options available. The two most commonly encountered models in practice, unified structural equation modeling (uSEM; Kim et al., 2007) and graphical vector autoregression (gVAR; Wild et al., 2010), estimate contemporaneous relations either as directed relations among the observed variables or as undirected relations among residuals, respectively. Importantly, neither approach allows for both types of contemporaneous relations to be modeled simultaneously. In this article, we define a "directed" relation as unidirectional, that is, it points from one variable to another, and an "undirected" relation as nondirectional, that is, it does not have an arrow pointing from one variable to another but rather just connects two variables. Mathematically, one can think of a series of directed relations represented by an asymmetric matrix (as in multivariate regression analyses) and undirected relations represented by a symmetric matrix (as in correlation matrices). In the uSEM framework, contemporaneous relations are estimated as directed relations, as opposed to in the VAR approach where contemporaneous relations are estimated as undirected among variables (errors). A uSEM can be transformed to an equivalent VAR representation as we will demonstrate later.

Statistical tests of directed contemporaneous relations attend to different research questions and carry different assumptions than tests of correlations — much like in cross-sectional research. Directed contemporaneous relations can imply that one variable explains variability in another variable after controlling for covariates. As an example, let's take two commonly used measures: anxiety and feeling sad. One research hypothesis might be that feeling sad relates to higher levels of anxiety after taking into account other variables. The interpretation is the same whether it is in the time series context or cross-sectional context: Having some information about sadness at time t explains some variability in anxiety levels (above and beyond other covariates) at the same time point. The test here is whether sadness explains variability in anxiety after controlling for other potential variables, and doesn't test the reverse direction. Similarly, contemporaneous directed relations in the time series context indicate that some knowledge about the value of one variable (say, sadness) explains variability in another variable at that time point, but perhaps not the reverse. This can help the research in generating hypotheses to test, such as if addressing an individual's sadness influences their anxiety levels.

The interpretation of the undirected relations differs slightly in the time series context from cross-sectional. Here in the time series context, the correlations are typically among residuals after already taking into account the lagged influence of other variables. So, it is not simply the correlation between two variables. Rather, it is the correlation between what was not explained by the lagged portion of the model (and directed contemporaneous portion, if included) for each of the two variables. One might expect correlated residuals in processes where the two variables have a common cause, or when the variables explain similar levels of variability in each other. Take two symptoms of depression: feelings of sadness and emptiness. After regressing out all other influences on these two variables such as lagged relations, the residuals for these two variables may correlate because they are both caused by the unmodeled latent construct of depression.

Oftentimes, it is not clear which type of relation best attends to the dynamic interplay of the data at hand. The two main options for modeling contemporaneous relations are the uSEM and gVAR. The uSEM approach estimates contemporaneous relations as directed relations among the observed variables, often after taking into account the variance explained by their autoregressive (or self-lagged) relation. This time series approach combines vector autoregressive modeling (VAR; Hamilton, 1994; Lütkepohl, 2005) with traditional structural equation modeling (SEM; Bollen, 1989), the latter of which is typically applied to data where there is an assumption of independent observations, as seen in cross-sectional data. Observation independence is rarely the case for time series data due to serial dependencies and lagged relations. In uSEM, the contemporaneous relations resemble the lagged relations: all relations are directed. Current implementations of the uSEM class of models are data-driven with sparsity typically induced by a sequential search for relations (i.e., within the Group Iterative Multiple Model Estimation (GIMME) framework; Gates & Molenaar, 2012). By estimating the model within the SEM framework, researchers can directly control for contemporaneous influences on target variables while estimating lagged relations, thus preventing spurious or false positive lagged relations (Gates et al., 2010). In addition, researchers can use fit indices to evaluate model-data correspondence.

Another approach for estimating contemporaneous relations is to consider the undirected relations of residuals from within a traditional VAR framework. As noted in the Introduction, we define an undirected relation here to mean that the residuals of two variables are correlated or partially correlated, which differs from a feedback loop where the variables both predict each other with two directed relations (Carver & Scheier, 1982). Correlating errors of a traditional VAR is standard practice. Graphical VAR (Epskamp, van Borkulo, et al., 2018; Wild et al., 2010) is a newer approach that is popular in psychological sciences, and similarly models contemporaneous relations as undirected among the residuals. Specifically, gVAR takes the partial correlation of the contemporaneous residuals (i.e., the correlation between the residuals of two contemporaneous variables after conditioning on all other contemporaneous residuals) following traditional estimation of a VAR model (Epskamp & Fried, 2018). Both the VAR coefficient estimates and residual covariance matrices have sparsity induced via regularization in the *graphicalVAR* package (Epskamp, Waldorp, et al., 2018). One benefit of correlating the residuals within the regularized VAR approach is that it can have more potential parameters than a saturated nonregularized VAR model (Epskamp, Waldorp, et al., 2018).

The two approaches carry different assumptions and interpretations. When contemporaneous relations are modeled as directed relations among observed variables, they can be interpreted as assessing if knowledge of a given variable explains the variance of another variable at the same time point while holding the lagged influences constant. It is assumed that the relations among variables occur among the available variables in the data set, and thus the contemporaneous variables are endogenous (Nakamura & Nakamura, 1998). When modeled as undirected relations among errors, the interpretation shifts. To start, lagged relations are estimated without controlling for contemporaneous relations and thus will have different coefficient estimates (Gates et al., 2010). From an interpretation standpoint, correlated residuals suggest a shared influence that is outside of the observed variables in the data (Lütkepohl, 2005). This shared influence could be a latent variable, as explained by Hallquist et al. (2019), or simply another variable not included in the model. Note that this interpretation suggests that undirected correlations are not the results of two directed relations between two variables, which could be captured with directed relations.

Selecting an improper structural form for the contemporaneous relations can impact inferences. When the true contemporaneous relations are directed relations among the observed variables and the model only allows for the search of undirected relations among residuals, the VAR estimates will be biased due to the exclusion of the contemporaneous variables as covariates in the model. Furthermore, spurious lagged effects will likely arise (Gates et al., 2010) which can be erroneously interpreted from a causal inference perspective given that it would appear there is evidence for temporal precedence. When the true contemporaneous relations are undirected among the residuals and the model only allows for the search of directed relations among the observed variables, it could likewise result in incorrect inferences. The directed relations among variables would suggest that one variable explains more variability in the other variable than the reverse, which may not always be the case. This is particularly true if the two variables are related via a third variable exogenous to the system that might be a common cause for both variables.

Currently available software for modeling ILD only allows for one of the above approaches, uSEM or gVAR, to selecting and estimating contemporaneous relations, as either directed or undirected, respectively. This requires researchers to have strong theoretical justifications in order to choose the more appropriate approach. In reality, however, researchers may not have enough information regarding the dynamic process being studied to make such decisions. Moreover, there might exist rationale to expect some contemporaneous relations to be directed and others to be undirected. In both cases, allowing only one type of specification to be estimated has the potential to miss the true relations, introduce some false relations, and lead to misleading model structures.

Molenaar (2019) proposed a hybrid-VAR approach that allows for both undirected contemporaneous covariances among residuals and directed contemporaneous relations among variables. This can be estimated within the SEM framework, with the model then referred to as hybrid-uSEM (Ye et al., 2021). Inspired by this recently introduced approach, this article aims first to further understand the differences and similarities between directed and undirected contemporaneous relations, as well as the impact in choosing one versus the other while modeling. Second, this article introduces the incorporation of hybrid-uSEM into a current data-driven search method, the group iterative multiple model estimation (GIMME; Gates & Molenaar, 2012). GIMME is a completely data-driven algorithm that can recover lagged and contemporaneous relations simultaneously from within a uSEM framework and is a well-suited algorithm for hybrid-uSEM to be implemented. We thus named the implementation of the hybrid-uSEM approach into the GIMME framework hybrid-GIMME.

For this article, we first discuss the technical details of VAR and uSEM and their similarities and distinctions. Then we introduce a new method, hybrid-uSEM, which conceptually combines the two currently most commonly used approaches (uSEM & gVAR) by allowing for both directed contemporaneous relations among observed variables and undirected relations among residuals. Working from this foundation, we present the integration of this modeling approach into the GIMME model search procedure. We then present results from an extensive data simulation study suggesting that this is a robust method for recovering the data-generating contemporaneous relations in an exploratory manner. Results of an empirical data example probing emotions by using emoji measurements collected across days are also presented to demonstrate the practical utility of hybrid-GIMME.

Methods

The hybrid-GIMME method introduced in this paper builds directly from hybrid-uSEM, a flexible model that allows for both types of contemporaneous relations (directed relations among variables and undirected among residuals) as well as lagged relations. Hybrid-uSEM is an extension of uSEM, which is a type of structural VAR (SVAR). We thus begin by first explaining SVAR's foundation, VAR, and the extensions that make it an SVAR. We then describe uSEM, an approach for estimating a specific type of SVAR models within a SEM framework. Next, we introduce hybrid-uSEM. Finally, we provide details of the hybrid-GIMME algorithm for arriving at the structure of relations among time series variables in a data-driven manner.

VAR

The VAR model is a standard model in time series analysis. It models the changes in variables over time as a linear function of their past values and the past values of other variables in the system. Equation 1 represents a first-order standard VAR discussed in Hamilton (1994), where only a single lag is considered. It is also referred to as VAR(1) for simplicity.

$$\boldsymbol{\eta}_t = \boldsymbol{c} + \boldsymbol{\Phi}_1 \boldsymbol{\eta}_{t-1} + \zeta_t, \zeta_t \sim N(0, \boldsymbol{\Psi}) \tag{1}$$

In the above equation, $\boldsymbol{\eta}_t = [\eta_{1,t}, \eta_{2,t}, \ldots, \eta_{p,t}]^T$ represents a p-variate time series (with $p > 1$) at time point t, with $t = 1, \ldots, T$. Time point t is usually used as the "current" time data with variance explained by prior time points. $\boldsymbol{c}$ is a p-vector of constants (intercepts). $\boldsymbol{\Phi}_1$ has the dimension of $p \times p$ and is the lagged coefficients matrix; the diagonal contains of the order 1 autoregressive (AR(1)) regression coefficients indicating the prediction of a given variable from itself at the prior time point and the off-diagonal represents the cross-lagged coefficients for how variables at the prior time point predict each other. Residuals (ζ_t) are assumed to be uncorrelated across time (but can be correlated with each other at t) with a mean of zero.

For example, a VAR(1) model with two variables can be written as:

$$\begin{bmatrix} \eta_{1,t} \\ \eta_{2,t} \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} + \begin{bmatrix} \phi_{1,1} & \phi_{1,2} \\ \phi_{2,1} & \phi_{2,2} \end{bmatrix} \begin{bmatrix} \eta_{1,t-1} \\ \eta_{2,t-1} \end{bmatrix} + \begin{bmatrix} \zeta_{1,t} \\ \zeta_{2,t} \end{bmatrix}$$

SVAR

Whereas the standard VAR model focuses on estimating lagged relations, contemporaneous relations—the other important piece in fully understanding and analyzing time series data—are not being estimated alongside the lagged relations. They are often modeled by correlating the residuals obtained for contemporaneous variables (i.e., correlating the residuals at a lag of 0), but this does not allow for directed relations. Structural VAR is derived from the standard VAR and incorporates estimation of directed contemporaneous relations in addition to lagged relations (Lütkepohl, 2005). Here we present an adaptation of the model specifications of a lag one SVAR model Type A, which models the contemporaneous relations as directed relations among variables:

$$\boldsymbol{\eta}_t = \boldsymbol{c} + A\boldsymbol{\eta}_t + \boldsymbol{\Phi}_1\boldsymbol{\eta}_{t-1} + \zeta_t, \zeta_t \sim N(0, \boldsymbol{\Psi}) \tag{2}$$

In Equation 2, contemporaneous relations are estimated as the $p \times p$ regression coefficients in **A**, with the residuals treated as white noise that are mutually independent. The diagonal of **A** is set to zero as a variable cannot explain its own variability contemporaneously.

By moving $A\boldsymbol{\eta}_t$ to the left hand side of the equation, we see what looks like a standard VAR on the right hand side of the equation. We can solve for $\boldsymbol{\eta}_t$ and in doing so, transform the SVAR into an equivalent VAR:

$$\boldsymbol{\eta}_t - A\boldsymbol{\eta}_t = \boldsymbol{c} + \boldsymbol{\Phi}_1\boldsymbol{\eta}_{t-1} + \zeta_t, \zeta_t \sim N(\boldsymbol{0}, \boldsymbol{\Psi}) \tag{2a}$$

$$\boldsymbol{\eta}_t = (\boldsymbol{I} - A)^{-1}\boldsymbol{c} + (\boldsymbol{I} - A)^{-1}\boldsymbol{\Phi}_1\boldsymbol{\eta}_{t-1} + (\boldsymbol{I} - A)^{-1}\zeta_t, \zeta_t \sim N(\boldsymbol{0}, \boldsymbol{\Psi}) \tag{2b}$$

Defining $\boldsymbol{c}^* = (\boldsymbol{I} - A)^{-1}\boldsymbol{c}$, $\boldsymbol{\Phi}_1^* = (\boldsymbol{I} - A)^{-1}\boldsymbol{\Phi}_1$, and $\zeta_t^* = (\boldsymbol{I} - A)^{-1}\zeta_t$, the contemporaneous relations will now be found among the residuals and Equation 2 can be rewritten as:

$$\boldsymbol{\eta}_t = \boldsymbol{c}^* + \Phi_1^*\boldsymbol{\eta}_{t-1} + \zeta_t^* \tag{3}$$

Based on the above transformation, one can see that these two equations are equivalent. Specifically, one could take estimates from the SVAR in Equation 2 and obtain an equivalent VAR representation in Equation 3. Note that the estimates for intercept, **Φ** and residuals will differ from those in the SVAR since now the contemporaneous effects are spread out across these estimates. The take away here is that one can transform back and forth from a model that has directed contemporaneous paths to a model that does not. These will explain an equivalent amount of overall variance in the data.

Having the contemporaneous relations estimated as directed relations among the observed variables versus having the undirected relations among the residuals, however, differs drastically in interpretation as mentioned above. Specifically, when relations are modeled as directed, the variability among all variables is thought to relate to other observed variables in the data set. In contrast, when the contemporaneous relations are modeled as covariances or correlations among residuals, the assumption is that shared variability between the two variables occurs due to mechanisms outside the system of the observed variables at hand (Lütkepohl, 2005). While the two representations can be transformed to each other (Gates et al., 2010), Molenaar (2019) demonstrated that a feed-forward search procedure was able to recover the data-generating structures when both types of relations existed. We explain below in the hybrid-GIMME section Identifying Directionality and Recovering Undirected Relations section how the true data-generating directionality can be obtained from within an SEM framework. This is critical because researchers are often unsure if they may encounter only one of the two types of contemporaneous relations in the data or both types. Hence, an appropriate approach that allows both types of contemporaneous relations to be simultaneously estimated and compared is needed to better understand the underlying relations in time series data.

uSEM

SEM is a widely used analytic approach in psychology for estimating relations between variables. However, it is mostly applied to estimate contemporaneous relations (as in cross-sectional data) rather than lagged relations, due to most SEM approaches' assumption of independent observations. Kim et al. (2007) first proposed unified SEM (uSEM). The uSEM method conducts SVAR estimation via SEM. It thus allows the estimation of lagged relations and directed contemporaneous relations simultaneously. Kim et al. introduced the method for use with functional MRI (fMRI) data applications. fMRI data is well-suited for this method because it is known to typically have very high sequential dependencies in addition to contemporaneous relations (Logothetis, 2008). Increasingly it is becoming apparent that some ecological momentary assessment data may also share these qualities (Fisher & Boswell, 2016; Lane, Gates, Pike, et al., 2019). Gates et al. (2010) demonstrated in detail how to transform a regular VAR model with correlated residuals to an equivalent uSEM model in which the contemporaneous relations are modeled as directed relations among observed variables, and vice versa, much like we showed in the previous section for standard SVAR.

The uSEM approach for estimating time series models has emerged as a fruitful way to analyze data as it allows the estimation of lagged and directed contemporaneous relations simultaneously (Beltz, Beekman, et al., 2013; Gates & Molenaar, 2012). To continue this line of work, we can estimate hybrid-VARs using hybrid-uSEM. In doing so, we reap the benefits of a long line of work using the uSEM framework. Equation 2 can be rewritten for SEM by having one matrix, $\boldsymbol{B}$, containing the coefficients for both lagged and contemporaneous relations.

$$\boldsymbol{\eta} = \boldsymbol{c} + \boldsymbol{B}\boldsymbol{\eta} + \zeta, \zeta \sim N(\boldsymbol{0}, \boldsymbol{\Psi}) \tag{4}$$

In this form, we have $\boldsymbol{\eta} = [\boldsymbol{\eta}_{t-1}, \boldsymbol{\eta}_t]$, where $\boldsymbol{\eta}$ becomes $2p$-variate time series data, where $\boldsymbol{\eta}_t = [\eta_{1,t}, \eta_{2,t}, \ldots, \eta_{p,t}]^T$ as before and $\boldsymbol{\eta}_{t-1} = [\eta_{1,t-1}, \eta_{2,t-1}, \ldots, \eta_{p,t-1}]^T$. The observations are now time embedded by appending each observation at previous time points to themselves at time point t. In doing so, we now have both lagged and contemporaneous relations stored in a new $2p \times 2p$ $\boldsymbol{B}$ matrix. More specifically, the $\boldsymbol{B}$ matrix is:

$$B = \begin{pmatrix} 0 & \cdots & \cdots & \cdots & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & & & \vdots & \vdots & \ddots & & & \vdots \\ \vdots & & \ddots & & \vdots & \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots & \vdots & & & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ \phi_{11} & \cdots & \cdots & \cdots & \phi_{1p} & 0 & a_{12} & \cdots & \cdots & a_{1p} \\ \vdots & \ddots & & & \vdots & a_{21} & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & \ddots & \vdots & \vdots & & \ddots & \ddots & a_{(p-1)p} \\ \phi_{p1} & \cdots & \cdots & \cdots & \phi_{pp} & a_{p1} & \cdots & \cdots & a_{p(p-1)} & 0 \end{pmatrix}_{2p \times 2p}$$

The upper left contains directed relations among the $\boldsymbol{\eta}_{t-1}$ variables, which are constrained to zero here and captured as covariances in $\boldsymbol{\Psi}$ (see below). The upper right is also constrained to zero because directed relations cannot explain variability backward in time; in other words, $\boldsymbol{\eta}_t$ cannot predict $\boldsymbol{\eta}_{t-1}$. The $\boldsymbol{\Phi}$ matrix is now the lower-left block of the $\boldsymbol{B}$ matrix, which contains all the VAR(1) relations with the autoregressive relations along the diagonal. The lower-right block is the previously introduced $\boldsymbol{A}$ matrix that contains estimates for directed contemporaneous relations. The diagonal of the lower-right block previously $\boldsymbol{A}$ matrix is constrained to zero so a variable cannot predict itself at the same time point.

$$\Psi = \begin{pmatrix} \psi_{11} & & & & & & & & & \\ \psi_{21} & \ddots & & & & & & & & \\ \vdots & \ddots & \ddots & & & & & & & \\ \vdots & & \ddots & \ddots & & & & & & \\ \psi_{p1} & \cdots & \cdots & \psi_{p(p-1)} & \ddots & & & & & \\ 0 & \cdots & \cdots & \cdots & 0 & \ddots & & & & \\ \vdots & \ddots & & & \vdots & 0 & \ddots & & & \\ \vdots & & \ddots & & \vdots & \vdots & \ddots & \ddots & & \\ \vdots & & & \ddots & \vdots & \vdots & & \ddots & \ddots & \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & \cdots & \cdots & 0 & \psi_{(2p)(2p)} \end{pmatrix}_{2p\times 2p}$$

The $\boldsymbol{\Psi}$ matrix is the variance-covariance matrix of the data with the variance of observed contemporaneous variables on the diagonal. The upper triangle above the diagonal is omitted here because the matrix is symmetrical. The first p elements on the diagonal represents the variance of the p variables in $\boldsymbol{\eta}_{t-1}$ whereas the remaining p elements (from $p + 1$ to $2p$) contain the residual variance estimates after the lagged and contemporaneous relations are estimated. The upper left off-diagonal portion is the covariance matrix of $\boldsymbol{\eta}_{t-1}$ as mentioned earlier. The lower right is the covariance matrix of residuals. They are constrained to zero for traditional uSEM because they are assumed to be independent after conditioning on the contemporaneous and lagged relations among the observed variables. With matrices defined as described here, traditional SEM estimation can then be carried out once a subset of the relations in the $\boldsymbol{\Phi}$ and $\boldsymbol{A}$ are selected to ensure identifiability. We discuss a robust approach for identifying the subset of relations below in the Hybrid-GIMME section. But first, we describe hybrid-uSEM.

Hybrid-uSEM

Although uSEM can estimate lagged and contemporaneous relations simultaneously, it has limitations in that all contemporaneous relations are required to be directed relations among observed variables. Molenaar (2019) first introduced to the field of psychology the hybrid-VAR concept, which incorporates the estimation of both directed and undirected contemporaneous relations into one single model, in addition to the estimation of lagged relations for time series data. This model can be estimated via SEM, which we denote hybrid-uSEM. The hybrid-uSEM approach is one representation of how this could be empirically applied. Borrowing from both the VAR model and the uSEM model, hybrid-uSEM is able to estimate lagged relations while also allowing both directed and undirected contemporaneous relations to coexist. This is done by freeing some constraints imposed on the residual covariance in the traditional uSEM model.

The $\boldsymbol{B}$ matrix specification is identical to Equation 4. However, the $\boldsymbol{\Psi}$ matrix is now different because the covariances among contemporaneous residuals are allowed to be included during estimation. This would also affect the values in the $\boldsymbol{B}$ matrix if we were estimating both directed and undirected contemporaneous relations simultaneously, although the $\boldsymbol{B}$ matrix still has the same structure as before (the lower right of the $\boldsymbol{B}$ matrix will become all zeros if we are only allowing undirected relations). More specifically, now the $\boldsymbol{\Psi}$ matrix is as follows:

$$\Psi^* = \begin{pmatrix} \psi_{11} & & & & & & & & & \\ \psi_{21} & \ddots & & & & & & & & \\ \vdots & \ddots & \ddots & & & & & & & \\ \vdots & & \ddots & \ddots & & & & & & \\ \psi_{p1} & \cdots & \cdots & \psi_{p(p-1)} & \ddots & & & & & \\ 0 & \cdots & \cdots & \cdots & 0 & \ddots & & & & \\ \vdots & \ddots & & & \vdots & \psi_{(p+1)(p)} & & & & \\ \vdots & & \ddots & & \vdots & \vdots & \ddots & \ddots & & \\ \vdots & & & \ddots & \vdots & \vdots & & \ddots & \ddots & \\ 0 & \cdots & \cdots & \cdots & 0 & \psi_{(2p)(p)} & \cdots & \cdots & \psi_{(2p)(2p-1)} & \psi_{(2p)(2p)} \end{pmatrix}_{2p \times 2p}$$

The difference between $\boldsymbol{\Psi}^*$ and $\boldsymbol{\Psi}$ is that the lower-right block is no longer constrained to zeros in $\boldsymbol{\Psi}^*$. Now, much like in traditional VAR and gVAR, the relationships among residuals can potentially model the contemporaneous relations in the data.

Because more coefficients in the residual matrix are freed to be estimated, the model becomes saturated and underidentified if all potential coefficients were estimated. In order to avoid model underidentification, hybrid-uSEM is expected to perform the best either in a confirmatory manner in which not all possible relations are being estimated, or in a data-driven algorithm that contains a fewer number of all possible relations in order to have enough degrees of freedom to continue model estimation. We next introduce such an algorithm—hybrid-GIMME—and show how hybrid-uSEM can be incorporated into an existing data-driven method for time series data and apply it to both simulated and empirical data.

Hybrid-GIMME

GIMME (Gates & Molenaar, 2012) is an algorithm that is freely available via the R package *gimme* (Lane, Gates, Fisher, et al.,

2019) on the Comprehensive R Archive Network (CRAN; R Core Team, 2019). GIMME is a completely data-driven method that can recover both the presence and the direction of directed contemporaneous and lagged relations. The algorithm has two main steps:

- *Group-level search*: Look for relations that consistently exist across individuals. Add these to the "group-level" model and obtain person-specific estimates for everyone.
- *Individual-level search*: Starting with the person-specific estimation of group-level relations as a foundation, search for relations to add at the individual level.

Starting with an empty model (typically a model with only AR(1) relations estimated), GIMME uses modification indices (MI; Sörbom, 1989), a measure of expected change in the log likelihood if a relation were added to the model, for feed-forward selection of relations. Starting with a model where no additional relations are estimated in either the $\boldsymbol{\Phi}$ or $\boldsymbol{A}$ components of the $\boldsymbol{B}$ matrix,[1] it first arrives at the group-level model by including only relations that improve the fit (as indicated by MIs) for the majority of individuals' models. What constitutes the majority should be driven by insights into the expected signal to noise ratio. For fMRI, large scale simulation studies have suggested that the data-generating relations can be expected to be recovered in about 75% of individuals under typical noise and time series lengths (Smith et al., 2011). The current GIMME default for group-level relation cutoff threshold is 75% indicating that at least this proportion of individuals must have a relation be significant for it to be included in the group-level model. This value can be changed by the user.

GIMME then moves on to the individual-level search using the group-level results as a baseline model for the search of relations to add, again using MIs to guide relation selection in a feed-forward manner. The search for individual-level relations ends once the model is found to be a good fit according to at least two of the following indices: comparative fit index, non-normed fit index, root mean square error of approximation, and standardized root-mean squared residual. The model search may stop even if there still are significant modification indices, favoring parsimony to prevent overfitting. At each step, GIMME arrives at individual-level estimates. GIMME has been shown to be highly reliable in obtaining lagged and contemporaneous relations across varied contexts (Gates et al., 2019; Gates & Molenaar, 2012; Lane, Gates, Pike, et al., 2019) largely because it uses shared information across individuals to bring each individual's model closer to their true data-generating structure of relations. Note that the group-level information is used solely to cut down on potential overfitting and spurious relations at the individual level. The group-level relations are used to get the individual-level search closer to the true final model at the start of that search, which has been recommended for any model building procedures using modification indices (MacCallum et al., 1992). In the end, GIMME produces an individual-level model for each individual, and all estimates are obtained for individuals separately—even for the group-level paths. The current GIMME finds relations from within the uSEM structure; in other words, it only allows lagged and directed contemporaneous relations to be estimated. For hybrid-GIMME, we are incorporating the hybrid-uSEM approach that we just presented, which allows for both directed and undirected contemporaneous relations to be estimated simultaneously in addition to lagged relations. For more details on the GIMME algorithm, we refer readers to Gates and Molenaar (2012).

Specifically, to enable hybrid-GIMME to detect undirected contemporaneous relations among residuals, we allowed the covariance between the residuals of contemporaneous variables (see the lower-right block of $\boldsymbol{\Psi}^*$) to also be included among the candidate relations to be considered when running model specification using modifications indices. Now hybrid-GIMME simultaneously compares the modification index values of three candidate contemporaneous relations between two variables, say A and B: the directed relation of A on B, the directed relation of B on A, and the undirected relation of the residuals for A and B. One benefit of conducting the analysis within a SEM framework is that there is no need for a two-step procedure whereby the VAR model is detected first, followed by investigation of residuals. In the hybrid-uSEM approach used in hybrid-GIMME, all potential relations are evaluated simultaneously for addition to the model, and once added they are estimated simultaneously in one step.

Identifying Directionality and Recovering Undirected Relations

As demonstrated in hybrid-uSEM, the lower-right block of the $\boldsymbol{\Psi}^*$ matrix will be allowed to potentially be estimated instead of being constrained to all zeros (as in the traditional uSEM framework, $\boldsymbol{\Psi}$). Given that SVAR can be transformed to an equivalent VAR with covaried residuals and the same has been demonstrated for uSEM and VAR, we investigate the rationale for whether or not a data-driven approach is able to detect which candidate relation (e.g., $b_{1,2}$ vs. $\psi_{1,2}$) is selected for a given data generating model. First we will start by explaining how one can differentiate the directed relation of η_1 on η_2 ($b_{1,2}$) from η_2 on η_1 ($b_{2,1}$).

As most researchers are familiar with regression analyses, we describe the concept from within that framework. Suppose we have only η_1 and η_2 in the model, and the directed relation (slope as in simple linear regression) using ordinary least square is given by:

$$b_{1,2} = \frac{Cov(\eta_1, \eta_2)}{Var(\eta_2)} \quad \text{and} \quad b_{2,1} = \frac{Cov(\eta_2, \eta_1)}{Var(\eta_1)}$$

The above equations show that b_{12} and b_{21} are just the covariance scaled according to the variance of the dependent variable in a simple regression. Furthermore, when the two variables are standardized $(Var(\eta_1) = Var(\eta_2) = 1, \mu_{\eta_1} = \mu_{\eta_2} = 0)$, it is known that we have $b_{12} = b_{21}$. However, this is not the case when we have other confounding covariates in the model, which

[1] While not the default, users can start with some relations freed for estimation in these matrices for a semiconfirmatory search.

is almost always the case in time series data due to the inclusion of AR relations.

By adding AR(1) relations to the simple regression we can quickly see how directionality can be discovered (cross-lagged relations and residuals are omitted here to simplify the equations). The model specification becomes:

$$\eta_1 = b_{1,2}\eta_2 + b_{1,(1,t-1)}\eta_{1,t-1} \quad \text{and}$$
$$\eta_2 = b_{2,1}\eta_1 + b_{2,(2,t-1)}\eta_{2,t-1}$$

Therefore we have the directed relations calculated as:

$$b_{1,2} = \frac{Var(\eta_{1,t-1})Cov(\eta_2,\eta_1) - Cov(\eta_2,\eta_{1,t-1})Cov(\eta_{1,t-1},\eta_1)}{Var(\eta_2)Var(\eta_{1,t-1}) - Cov(\eta_2,\eta_{1,t-1})^2}$$

$$b_{2,1} = \frac{Var(\eta_{2,t-1})Cov(\eta_1,\eta_2) - Cov(\eta_1,\eta_{2,t-1})Cov(\eta_{2,t-1},\eta_2)}{Var(\eta_1)Var(\eta_{2,t-1}) - Cov(\eta_1,\eta_{2,t-1})^2}$$

The equations demonstrate that by having additional covariates in the model (here, lagged variables), the directed contemporaneous relation of one variable being explained by the other is unlikely to be equal to the reverse. Therefore the direction (i.e., which one is considered the target or dependent variable) can be detected in that one direction might explain more variance in the data than selecting the opposite direction. What we have demonstrated here is the premise for Granger Causality (Granger, 1969), which builds models from within a VAR approach to arrive at lagged and/or contemporaneous relations by the inclusion of autolagged covariates (Henry & Gates, 2017).

Not only do the directions of relations matter, but also whether the relation is better quantified as a directed relation or undirected relation matters. In the previous sections we introduced the theoretical difference of the two types of relations; in the Appendix we detail how the selection of a directed relation among two observed variables provides a different model-implied covariance matrix than the selection of an undirected relation among residuals for SEM. To summarize, we show that one will arrive at different model-implied covariance matrices depending on whether one is including a directed relation in $\boldsymbol{B}$ (as b_{43} in the example) matrix or an undirected relation (ψ_{34}) in the $\boldsymbol{\Psi}$ matrix. The model implied covariance matrices differ because of the presence of autoregressive relations, which serve as covariates. It follows that fit values will also differ. In this way the MIs, which are related to the expected change in overall model log likelihood, will differ between the directed relation among observed variables and the covariance among residuals when autoregressive effects are included as a baseline or "null" model. One advantage of GIMME (and also of hybrid-GIMME) is that it uses MIs to determine the addition and deletion of candidate relations. Here we have shown that the model-implied covariance matrix—and thus the fit indices and MI based on this—will differ depending on the directionality (whether the relation is directed or undirected, and which direction if it is directed) of the relation selection. Hence, we expect hybrid-GIMME to be able to detect the correct direction and type of a relation using MIs.

Simulations

Data Generation

Simulations were conducted to evaluate the performance of hybrid-GIMME. Data for a single individual was generated according to

$$\boldsymbol{\eta}_t = \boldsymbol{A}\boldsymbol{\eta}_t + \boldsymbol{\Phi}\boldsymbol{\eta}_{t-1} + \zeta_t. \tag{5}$$

where we have p = 10 variables. Time series lengths of T = 60, 100, 120, 150, 200, and 1,000 were considered, with 100 replications in total for each time series length representing different samples of individuals. For each replication, there are N = 100 individual time series. The time series lengths of simulated data were chosen as they are commonly encountered in daily diary and fMRI data.

All replications had the same diagonal $\boldsymbol{\Phi}$ matrix structure (with specific values of the relations differ), where only AR relations were included at the group level. All AR relations were randomly generated with a mean of .4 and standard deviation of .1 with a normal distribution. Having parameters deviate across individuals better matches what is expected to be seen across individuals in empirical studies due to sampling fluctuations. Each individual also had two off-diagonal relations in the $\boldsymbol{\Phi}$ matrix (cross-lagged relations) randomly generated, with a mean of .3 and standard deviation of .05. For each replication of each length of simulated data, all individuals share the same randomly generated *group-level* contemporaneous relation structure: five directed relations (in the $\boldsymbol{A}$ matrix) and three undirected relations (in the $\boldsymbol{\Psi}$ matrix). Each individual also had four directed relations and two undirected contemporaneous relations randomly generated at the *individual level*. This proportion of sparsity in the final individual-level patterns are consistent with prior simulations aiming to assess the performance of methods in terms of recovering true network relations (e.g., Nestler & Humberg, 2021; Ramsey et al., 2011; Smith et al., 2011) as well as empirical results on data gathered on humans (e.g., Epskamp, van Borkulo, et al., 2018). All relations in the $\boldsymbol{A}$ and $\boldsymbol{\Psi}$ matrices (directed and undirected relations at both the group level and the individual level) were again generated with a mean of .4 and standard deviation of .1. The randomness in group-level relations (in magnitude) and individual level relations (in both location and magnitude) was included to break up the homogeneous nature of simulated data and to better resemble empirical data which has more interindividual variability even when some similarities exist. The code for generating and analyzing the simulated data can be found online at OSF: https://osf.io/6c3g5/?view_only=55a679495c9f4bd5abf6e1059d00ee77.

For example, for T = 60, Individual 1 and Individual 2 of Replication 1 would share the same five directed and three undirected contemporaneous group-level relations, while their specific values differ. They would also have additional four directed and two undirected contemporaneous relations, both differing from the other individuals in location and magnitude. In addition, for T = 60, Individual 1 of Replication 1 would have different group-level and individual-level contemporaneous relations from Individual 1 of Replication 2. The $\boldsymbol{A}$ and $\boldsymbol{\Psi}$ matrices for Individual 1 of Replication 1 for T = 60 are as following to assist in demonstrating the data generating models:

$$\boldsymbol{A}_{ind1,rep1} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.49 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.35 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.44 & 0.41 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.41 & 0 & 0.49 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.58 & 0 & 0.35 & 0.58 & 0 & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{\Psi}_{ind1,rep1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0.36 & 0 & 0 & 0 \\ 0 & 1 & 0.41 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.41 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0.18 \\ 0 & 0 & 0 & 1 & 0.44 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.44 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0.36 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0.18 \\ 0 & 0 & 0.18 & 0 & 0 & 0 & 0 & 0 & 0.18 & 1 \end{pmatrix}$$

Performance Criteria

We will examine the results by first looking at recovery of the group-level relations that are present in all individuals and then examining overall performance for all types of relations. Because each replication has different group level relations even for the same number of time points, there will not be relation-specific recovery, and the numbers are averaged across all 100 replications within each number of time points. Performance will largely be assessed based on two criteria, "sensitivity" and "specificity," with the focus mostly on sensitivity. Sensitivity measures the proportion of actual data-generating relations that are correctly recovered, and is also known as the true positive rate. Specificity measures the proportion of actual negatives that are correctly recovered as negative. In all machine learning approaches balancing the rate of true positives and true negatives is required because increasing sensitivity (i.e., recovering relations that existed in the data generating model) sometimes comes at the cost of increasing the rate of false positives. The GIMME algorithm errs on the side of missing true relations so that false positives are not introduced into the model.

Examining Recovery of Data-Generating Relations Found at the Group Level

We first will examine the group-level relations in depth by providing figures depicting how frequently they were correctly recovered in the appropriate matrix as well as false positives in the wrong matrix. For example, if $a_{2,1}$ was correctly recovered for one individual, it would contribute to the count of recovery for that data-generating relation. We will also count how often this relation erroneously occurred in the $\boldsymbol{\Psi}$ matrix, or recovered reversely as $a_{1,2}$. Similarly, we will provide a count of how often the group-level relation that was simulated to be in the $\boldsymbol{\Psi}$ matrix erroneously surfaced in the $\boldsymbol{A}$ matrix, and also provide results for how frequently it was correctly identified in the $\boldsymbol{\Psi}$ matrix.

We will also explore two types of relation-specific sensitivity measures: "presence sensitivity" and "direction sensitivity." Presence sensitivity measures the proportion of data-generating contemporaneous relations being recovered as any direction or type of relation. That is, if it surfaces in either the $\boldsymbol{A}$ matrix or the $\boldsymbol{\Psi}$ matrix, it would be counted as detection of the presence of a contemporaneous relations (regardless of the direction). Direction sensitivity captures the percent of times a given relation is recovered across individuals for those relations for which the presence is correctly recovered.

Note that presence sensitivity does not measure if the relation's direction is correctly identified. For instance, if there were truly 100 individuals in one repetition who share the $a_{2,1}$ directed relation, and hybrid-GIMME detected $a_{2,1}$ for 90 individuals, $a_{1,2}$ for five individuals (without overlapping with the previous 90 individuals), and for three individuals the relation was captured as $\psi_{2,1}$ in the undirected $\boldsymbol{\Psi}$ matrix, then the presence sensitivity rate would be $\frac{90+5+3}{100} = 98\%$. Although presence sensitivity doesn't take into account the direction, it is still important to assess if any relation was detected among variables that do in fact have a relation. Researchers may make inferences regardless of directionality. For instance, to quantify the degree or number of relations for a given variable, one might not differentiate directionality but simply add the number of other variables it has relations with.

Direction sensitivity is a bit more conservative and a stricter criterion. It will always be equal to or less than presence sensitivity as it requires that the contemporaneous relation between two variables be detected *and* in the right direction to be counted as correctly recovered. Continuing with the example above, direction sensitivity for the specific $a_{2,1}$ relation would be $\frac{90}{100} = 90\%$. Note that although undirected contemporaneous relations technically do not have a "direction" per se, as they do not point from one variable to another, direction sensitivity still applies. With direction sensitivity, we can assess if hybrid-GIMME correctly recovered these relations as undirected as opposed to as directed.

Overall Metrics of Recovery

Besides relation-specific probing and sensitivity measures, mean sensitivity and specificity will also be measured for each simulation condition. This will help to obtain an overall picture of how well the algorithm works by summarizing recovery across all types of matrices as well as including group- and individual-level relations. The mean sensitivity and mean specificity are calculated as

$$\text{Mean sensitivity} = \frac{1}{N}\sum_{n=1}^{N}\left(\frac{\Sigma_j(\hat{\theta}_{n,j} \neq 0 \text{ and } \theta_{n,j} \neq 0)}{\Sigma_j(\theta_{n,j} \neq 0)}\right), \tag{6}$$

$$\text{Mean specificity} = \frac{1}{N}\sum_{n=1}^{N}\left(1 - \frac{\Sigma_j(\hat{\theta}_{n,j} \neq 0 \text{ and } \theta_{n,j} = 0)}{\Sigma_j(\theta_{n,j} = 0)}\right) \tag{7}$$

where $\theta_{n,j}$ and $\hat{\theta}_{n,j}$ are the true and estimated elements of $\boldsymbol{\Phi}$, $\boldsymbol{A}$ and $\boldsymbol{\Psi}$, respectively, for individual n in a given design condition. Again we note the composition of $\theta_{n,j}$ is different depending on whether one is considering presence or direction measures. Direction sensitivity and specificity are straightforward in that $\hat{\theta}_{n,j}$ and $\theta_{n,j}$ correspond directly to the fitted and data generating model parameters, respectively. Presence sensitivity and specificity at the condition level requires some additional explanation.

To understand average presence sensitivity consider a single element of θ_j for individual n from Equation 6. For example consider $\theta_j = \psi_{2,10}$ is in the data generation model (DGM), (i.e., a covariance between the errors of the η_2 and η_{10} equations). Because this relation exists in the data generating model θ_j will be nonzero. Now, the corresponding element for the recovered parameter $\hat{\theta}_j$ will be nonzero if any of the following three conditions are satisfied: $\hat{\psi}_{2,10} \neq 0$, $\hat{a}_{2,10} \neq 0$, $\hat{a}_{10,2} \neq 0$. Any of these relations indicate accurate recovery of the presence of a contemporaneous relation between η_2 and η_{10}. Equivalently, if we consider the situation where $\theta_j = \psi_{1,10}$, which does not exist in the data generating model, satisfying any of the following conditions ($\hat{\psi}_{1,10} \neq 0$, $\hat{A}_{1,10} \neq 0$, $\hat{A}_{10,1} \neq 0$) would be considered a false-positive, as any would indicate the presence of a contemporaneous relation that does not exist in the data generating model. This information is used when arriving at presence specificity and would decrease the percentage of DGM negatives (i.e., no relation) found to be negative in the estimated model.

Simulation Results

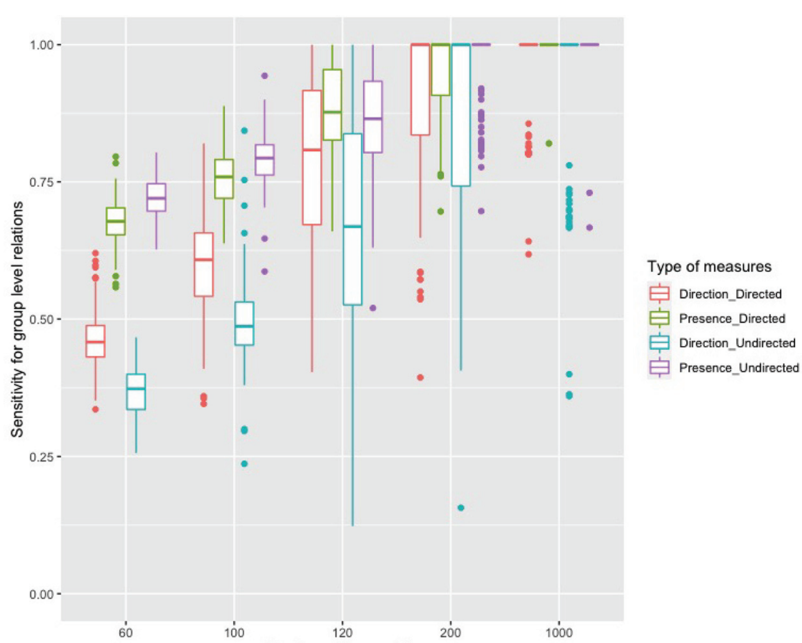
All repetitions for each of the number of time points were run using the *gimme* R package (Lane, Gates, Fisher, et al., 2019) with the newly added hybrid option invoked ("hybrid = TRUE"), and with the threshold of group level relation set at .75, which means a relation has to be identified in no less than 75% of the sample to be labeled as a group level relation. Out of 60,000 individuals (100 individuals for each of 100 replications for all six numbers of time points), only eight individuals failed to converge, resulting in a total of 59,992 individual level models estimated by hybrid-GIMME. These eight individuals' data were thus not included in our analyses.

We include two box plots here to represent the overall sensitivity for both group and individual level contemporaneous relations. The red and green boxes in Figure 1 depict the overall average presence and direction sensitivity for group-level directed contemporaneous relations. These are the relations present in the ***A*** matrices in the DGM. Relation-specific sensitivity rates are omitted here because each replication had different group level relations. For example, in Replication 1 there could be a directed contemporaneous relation from *x*2 to *x*4, while such a relation might not necessarily be present in Replication 2. Therefore, only averaged sensitivity rates are compared. In Figure 1, we see that both presence and direction sensitivity rates increased as the number of time points increased. The difference between the presence and directed contemporaneous sensitivity rates decreased as the number of time points increased. This indicates that when we have more time points in the data, directed contemporaneous relations are not only more likely to be detected, but also are more likely to be correctly recovered regarding their directions. In fact, the median presence sensitivity exceeded 75% when the number of time points was 100, and median direction sensitivity exceeded 75% when the number of time points was 120. When T = 1,000; average presence sensitivity reached 99.82%. The almost-disappearing box plots at T = 1,000 is because most replications consistently had a sensitivity rate of 1. We list averages in Table 1.

The blue and purple box plots in Figure 1 present the average presence and direction sensitivity for group-level undirected

Figure 1

Sensitivity for Group Level Contemporaneous Relations by the Number of Time Points



Note. See the online article for the color version of this figure.

Table 1
Mean Sensitivity and M Specificity Summary

Measures	$T = 60$	$T = 100$	$T = 120$	$T = 150$	$T = 200$	$T = 1{,}000$
Group-level directed Presence sensitivity	67.63%	75.86%	83.28%	93.05%	95.93%	99.82%
Group-level directed Direction sensitivity	46.39%	59.61%	71.02%	87.03%	90.13%	96.85%
Group-level undirected Presence sensitivity	71.88%	79.18%	80.67%	93.25%	96.67%	99.40%
Group-level undirected Direction sensitivity	36.72%	49.87%	56.04%	79.17%	85.52%	92.69%
Individual-level directed Presence sensitivity	66.26%	72.68%	74.32%	73.98%	71.81%	66.23%
Individual-level directed Direction sensitivity	44.57%	54.17%	57.47%	61.87%	62.76%	61.68%
Individual-level undirected Presence sensitivity	71.38%	76.30%	77.81%	77.06%	76.97%	68.34%
Individual-level undirected Direction sensitivity	36.61%	45.15%	49.69%	53.56%	56.95%	55.91%
Mean direction Sensitivity	42.40%	53.90%	60.89%	73.37%	76.58%	80.01%
Mean presence Sensitivity	68.69%	75.73%	79.37%	85.36%	86.49%	85.57%
Mean specificity	94.59%	96.69%	97.44%	98.49%	98.77%	98.34%

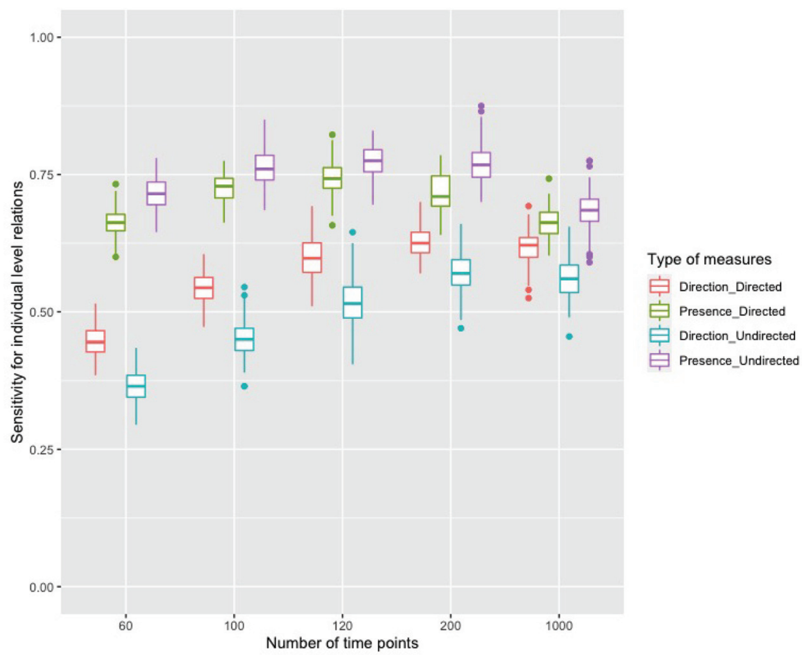
contemporaneous relations. These are the relations present in the $\boldsymbol{\Psi}$ matrices in the DGM. Note that although undirected relations no dot have a "direction," we say their direction is recovered when these relations were recovered correctly as undirected, as opposed to being falsely recovered as directed relation. Overall, there is a very similar pattern to what was seen for the directed contemporaneous paths. Both presence and direction sensitivity increased as the number of time points increased, and the difference between them decreased as well. It is worth noticing that while presence sensitivity did not differ very much for directed and undirected contemporaneous relations, direction sensitivity appeared to be consistently lower for undirected relations. This suggests that undirected relations are erroneously considered directed at a high rate, particularly when $T < 120$. Considering the results all together, compared with directed contemporaneous relations, undirected contemporaneous relations appeared to be more difficult to be recovered correctly as undirected, while their presence is generally as well detected as were directed contemporaneous relations by hybrid-GIMME. In addition, Figure 1 offers some insight on the minimum number of time points needed for a reliable estimation of contemporaneous relations at the group level. More than 75% of contemporaneous relations, both directed and undirected, were already successfully detected by hybrid-GIMME at $T = 100$. Additionally, more than 75% of the relations' directions were correctly recovered at $T = 150$. Hybrid-GIMME has demonstrated extremely robust performance on recovering the true data-generating model.

Individual-level contemporaneous relations show a slightly different recovery pattern compared with group-level contemporaneous relations. Figure 2 presents the overall presence and direction sensitivity for individual-level directed and undirected contemporaneous relations for all 100 replications at each number of time points in one plot. In general, individual-level contemporaneous relations had lower sensitivity rates compared with their group-level counterparts. It's worth noting that when there were not many time points in the data (i.e., $T = 60$), sensitivity rates did not differ much between group- and individual-level contemporaneous relations. Similar to group-level contemporaneous relations, undirected relations were recovered slightly better than directed relations in terms of their presence, but not as well for their true direction. This implies that although undirected relations were more often detected by hybrid-GIMME, they were also more likely to be falsely recovered as directed. Still, they were recovered as the true direction (i.e., undirected) greater than what would be expected by chance for $T > 60$.

The main difference of the recovery pattern between group- and individual-level contemporaneous relations is that sensitivity rates did not increase as much for individual-level relations as the number of time points increased; in fact, sensitivity even decreased when the number of time points increased to 1,000. The reason likely is that the GIMME has a conservative stopping point for adding paths to avoid false positives. Specifically, the algorithm stops adding paths—even if they would be significant—if the fit indices indicate a good enough fit. As stated above when introducing the GIMME framework, hybrid-GIMME utilizes group-level information as a starting point for the individual-level models in order to pick signal out of noise. Therefore, in favoring parsimony and reducing the risk of false positives, hybrid-GIMME misses some individual-level relations that exist in the data-generating model. This finding is in line with prior studies evaluating the main algorithm's performance (e.g., Beltz & Molenaar, 2016; Lane, Gates, Pike, et al., 2019; Nestler & Humberg, 2021). This explanation also aligns with what Figure 1 represents—both presence and direction sensitivity increased greatly at the group level as the number of time points increased. In Figure 2, we see a decrease in both presence and direction sensitivity when $T = 1{,}000$ which likely reflects the fit indices overcorrecting for the number of time points and stopping the search procedure too soon.

The above graphs which compare the recovery of group- as well as individual-level contemporaneous directed and undirected

Figure 2
Sensitivity for Individual Level Contemporaneous Relations by the Number of Time Points



Note. See the online article for the color version of this figure.

relations are intuitive in representing the simulation results directly, but they do not summarize the full picture of accurate model recovery. In addition to the overall sensitivity measures that the graphs above represent, Table 1 also includes the specific values of mean sensitivity and specificity at each time point. As we have seen in prior work (e.g., Gates & Molenaar, 2012; Lane, Gates, Pike, et al., 2019; Nestler & Humberg, 2021), presence sensitivity rates increase as the number of time points increases. In general, T = 100 appears to be a large enough number of time points in order to reliably recover the presence of relations in hybrid-GIMME, and T = 150 is large enough to recover the directions of contemporaneous relations correctly (more than 75%). Importantly, specificity rates stayed extremely high, almost always larger than 95%, regardless of the number of time points. This indicates that hybrid-GIMME, even for the number of time points as low as 60, performed extraordinarily well in terms of not capturing false positives. Overall, hybrid-GIMME demonstrated acceptable performance and significant potential on the implementation of hybrid-uSEM in the current GIMME framework.

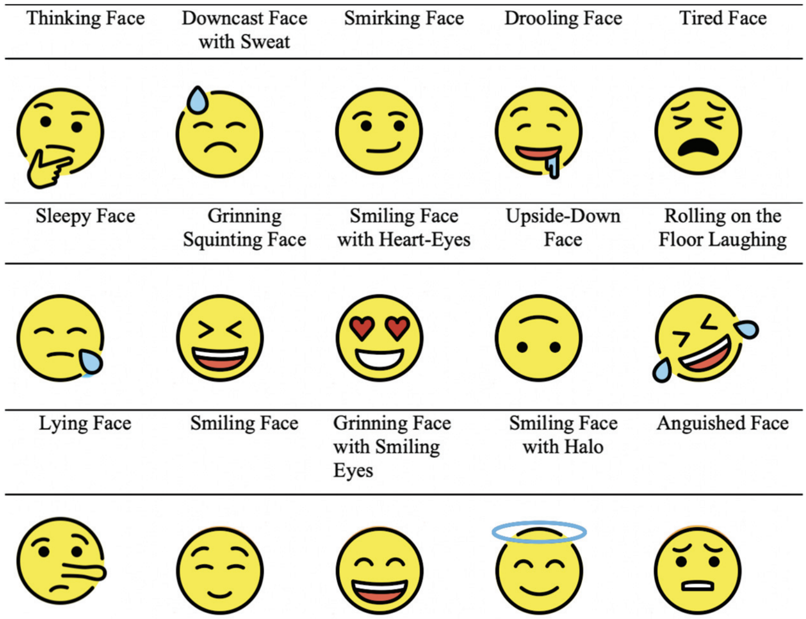
Empirical Example

An empirical data set was also used in this article to demonstrate hybrid-GIMME's potential for providing novel insights into current research questions about emotion and depression. Collection of this empirical data was supported by National Institutes of Health grant UL1TR002240 and a Rachel Upjohn Clinical Scholars award from the University of Michigan Comprehensive Depression Center to A. Beltz, who was also supported by the Jacobs Foundation. This data is a 100-day recently completed daily diary study on the relations of emotions and depressive symptomology in individuals' day-to-day lives. Participants completed a newly developed, emoji-based emotion measure (Emoji Positive and Negative Affect Schedule; E-PANAS) in addition to standard daily experience and depression measures. A community-based sample of adults varying in mental health was recruited and contains an equal number of men and women. A total number of 75 emoji scales are included in the study and a subset of 15 emojis was used for this article. Participants were asked to rate all 75 emojis on a scale from 0 to 100 every time they received the survey—the higher the rate, the more accurately the emojis represented how the participants felt at the time they took the survey.

Figure 3 shows the specific 15 emojis used for this article (all emojis shown in tables and figures with emojis were designed by OpenMoji, the open-source emoji and icon project.). It includes a wide range of emotions, from some more common emojis (i.e., "smiling face," "sleeping face") to emojis that could be interpreted very differently (i.e., "upside-down face," "smirking face"). The selection of emojis was motivated by the hypothesis that emojis of similar emotions (such as the two smiling emojis) may relate to each other in an undirected way as they may relate to an unmeasured construct and emojis of different emotions (such as one tired face emoji and one happy emoji) may relate in a directed way. The subset includes measurements from a total of N = 50 participants (female = 21) who have completed at least 80% of their daily self-reports (mean T = 100 days). The age of participants ranged from 18 to 45 (M = 26.54, SD = 7.41).

Given the exploratory nature of the hybrid-GIMME procedure we also tested the validity of the results. To do so, we used only the initial 95 observations from each individual's data to train the

Figure 3
Emojis From Empirical Data



Note. All emojis shown in this figure were designed by OpenMoji, the open-source emoji and icon project. See the online article for the color version of this figure.

hybrid-GIMME model. Consequently, we retained the final five time points from each series as a test set on which we could evaluate the final model obtained for each individual. By using the final model results obtained by hybrid-GIMME to develop five-step-ahead forecasts we can compare the model-predicted values to the true values for each series. Furthermore, we can compare the results from GIMME to standard approaches, such as the canonical VAR, as another tool for model validation. As future time points are being forecasted, in both cases only lagged relations are used.

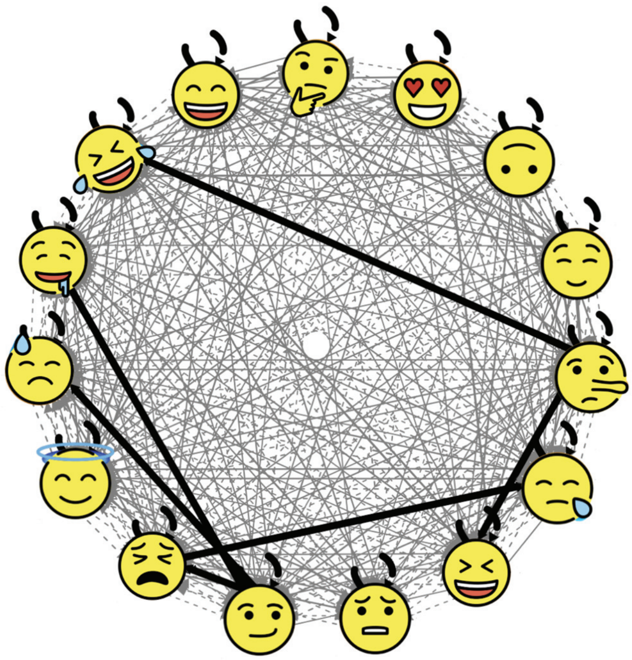
Empirical Data Results

Again, all analyses were run using hybrid-GIMME. AR relations were estimated as a start of the model search for all individuals in following the recommended default of GIMME. In this empirical example, no undirected contemporaneous relations were detected at the group level, and six directed contemporaneous relations were recovered at the group level. There were many individual-level contemporaneous paths that were both directed and undirected, suggesting a high degree of heterogeneity in emotional processes, a finding seen elsewhere (e.g., Fisher & Boswell, 2016; Wright & Simms, 2016). Figures 4 and Figure 5 show the two plots of the emoji data, with the first being the directed contemporaneous relations found in the $\boldsymbol{A}$ matrix and the latter being the undirected ones found in the $\boldsymbol{\Psi}$ matrix. The solid gray lines indicate individual level contemporaneous relations and black lines indicate group level relations (the arrows on each node indicate the AR relations). Line width corresponds with the proportion of people who had that path—the wider the line was, the larger the proportion was of people who were recovered to have that path. The two plots depict that despite the existence of many individual contemporaneous relations, there are not many relations shared by at least 75% of the individuals in the sample, a threshold set for group-level relations in this article. Gates et al. (2019) showed that by lowering the group-level threshold to 51%, the true positive rate increased without a corresponding increase in the false positive rate. Users have the option to alter this hyperparameter if they wish to change what percentage dictates the majority in their data. However, to keep the empirical results consistent with our simulation (which follows the bulk of simulation work in this area), which used a 75% group-level threshold, we kept the threshold at 75%.

The results offered some useful information in interpreting the novel emoji data, and reflected the complexity of emotional data measured by emojis. For instance, one of the most shared directed contemporaneous relations is “tired face” to “sleepy face” (94% significant). However, there are also other directed relations recovered at the group level that do not seem to be very intuitive, that is, “smirking face” to “downcast face with sweat.” There was also a significant amount of detected positive cross-category directed contemporaneous relations (e.g., “downcast face with sweat” to “drooling face”) at the individual level. For instance, there were seven participants who shared the relation from “thinking face” to “smiling face with halo.” Another example is the relation shared by 16 participants from “smiling face” to “lying face.” The presence of these positive cross-category directed contemporaneous relations indicates the complexity of this new data using emojis to rate emotions.

The most shared undirected contemporaneous relation is between “downcast face with sweat” and “smirking face” which was seen in seven participants. This is represented as the thickest

Figure 4
Hybrid-GIMME Plot of Directed Relations of Emoji Data



Note. All emojis shown in this figure were designed by OpenMoji, the open-source emoji and icon project. GIMME = group iterative multiple model estimation. See the online article for the color version of this figure.

gray line shown in Figure 5. Note that a directed contemporaneous relation was also identified for some participants for the same two variables. The two second most shared undirected contemporaneous relations are between "grinning squinting face" and "rolling on the floor laughing" in six individuals out of 50. These are two more extreme emojis that are usually associated with happiness and joy among the 15 emojis in the data. It could be a sign suggesting a potential latent factor for these positive construct emojis. One possible explanation of why there were not more individuals sharing this undirected relation could be because "rolling on the floor laughing" can be interpreted very differently by different people, ranging from being genuinely happy or just being sarcastic, thus not necessarily related to the "grinning squinting face" emoji.

On average, each individual in our empirical example data set was recovered to have around 17 directed contemporaneous relations (M = 17.36, SD = 4.70) and three undirected contemporaneous relations (M = 2.81, SD = 2.82). This large variation in the number of recovered contemporaneous relations contributes to the small number of shared group level contemporaneous relations. Based on our simulation results which showed a relatively low sensitivity for individual level undirected contemporaneous relations (around 55% for $T = 100$), hybrid-GIMME could be missing some undirected contemporaneous relations that are potentially present in the data. We also randomly selected two out of the 50 individuals (individual 15 and 34) in our empirical example data to demonstrate what a typical recovered model looks like for this novel emoji data set. Individual 15 had 19 directed contemporaneous relations and six undirected contemporaneous relations, while Individual 34 only had 10 directed and one undirected contemporaneous relations. Figure 6 and Figure 7 show their directed relations, both lagged and contemporaneous, respectively. A solid line represents a contemporaneous relation and a dashed line represents a lagged relation; a red line represents a positive relation and a blue line represents a negative relation.

Model Validation

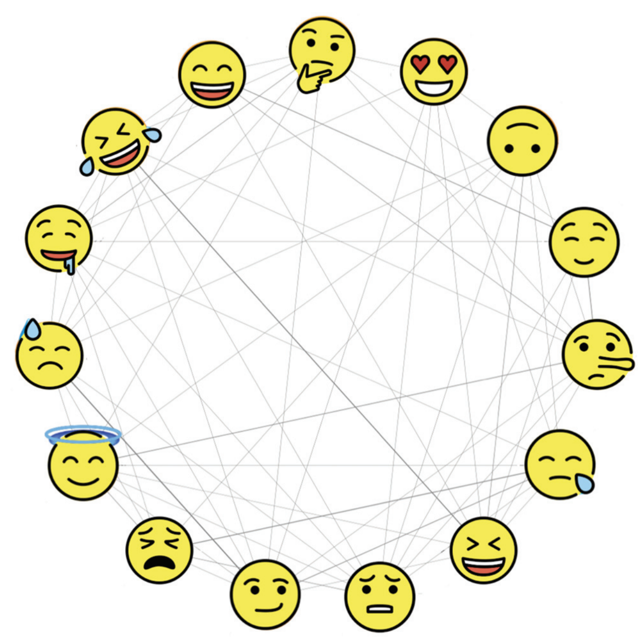
Given the exploratory nature of our procedure we chose to validate the hybrid-GIMME results by comparing the five-step-ahead forecasts to a hold-out-sample of the final five time points from each individual's component time series. Forecast accuracy was assessed using the root mean square forecast error (RMSFE). To communicate the results we aggregated RMSFE across individual time series as follows,

$$\text{Mean RMSFE} = \frac{1}{K}\sum_{k=1}^{K}\sqrt{\frac{1}{d}\sum_{j=1}^{d}\left(\hat{\boldsymbol{\eta}}^{(k)}_{j,t-5+h} - \boldsymbol{\eta}^{(k)}_{j,t-5+h}\right)^2} \quad (8)$$

where $(\hat{\boldsymbol{\eta}}^{(k)}_{j,t-5+h} - \boldsymbol{\eta}^{(k)}_{j,t-5+h})$ is the h step ahead forecast error for individual k on variable j and $h \in \{1, 2, 3, 4, 5\}$.

Furthermore, we compare the performance of the hybrid-GIMME approach to that of the canonical VAR(1) model fit to each individual's multivariate time series. Table 2 contains the results for both approaches. For the data considered here, the forecasts obtained from hybrid-GIMME are more accurate than those obtained from the individual-level canonical VAR(1) models, at each step of the forecast

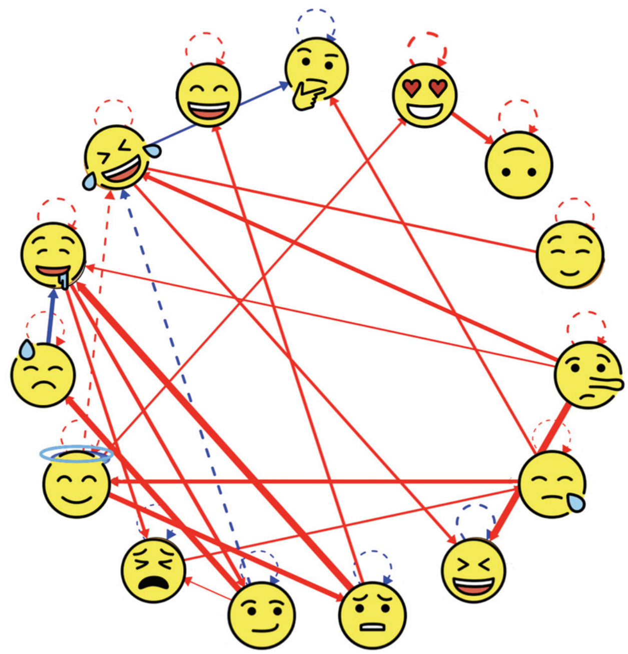
Figure 5
Hybrid-GIMME Plot of Undirected Contemporaneous Relations of Emoji Data



Note. All emojis shown in this figure were designed by OpenMoji, the open-source emoji and icon project. GIMME = group iterative multiple model estimation. See the online article for the color version of this figure.

Figure 6

Hybrid-GIMME Plot of Directed Relations of Emoji Data for Individual 15



Note. All emojis shown in this figure were designed by OpenMoji, the open-source emoji and icon project. GIMME = group iterative multiple model estimation. See the online article for the color version of this figure.

horizon. This provides some preliminary evidence in support of the utility of hybrid-GIMME results.

Discussion and Limitations

We introduce here a novel method, hybrid-GIMME for capturing two types of contemporaneous relations in time series models: directed and undirected. The simulation results demonstrate that hybrid-GIMME can appropriately detect directed and undirected contemporaneous relations simultaneously in a data-driven manner. When the number of time points reached 100, presence sensitivity for group-level relations became larger than 75%; and when the number of time points reached 150, direction sensitivity as well exceeded 75%. The rates of recovery for group-level paths neared 100% as time points increased even higher. As for individual-level relations, we saw less optimal recovery of paths which is due to the algorithm favoring parsimony by stopping the model search once fit indices are acceptable (Gates & Molenaar, 2012). As fit indices are influenced by the number of observations, sensitivity of the individual-level paths actually is larger when T is smaller, and decreasing as T grows larger.

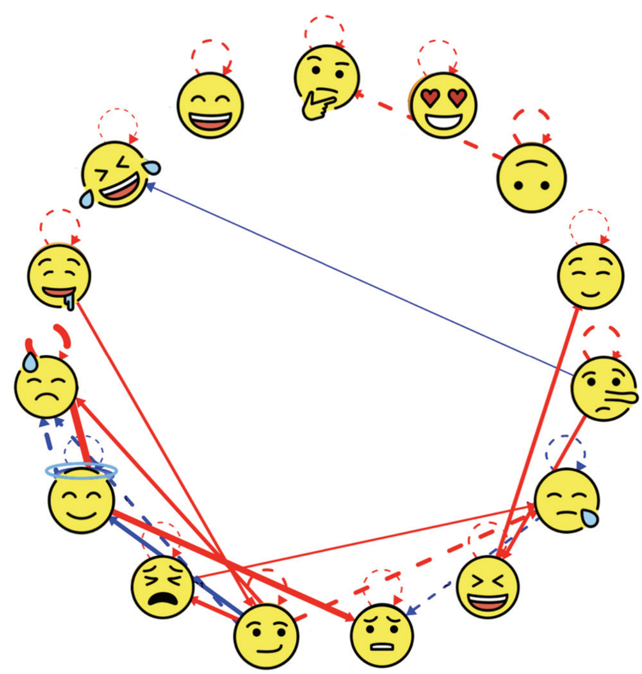
Taken together, this is strong evidence that hybrid-GIMME can successfully capture undirected contemporaneous relations nearly as well as it detects directed contemporaneous relations in types of data increasingly encountered by and of interest to researchers. However, for hybrid-GIMME the number of time points suggested is 150, which is higher than seen for the regular GIMME conducted with the uSEM. This may be an unrealistic number of time points in some research settings. When the number of time points is smaller than this, caution must be made when interpreting the directed contemporaneous relations as some of them might truly be undirected relations. Additionally, that group-level paths are more reliably found than individual-level paths warrants further exploration, as some individual-level paths may be missed. Similar to prior implementations of the GIMME algorithm, specificity rates were also almost always greater than 95% for all conditions, suggesting a very low number of false positives.

While the simulation results show high sensitivity rates of the contemporaneous relations using hybrid-GIMME, the empirical results also provided a proof of concept on the interpretation of the results. The findings highlight expected heterogeneity in emotional experiences. The fact that not many group-level contemporaneous undirected relations were detected may be due to the nature of the data. It is unknown if one can expect generalizable relations among this new form of measurement. The empirical data is a daily diary data that utilizes emojis as the items, which is a very innovative approach that adds another layer of complexity to the data because individuals could easily be interpreting and using the same emojis very differently. Therefore, individuals in the sample could completely reasonably share zero contemporaneous relations, especially when the threshold for a group-level relation was set at .75 (a relation needs to be shared by at least 75% of the sample to be categorized as a group-level relation), which could be too high considering the high interindividual variability in most empirical data in conjunction with this nonstandard measurement approach.

Another likely reason for the lack of group-level undirected relations is that they may have been detected, but erroneously

Figure 7

Hybrid-GIMME Plot of Directed Relations of Emoji Data for Individual 34



Note. All emojis shown in this figure were designed by OpenMoji, the open-source emoji and icon project. GIMME = group iterative multiple model estimation. See the online article for the color version of this figure.

Table 2
Root Mean Square Forecast Error for Five-Step Ahead Forecast Horizon

	Method	
Horizon	Gimme	Var(1)
1	0.67	0.77
2	0.66	0.69
3	0.66	0.74
4	0.67	0.73
5	0.67	0.76

given a directed relation. The simulation study revealed that data generating undirected contemporaneous relations were sometimes erroneously recovered as directed relations, especially when the number of time points is low. Hence, the lack of group-level undirected relations may be because some of them were captured as directed. More work is needed to improve upon recovery of these paths. Nonetheless, the present work is a critical and important contribution as it is the only method available that simultaneously searches for both types of contemporaneous relations without giving preference to one type or another.

A word of caution must be provided when interpreting directed relations. Causality cannot be ascertained using these statistical tests alone. To start, the approach is data-driven, and thus best used for hypothesis-generating. Those wishing to make causal inferences should refer to the large body of work focused on the topic. A nice overview is provided by Pearl (2009). In ideal cases, an experimental design, confirmatory analyses, and clear research questions (as well as hypotheses) are needed. Directed contemporaneous relations can be interpreted similarly to cross-sectional studies. That is, one variable explains variability in the other variable, after accounting for other covariates. In the time series context, the covariates include prior time points of the same variables for AR effect estimation. This differs from the interpretation of the undirected relations, wherein the variables are interpreted as co-occurring after taking covariates into account. The possibility to discover both types of relations at the same time, as demonstrated here, removes the requirement that the researcher have strong hypotheses or assumptions regarding which type of directionality is present in their data.

There also exist several decision points in the simulation study to note. First, the simulation data were generated to share the same number of group- and individual-level directed and undirected contemporaneous relations. The locations and specific values of all contemporaneous relations were randomly generated for each replication, intending to add as much heterogeneity to the simulation as possible so results were not skewed by an arbitrary choice in model structure. It is unknown if this is realistic or to be expected in empirical data as studies that have both types of contemporaneous relations are lacking. Second, although the results were able to show that the number of time points in time series data highly influences the recoverability of the correct relations in the data, they do not provide information on the influence of the magnitude of those relations and recoverability. However, prior work has shown that GIMME can recover relations along a range of absolute values for the relations, doing more poorly with low values (Lane, Gates, Pike, et al., 2019; Nestler & Humberg, 2021), suggesting that inquiry into this specific question here was outside the necessary scope of the paper and would have been potentially redundant. Some possible next steps to further test the stability and recoverability of hybrid-GIMME in different conditions include changing the values of contemporaneous relations and varied ratios of directed to undirected paths.

Third, by allowing the search procedure to include undirected contemporaneous relations, there is a greater chance of overfitting the data. Overfitting happens when the model is more complicated than necessary and explains variability in noise rather than recover true relations. For example, in the simulation when $T = 1{,}000$, there were replications where the true directed contemporaneous relations were identified at the group level both as directed and undirected. While such patterns could be true in some empirical data, this was not the case in the DGM used here as we know the ground-truth in simulation studies. Although the method attempts to limit overfitting by, for instance, including a pruning stage and favoring parsimony in its stopping criteria (Gates & Molenaar, 2012), it is unlikely that overfitting can be completely prevented, which is a common problem shared in many data-driven methods in general (Mumford & Ramsey, 2014). One possible fix specific to this approach would be to restrict the simultaneous presence of both directed and undirected relations between the same two variables. Another potential implementation would be to introduce other criteria besides MIs and fit indices in the model search procedure.

Fourth, having only one data set restricted the performance testing of hybrid-GIMME on empirical data. The empirical data used in this paper most closely resembles the condition where $T = 100$, which did not have an excellent sensitivity rate for recovering the direction of either directed or undirected contemporaneous relations. The need for a large number of time points ($T = 150$) to improve recovery of directionality is a limiting factor for many studies, and future work is needed to accommodate shorter time series lengths. This could be one reason there were no group level undirected relations detected in the emoji empirical data. However, for empirical data with possible large interindividual variability like this, it might not be possible to arrive at a tentative general model that fits the majority of the sample. Another aspect of this is that the homogeneous simulation has very different, almost opposite, nature as the heterogeneous empirical data. It is worth noting that hybrid-GIMME not only performed very well on the simulated data in recovering both types of contemporaneous relations, but also provided results on the empirical data that aligned with expectations.

Fifth, we used the conservative and default group cutoff of 75% in our simulation study as well as empirical data example. This means that for a path to be added to the group-level model, and thus estimated for everyone, it had to have a significant MI for at least 75% of individuals. Recent work on integrating latent variables into GIMME (Gates et al., 2019) found that decreasing the group cutoff to 51%, the technical majority, improved sensitivity rates without introducing false positives. The sensitivity rates here may have increased with a more lenient group cutoff. As there are many things to consider when adjusting the hyperparameter of group cutoff, such as whether or not subgroups are present, we did not explore this complex topic here. More work is needed to address the optimal group cutoff value given the qualities of the data.

Finally, we saw that recovery of individual-level paths decreased as the number of time points increased. This likely is due to the stopping criteria, which rests on fit indices that adjust for the number of parameters and number of observations, being too strict. That is, the model searches were stopped in some cases before finding the data generating paths. This approach has the benefit of introducing very few false positives into the results. However, better recall —particularly at smaller numbers of time series—may occur if the stopping criteria values were shifted given the qualities of the data. This topic is outside the scope of the present paper but warrants more explorations.

Conclusion

This article showed the successful implementation of hybrid-uSEM in one existing data-driven method, GIMME. Simulation results suggested that hybrid-GIMME performed well in recovering the presence and direction of contemporaneous relations in time series data, especially when the number of time points is large (ideally at least larger than 60). The empirical example showed the need to differentiate directed and undirected contemporaneous relations and also demonstrated practical potentials of hybrid-GIMME in doing so. One main future next step is to better address false negatives rates in the algorithm, and to apply and test hybrid-GIMME on more simulations and empirical data. In summary, hybrid-GIMME was a successful implementation of hybrid-uSEM (Molenaar, 2019), and provides a new method for understanding and analyzing of contemporaneous relations in time series data.

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Appendix

Variance-Covariance Matrix Demonstration

For simplicity, here we use $p = 2$ (number of variables at time point t) for as an example, which results in the $\boldsymbol{B}$ and $\boldsymbol{\Psi}$ matrices to be 4×4 because the previous time point measurements are embedded, as demonstrated in the main text. We have two models to consider: (1) $\boldsymbol{B}_1$ and $\boldsymbol{\Psi}_1$ which represent the matrices for when the contemporaneous relation are measured as directed relations among the observed variables, and (2) $\boldsymbol{B}_2$ and $\boldsymbol{\Psi}_2$ which contain an undirected relation among the residuals and no contemporaneous directed relations among observed variables. Note that b_{31} and b_{42} are estimates for autoregressive relations and exist in both exemplar models.

More specifically, the matrices as following:

$$\boldsymbol{B}_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ b_{31} & 0 & 0 & 0 \\ 0 & b_{42} & b_{43} & 0 \end{pmatrix} \qquad \boldsymbol{\Psi}_1 = \begin{pmatrix} \psi_{11} & \psi_{21} & 0 & 0 \\ \psi_{21} & \psi_{22} & 0 & 0 \\ 0 & 0 & \psi_{33} & 0 \\ 0 & 0 & 0 & \psi_{44} \end{pmatrix}$$

$$\boldsymbol{B}_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ b_{31} & 0 & 0 & 0 \\ 0 & b_{42} & 0 & 0 \end{pmatrix} \qquad \boldsymbol{\Psi}_2 = \begin{pmatrix} \psi_{11} & \psi_{21} & 0 & 0 \\ \psi_{21} & \psi_{22} & 0 & 0) \\ 0 & 0 & \psi_{33} & \psi_{34} \\ 0 & 0 & \psi_{34} & \psi_{44} \end{pmatrix}$$

The model implied variance-covariance matrix is given by:

$$\boldsymbol{\Sigma} = (\boldsymbol{I} - \boldsymbol{B})^{-1} \boldsymbol{\Psi} (\boldsymbol{I} - \boldsymbol{B}^T)^{-1}$$

Therefore, we have the two $\boldsymbol{\Sigma}$ matrices as following:

$$\boldsymbol{\Sigma}_1 = \begin{pmatrix} \psi_{11}, & \psi_{21}, & b_{31} \cdot \psi_{11}, & b_{42} \cdot \psi_{21} + b_{31} \cdot b_{43} \cdot \psi_{11} \\ \psi_{21}, & \psi_{22}, & b_{31} \cdot \psi_{21}, & b_{42} \cdot \psi_{22} + b_{31} \cdot b_{43} \cdot \psi_{21} \\ b_{31} \cdot \psi_{11}, & b_{31} \cdot \psi_{21}, & \psi_{11} \cdot b_{31}^2 + \psi_{33}, & \sigma_{34} \\ b_{42} \cdot \psi_{21} + b_{31} \cdot b_{43} \cdot \psi_{11}, & \sigma_{42}, & \sigma_{43}, & \sigma_{44} \end{pmatrix}$$

(*Appendix continues*)

Where:

$$
\begin{aligned}
\sigma_{34} &= b_{43} \cdot \psi_{11} \cdot b_{31}^2 + b_{42} \cdot \psi_{21} \cdot b_{31} + b_{43} \cdot \psi_{33} \\
\sigma_{42} &= b_{42} \cdot \psi_{22} + b_{31} \cdot b_{43} \cdot \psi_{21} \\
\sigma_{43} &= b_{43} \cdot \psi_{33} + b_{31} \cdot (b_{42} \cdot \psi_{21} + b_{31} \cdot b_{43} \cdot \psi_{11}) \\
\sigma_{44} &= \psi_{44} + b_{43}^2 \cdot \psi_{33} + b_{42} \cdot (b_{42} \cdot \psi_{22} + b_{31} \cdot b_{43} \cdot \psi_{21}) + b_{31} \cdot b_{43} \cdot (b_{42} \cdot \psi_{21} + b_{31} \cdot b_{43} \cdot \psi_{11})
\end{aligned}
$$

$$
\boldsymbol{\Sigma}_2 = \begin{pmatrix} \psi_{11}, & \psi_{21}, & b_{31} \cdot \psi_{11}, & b_{42} \cdot \psi_{21} \\ \psi_{21}, & \psi_{22}, & b_{31} \cdot \psi_{21}, & b_{42} \cdot \psi_{22} \\ b_{31} \cdot \psi_{11}, & b_{31} \cdot \psi_{21}, & \psi_{11} \cdot b_{31}^2 + \psi_{33}, & \psi_{34} + b_{31} \cdot b_{42} \cdot \psi_{21} \\ b_{42} \cdot \psi_{21}, & b_{42} \cdot \psi_{22}, & \psi_{34} + b_{31} \cdot b_{42} \cdot \psi_{21}, & \psi_{22} \cdot b_{42}^2 + \psi_{44} \end{pmatrix}
$$

The equations show that the two model implied variance-covariance matrices are not identical and we should expect to see different results depending on whether the contemporaneous relation are measured as directed relations among the observed variables or as undirected relations among the residuals.

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