Conducting Simulations in Causal Inference with Networks-Based Structural Equation Models

Oleg Sofrygin (sofrygin@berkeley.edu, Department of Biostatistics, University of California, Berkeley, USA)

Romain Neugebauer (Division of Research, Kaiser Permanente Northern California, Oakland, USA)

Mark J. van der Laan (Department of Biostatistics, University of California, Berkeley, USA)

Abstract

The past decade has seen an increasing body of literature devoted to the estimation of causal effects in network-dependent data. However, the validity of many classical statistical methods in such data is often questioned. There is an emerging need for objective and practical ways to assess which causal methodologies might be applicable and valid in network-dependent data. This paper describes a set of tools implemented in the simcausal R package that allow simulating data based on user-specified structural equation model for connected units. Specification and simulation of counterfactual data is implemented for static, dynamic and stochastic interventions. A new interface aims to simplify the specification of network-based functional relationships between connected units. A set of examples illustrates how these simulations may be applied to evaluation of different statistical methods for estimation of causal effects in network-dependent data.

1 Introduction

The past decade has seen an increasing body of literature devoted to estimation of causal effects in network-dependent data. Many of these studies seek to answer questions about the role of social networks on various aspects of public health. For example, Christakis et al. used the observational data on subjects connected by a social network to estimate the causal effects of contagion for obesity, smoking and a variety of other outcomes (Christakis and Fowler, 2007, 2013), finding that many of these conditions are subject to social contagion, e.g., in one of the studies the authors found that the person’s risk of becoming obese increases with an additional obese friend, even when one controls for all measured confounding factors. However, the statistical methods employed by these studies have come under scrutiny due to possibly anti-conservative standard error estimates that did not account for network-dependence among the observed units (Lyons, 2010), and possibly biased effect estimates that could have resulted from: model misspecification (Lyons, 2010; VanderWeele and An, 2013), network-induced homophily (Shalizi and Thomas, 2011), and unmeasured confounding by environmental factors (Shalizi and Thomas, 2011). Given the potential high impact of such studies on future policy and public health decisions, it is important to be able to verify the robustness of statistical methods employed in these and similar studies. Clearly, there is an emerging need for methods which can test the validity of various statistical methods for social network data and we argue that one of the possible approaches involves the conduct of simulation studies. That is, a practical way to test the validity of a certain statistical method involves its application against a large set of plausible data generating scenarios, specifically in relation to the types of dependent data one might see in social networks. Moreover, a carefully designed simulation study can test the method’s sensitivity to violations of its key assumptions, highlight its limitations for specific types of data, and provide an important proof of concept that complements the results based on statistical theory. Finally, simulations can be also helpful in identifying errors in the implementation of complex statistical algorithms.

While estimation of causal effects in social network settings is challenging, it is also an active area of ongoing research (Halloran and Hudgens, 2016). Some of the challenges for inference are due to the fact that the frequently made assumption of independence among units is generally invalid. Consider a setting with single
time point exposure where we collect data on the baseline covariates, the exposures and the outcomes on \( N \) units. When these units are also connected by a network we might expect that the interactions between any two connected units can cause the exposure of one unit to have an effect on the outcome of the other unit - an occurrence often referred to as interference or spillover (Sobel, 2006; Hudgens and Halloran, 2008). Moreover, it is possible that both, the outcome and the exposure of one unit, are dependent on the baseline covariates of other connected units. This paper is concerned with design and implementation of simulation studies for these types of network-dependent data. We describe a comprehensive set of tools implemented in the \texttt{simcausal}\(^1\) \texttt{R} package (Sofrygin et al., 2015; Sofrygin et al.), which allow simulating the types of dependent data one might collect on a community connected by a social or geographical network. We then illustrate potential application of \texttt{simcausal} by describing a simulation study that assesses the performance of several estimators of causal effects among network-dependent observations.

In general, \texttt{simcausal} uses the following two-step process for specifying the data generating distribution for \( N \) connected units. First, one describes the network of connections between these units (e.g., social or geographical network) by specifying either a known network graph or a probabilistic network graph model for \( N \) nodes. Next, one specifies the distribution of the unit-level covariates (node attributes) by parameterizing a structural equation model (SEM) for connected units (van der Laan, 2014). This SEM allows the covariates of one unit to be dependent on the covariates of other connected units via some known functional form which is controlled explicitly by the user. For this purpose, we developed a novel \texttt{R} interface which simplifies the specification of complex network-based functional relationships between such units. Moreover, the network-based syntax can be combined with the existing syntax for specifying longitudinal data structures, allowing for simulations of network-based processes that also evolve in time. We refer to Sofrygin et al. for general information about the \texttt{simcausal} package and the description of its syntax for simulating longitudinal independent and identically distributed (IID) data.

Network simulation studies have been previously applied to assess the validity of different estimation approaches in causal inference (for example, see Noel and Nyhan (2011), Eckles et al. (2014) and Athey et al. (2015)). Such simulation studies have also been used as a guiding tool for comparison of the benefits of different experimental design strategies in network settings (Aral and Walker, 2011; Walker and Muchnik, 2014; Basse and Airoldi, 2015; Harling et al., 2016). However, to the best of our knowledge, there is no open-source simulation software for conducing network-based causal inference research that is similar to the tools and syntax implemented in the \texttt{simcausal} package. While our package provides the user with a broad range of possible data-generating distributions, it is specifically targeted towards causal inference research on the types of observational data that might be collected when observing members of a single social network. In other words, \texttt{simcausal} allows specification of a model based on a causal Directed Acyclic Graph (DAG), and in conjunction with previously specified network model, this causal DAG can be used to define ways in which connected units depend on each other. Moreover, any \texttt{R} package that can simulate a network graph can be used within \texttt{simcausal}. For example, in this article we rely on the \texttt{igraph} \texttt{R} package (Csardi and Nepusz, 2006) for simulating various network graphs.

In summary, our newly developed software provides a simple and concise interface for specifying a network data-generating distribution and incorporating the network structure into various forms of functional dependence of one unit on other connected units. It permits the simulation of such interconnected data structures, as well as the generation of the counterfactual data under single or multiple time-point interventions. The user-defined causal parameters can then be evaluated from the counterfactual data and serve as gold-standards in testing the validity of various statistical methods. Finally, the \texttt{simcausal} package provides the syntax for specifying complex longitudinal data structures in combination with the network-dependent syntax, allowing one to simulate complex network processes that also evolve over time.

### 1.1 Other related \texttt{R} packages

As of May 29, 2016, there were 208 \texttt{R} packages on CRAN that contain the word “network” in their title sentence. A large number of these packages are dedicated towards visual analysis and representation of

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1\texttt{simcausal} package was developed using the \texttt{R} system for statistical computing (\texttt{R Core Team}, 2016) and it is available from the Comprehensive \texttt{R} Archive Network (CRAN) at \url{http://CRAN.R-project.org/package=simcausal}. 

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networks (e.g., ggnetwork (Briatte, 2016), igraph (Csardi and Nepusz, 2006), d3Network (Gandrud, 2015)), re-constructing the network based on biological, neural and other field-specific data (e.g., interventionalDBN (Spencer, 2014), LogitNet (Wang et al., 2009), RSNNS (Bergmeir and Benitez, 2015), dina (Gill et al., 2014)), statistical analysis of networks based on specific network-generating models (multiplex (Rivero Ostoic, 2016), lv4net (Gollini, 2015)). In addition, a large collection of packages often referred to as a “statnet suite of packages” provides various tools for social network analysis, visualization, simulation and diagnoses based on the statistical methods of exponential-family random graph models (ERGMs) or other related parametric model families for networks (e.g., statnet (Handcock et al., 2008), sna (Butts, 2014), EpiModel (Jenness et al., 2016), ergm (Handcock et al., 2016), tergm (Krivitsky and Handcock, 2016)). Other packages for statistical analysis of network or network-related data include, among others, netdiffuseR (Vega Yon et al., 2016), nets (Brownlees, 2016), ebdbNet (Rau, 2013) and tmlenet (Sofrygin and van der Laan, 2015). Finally, a large number of R packages are targeted towards analyses and simulation of various networks, network evolution over time and the modeling various network features, such as the creation of the tie between two nodes and answering questions such as, how and why certain network ties are formed? Among the packages that are tailored to such analyses are CIDnetworks (Adhikari et al., 2015), tsna (Bender-deMoll and Morris, 2016), networkDynamic (Butts et al., 2016) and egonet (Sciandra et al., 2012). Another class of packages that is worth noting are those specifically targeted towards modeling of epidemics on a network graph, such as packages epinet (Groendyke and Welch, 2016), netdiffuseR (Vega Yon et al., 2016), EpiModel (Jenness et al., 2016), for example, by relying on the agent-based modeling or ERMG techniques. In addition, the following packages are specifically designed for simulations of the network-graph data: SocialMediaLab (Graham et al., 2016), which provides tools for collecting and generating social media data for networks; hybridModels (S. Marques et al., 2016), which allows simulations of stochastic models for transmission of infectious diseases in longitudinal networks; NetSim (Stadtfeld, 2013), a package for simulating social networks; and finally, RSienna (Ripley et al., 2013), a package designed for simulation-based analysis of networks as well as model fitting for longitudinal network data.

1.2 Organization of this article

The rest of this article is organized as follows. In Section 2, we formally describe our assumed observed data structure and provide the technical definition of the underlying structural equation model (SEM) for possibly connected units. In Section 3 we provide some technical details of the simcausal interface for simulating data according to the user-specified parameterization of this SEMs. In Section 4, we illustrate the use of simcausal in a typical simulation study, evaluating the true sample-average mean causal outcome (the gold-standard) of a single time-point stochastic intervention on continuous exposure. We also demonstrate how this network simulation examples can be used in practice for assessing the performance of statistical methods for estimation of causal effects among network-dependent observations. We conclude with a discussion in Section 5.

2 Structural Equation Model for Connected Units

We start by introducing some notation. Suppose that we can simulate a sample of $N$ connected observations, where each observed unit is indexed as $i = 1, \ldots, N$. We let $F_i \subseteq \{1, \ldots, N\} \setminus \{i\}$ denote the set of observations that are assumed “connected” to $i$ or, as we will refer to it, the units in $F_i$ are “friends” of $i$. In other words, we assume that each set $F_i$ consists of a unique set of indices $j$ in $\{1, \ldots, N\}$, except for $i$ itself. We also allow $F_i$ to be empty, which would imply that observation $i$ is not receiving input from any other units. We assume that $i$ may receive input from other observations only if those observations are listed as part of $F_i$. We will refer to the union of all $F_i$ as a “network profile” on all $N$ observations, which will be denoted by $F$. Let $O_i = (W_i, A_i, Y_i)$ denote the data collected on each observation $i$, for $i = 1, \ldots, N$, where $W_i$ denotes all the baseline covariates for $i$, $A_i$ denotes the exposure of $i$ and $Y_i$ denotes the outcome of $i$. Let $W = (W_i)_{i=1}^{N}$, $A = (A_i)_{i=1}^{N}$, $Y = (Y_i)_{i=1}^{N}$, and $O = (W, A, Y)$. Finally, we assume $F_i \subseteq W_i$, that is, the network of friends of $i$ is assumed to be part of $i$’s baseline covariates. Below we define the structural equation model (SEM) (Pearl, 2009) for $N$ connected units, similar to that presented in van der Laan (2014). This model will form
the basis for describing the types of network-based data generating distributions that are considered in this article.

2.1 General Structural Equation Model for Connected Units

Suppose that $N$ connected observations in $O$ are generated by applying the following structural equation model (SEM): first generate a collection of exogenous errors $U_N = (U_i : i = 1, \ldots, N)$ across the $N$ units, where the exogenous errors for unit $i$ are given by

$$U_i = (U_{W_i}, U_{A_i}, U_{Y_i}), \ i = 1, \ldots, N,$$

and then generate $O$ deterministically by evaluating functions as follows:

$$W_i = f_{W_i}(U_{W_i}), \text{ for } i = 1, \ldots, N$$
$$A_i = f_{A_i}(W_i, (W_j : j \in F_i), U_{A_i}), \text{ for } i = 1, \ldots, N$$
$$Y_i = f_{Y_i}(A_i, W_i, (A_j, W_j : j \in F_i), U_{Y_i}), \text{ for } i = 1, \ldots, N$$

The above SEM is general in the sense that it makes no functional restrictions on $f_{W_i}, f_{A_i}$ and $f_{Y_i}$, allowing each $i$-specific set of covariates $(W_i, A_i, Y_i)$ to be generated from their own $i$-specific functions. However, the functions $f_{W_i}, f_{A_i}$ and $f_{Y_i}$ will be subjected to modeling below. This SEM could be visualized as a causal graph describing the causal links between the $N$ units. That is, one could represent the SEM in 1 as a Directed Acyclic Graph (DAG) (Pearl, 1995), by drawing arrows from causes to their effects. However, such a DAG would have to include all $N$ dependent observations (the entire network), since the above SEM includes a separate equation for each observed unit $i = 1, \ldots, N$. Furthermore, one can imagine that this structural causal model might be also time-dependent, in which case the causal links among $N$ units would evolve over time and the visualization of such structural causal model would describe what one might call a dynamic causal network (van der Laan, 2014). For example, for a network with two units ($N = 2$), in which unit $i = 1$ is dependent on unit $i = 2$, but not vice-versa, this type of the SEM could be depicted with a DAG shown in Figure 1. We also note that the error terms $(U_{W_i}, U_{A_i}, U_{Y_i})$, for $i = 1, 2$, are excluded from this causal DAG (Pearl, 2012), with the implication that each of the remaining variables is subject to the influence of its own error.

![Figure 1: An example of a directed acyclic graph (DAG) for two observations, where unit 1 is dependent on unit 2, but not vice-versa.](image)

2.2 Dimension Reduction Assumptions

To simplify the notation and to control the dimensionality of the above SEM, we assume that there are also some known summary measures:

$$W^s_i := w^s_i(W_i, W_j : j \in F_i)$$

and

$$A^s_i := a^s_i((A_i, W_i), (A_j, W_j : j \in F_i)),$$
and we use the short-hand notation $W_i^s$ for $w_i^s(\cdot)$ and $A_i^s$ for $a_i^s(\cdot)$. We assume that these summary measures $W_i^s$ and $A_i^s$ are of constant-in-$i$ dimension (that does not depend on $N$). Finally, we assume that for each node $A_i$ and $Y_i$, we can define the corresponding common (in $i$) functions $f_A$ and $f_Y$, so that

\begin{align}
W_i &= f_W(U_{W_i}), \text{ for } i = 1, \ldots, N \\
A_i &= f_A(W_i^s, U_{A_i}), \text{ for } i = 1, \ldots, N \\
Y_i &= f_Y(A_i^s, W_i^s, U_{Y_i}), \text{ for } i = 1, \ldots, N.
\end{align}

Examples of such dimension reductions are provided in Section 3 and 4. In particular, one could define $a_i^s(W) = (A_i, (A_j : j \in F_i))$, i.e., the observed exposure of unit $i$ itself and the observed exposures of its friends. Similarly, one could define $w_i^s(W) = (W_i, (W_j : j \in F_i))$. By augmenting these reductions to data on maximally $K$ friends, filling up the empty cells for units with fewer than $K$ friends with a missing value, these dimension reductions have a fixed dimension, and include the information on the number of friends.

### 2.3 Independence Assumptions on Exogenous Errors

We now make the following (conditional) independence assumptions on the exogenous errors. First, we assume that each $U_{W_i}$ is independent of all $U_{W_j}$, such that $F_i \cap F_j = \emptyset$, for $i = 1, \ldots, N$ (weak dependence of $W$). For example, one of the possible ways to simulate such dependent $W_1, \ldots, W_N$ in simcausal is to define a latent (hidden) covariate $W_i^s$ which is shared between all observations connected to $i$ and then defining the observed baseline covariate for $i$ and all $j \in F_i$ conditionally on $W_i^s$. Such simulation procedure allows one to introduce dependence between the observed $W_i$ and $W_j$, whenever $i$ and $j$ are connected. One could make further restrictions on $W$, for example, by assuming that all $U_{W_i}$ are unconditionally independent, which would imply the independence of $W$. Second, we assume that conditional on $W$, all $(U_{A_i} : i = 1, \ldots, N)$ are independent and identically distributed (IID). Finally, we assume that conditional on $A$, all $(U_{Y_i} : i = 1, \ldots, N)$ are also IID.

The important implication of the latter assumptions is that, given the observed past on $N$ baseline covariates and treatments $(W, A)$, for any two units $i$ and $j$ that have the same value for their summaries $W_i^s = W_j^s$ and $A_i^s = A_j^s$, we have that $Y_i$ and $Y_j$ are independent and identically distributed. Similarly, the same statement holds for two treatment nodes $A_i$ and $A_j$, whenever the baseline summaries of $i$ and $j$ are equal, i.e., $W_i^s = W_j^s$. These assumptions on errors $U_i := (U_{W_i}, U_{A_i}, U_{Y_i})$, for $i = 1, \ldots, N$ imply that: 1. $W_1, \ldots, W_N$ are (at most) weakly dependent; 2. Conditional on $W$, the random variables $(A_1, \ldots, A_N)$ are mutually independent; and 3. Conditional on $(A, W)$, the random variables $(Y_1, \ldots, Y_N)$ are mutually independent. Thus, all the dependence between units is explained by the observed pasts of the units themselves and of their friends. Furthermore, the above structural assumptions will imply restrictions on the conditional distribution of $Y_i$ and $A_i$. However, the full description of the resulting statistical model based on the above SEM is outside the scope of this article and we refer the interested reader to Sofrygin and van der Laan (2016) for additional details.

The SEM in 2 and the above independence assumptions define the set of possible data-generating distributions that are considered in this article. In particular, one could utilize the simcausal package to simulate $N$ dependent observations $O$ based on the following algorithm:

1. Start by generating $N$ baseline covariates $(W_1, \ldots, W_N)$, by first drawing $N$ weakly dependent errors $(U_{W_i} : i = 1, \ldots, N)$ and then applying the equations $f_W(U_{W_i})$, for $i = 1, \ldots, N$;
2. Generate $N$ baseline summaries $(W_1^s, \ldots, W_N^s)$, by applying the baseline summary measures $w_i^s(\cdot)$ to $W_i$ and $(W_j : j \in F_i)$, for $i = 1, \ldots, N$;
3. Generate $N$ exposures $(A_1, \ldots, A_N)$, by first drawing $N$ IID errors $(U_{A_i} : i = 1, \ldots, N)$ and then applying the common equation $f_A(\cdot)$ to each $W_i^s$ and $U_{A_i}$, for $i = 1, \ldots, N$;
4. Generate $N$ exposure summaries $(A_1^s, \ldots, A_N^s)$, by applying the exposure summary measures $a_i^s(\cdot)$ to $(A_i, W_i)$ and $(A_j, W_j : j \in F_i)$, for $i = 1, \ldots, N$; and

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2. Generate $N$ baseline summaries $(W_1^s, \ldots, W_N^s)$, by applying the baseline summary measures $w_i^s(\cdot)$ to $W_i$ and $(W_j : j \in F_i)$, for $i = 1, \ldots, N$;
3. Generate $N$ exposures $(A_1, \ldots, A_N)$, by first drawing $N$ IID errors $(U_{A_i} : i = 1, \ldots, N)$ and then applying the common equation $f_A(\cdot)$ to each $W_i^s$ and $U_{A_i}$, for $i = 1, \ldots, N$;
4. Generate $N$ exposure summaries $(A_1^s, \ldots, A_N^s)$, by applying the exposure summary measures $a_i^s(\cdot)$ to $(A_i, W_i)$ and $(A_j, W_j : j \in F_i)$, for $i = 1, \ldots, N$; and
5. Generate $N$ outcomes $Y_1, \ldots, Y_N$, by drawing $N$ IID errors $(U_{Y_i} : i = 1, \ldots, N)$ and then applying the common equation $f_Y(\cdot)$ to $(A_i^*, W_i^*)$ and $U_{Y_i}$, for $i = 1, \ldots, N$.

2.4 Counterfactuals, Interventions and the Target Parameter as the Average Causal Effect (ACE)

The SEM in 2 also implicitly encodes the definition of counterfactual variables, i.e., variables which would result from some particular interventions on a set of endogenous variables. For example, for a particular vector of treatment assignments $\mathbf{a} = (a_1, \ldots, a_N)$, we could modify the SEM as follows:

$$
W_i = f_{W_i}(U_{W_i}), \quad i = 1, \ldots, N,
$$

$$
A_i = a_i, \quad i = 1, \ldots, N,
$$

$$
Y_{i,a} = f_Y(a_i^*(\mathbf{a}, \mathbf{W}), W_i^*, U_{Y_i}), \quad i = 1, \ldots, N,
$$

where the equations for $W_i$ were kept unchanged, each $A_i$ was set to $a_i$, and each $Y_{i,a}$ denotes the counterfactual outcome of unit $i$, under the network intervention on all $N$ units that sets $A = \mathbf{a}$. In this article, we will refer to $(\mathbf{W}, \mathbf{a}, \mathbf{Y}_a)$ as counterfactual data for $N$ units and we define our target causal parameter as a function of such counterfactual data distribution. For example, the average treatment effect (ATE) can be simply expressed as $E[Y_1 - Y_0]$.

3 Syntax for Simulating Networks and Network-Dependent Data

To define the distribution of the data (and to simulate such data), simcausal uses a DAG object, which will typically consist of a collection of individual nodes (random variables). Such nodes are defined each time the user calls the `node()` function. That is, each call to `node()` defines the conditional distribution(s) of either a single or time-varying node. Collectively, these `node()` calls define a single DAG object, which parametrizes the distribution of the data that the user wants to simulate. By default, the distribution of any new node for a single observation $i$ can be dependent only on $i$'s values of the previously defined nodes, and not the node values of other observations. As a result, any two observations sampled from such DAG object will be independent. However, there are many real-life examples when one wishes to simulate data based on some either a priori known or hypothesized information about the network of connections between different observations. The new functionality we describe here allows the user to specify the distribution of a network graph and then use that network to define the distribution of covariates for each observation $i$ conditionally on the covariates of other observations. For example, if we assume that the observation $j$ is part of $i$'s social or geographical network (or as we will call it, the observation $j$ is a friend of $i$), then the nodes of $j$ are allowed to influence the distribution of the nodes of $i$. Moreover, we assume that the functional form of such dependence can be described by some user-specified network-based summary measures. For that purpose, we used the R list subsetting operator “[[...]]” and re-defined it specifically for indexing and building of such network summaries based on observations that are friends of $i$ (e.g., “\text{Var}[[\text{indx}]]”). We also note that simcausal does not allow simultaneous friend references of the same node, that is, each newly added node can be defined only as a function of the nodes that have been previously added to the DAG object.

3.1 Defining the network

In order to perform network-based simulations with the simcausal package, the user has to declare a function which will return a specific network matrix, and we will refer to any such function as the network generator. In particular, a network generator is any user-specified function that returns a network profile $\mathbf{F}$ on $N$ observations, defined as a matrix of $N$ rows, each row $i$ containing the set of friends $F_i$ of observation $i$, i.e., row $i$ consists of a vector of observations from $\{1, \ldots, N\}$ that are assumed connected to $i$. The network generator function should accept at least one named argument, $\mathbf{n}$, and it must return a network matrix with $\mathbf{n}$ rows and $K_{max}$ columns, where $K_{max}$ stands for a maximal possible number of friends for any observation.
When observation \( i \) happens to have fewer than \( K_{\text{max}} \) friends, i.e., \(|F_i| < K_{\text{max}}\), the remainder of the matrix row \( i \) must be filled with \text{NA} (missing) values. Note that an observation \( i \) is allowed to have no friends, which is denoted by an empty friend set \( F_i \), in which case the row \( i \) of the network matrix should only consist of \text{NA} (missing) values.

Once such a network generator has been defined, the next step is to add this network to a specific \text{DAG} object. This is accomplished by simply calling the \text{network} function, specifying the name of the network generator as its argument “\text{netfun}” and adding this network function call to the current \text{DAG} object with the \text{R} operator “\text{+}”. In other words, the \text{network} function call defines the network and is added to an existing \text{DAG} object with a syntax “\text{+ network(...)\text{}}”. Note that this is identical to the simcausal syntax for adding new \text{node} function calls to a growing \text{DAG} object when defining data for IID observations. This network can then serve as a backbone for defining the dependent-data structural equation models within such a \text{DAG} object. More specifically, the previously defined node values of \( i \)’s friends can be now referenced as part of the new \text{node} function calls, defining the conditional distribution of the node for each observation \( i = 1, \ldots, N \). The examples following this section illustrate this functionality for various network models.

Finally, we note that the \text{network} function can accept any number of user-specified optional arguments, where each of such optional arguments must be an evaluable \text{R} expression. These expressions will not be evaluated until the data simulation step, at which point all of them are passed as arguments to the function that defines the network generator. Thus, just like the regular \text{node} function expressions, the \text{network} function expressions can refer to any standard or user-specified \text{R} functions and can reference any of the previously defined \text{DAG} nodes (i.e., \text{DAG} nodes that were added prior to \text{network} function call). This feature can be useful when, for example, one wishes to simulate the network in which the probability of forming a tie between two units depends on the previously simulated unit-specific variable values (such as the baseline risk factors on each unit).

### 3.2 Using the syntax \text{[[...]]} for network-based variable subsetting

Following the \text{network} function call, subsequent calls to \text{node} function can employ our re-purposed list subsetting operator “\text{[[...]]}” for indexing the node values of friends. First, the variable which is to be used for network subsetting is specified in front of the subsetting operator, e.g., “\text{A[[...]]}”. Second, the friend values of the variable \( A \) are specified by the subsetting index, e.g., “\text{A[[1:5]]}”. This expression will look up the values of node \( A \) for friends indexed from 1 to 5 and it will be evaluated for all observations \( i = 1, \ldots, N \). The specific ordering of friends is determined by the column ordering of the network matrix returned by the network generator. Such network-indexing expressions can be also used as inputs of different \text{R} functions, enabling evaluation of various network-based summaries. For example, the expression “\text{sum(A[[1:Kmax]]\text{})\text{}}” will specify a vector of length \( N \) that will consist of a sum of \( A \) values among all friends of \( i \), for each observation \( i = 1, \ldots, N \). This syntax is fully generalizable towards any function which can operate on matrices, such as the matrix result of the expression “\text{A[[1:Kmax]]\text{}}”. Moreover, two of the commonly used \text{R} functions, \text{sum} and \text{mean}, are automatically replaced with their row-based counterparts: the functions \text{rowSums} and \text{rowMeans}. Thus, the expressions “\text{sum(A[[1:Kmax]]\text{})\text{}}” and “\text{rowSums(A[[1:Kmax]]\text{})\text{}}” can be used interchangeably.

We illustrate this syntax with a simple example. Suppose that we have a \text{DAG} object, named “\text{D}” and we use the network generator, named “\text{rnet.gnp}\text{\text{\textsuperscript{2}}\text{\text{}}\text{}}”. As shown in the code snippet below, we first define an empty \text{DAG} object \( \text{D} \), then we add the network named “\text{net}” to object \( \text{D} \) and we also define an IID Bernoulli variable named “\text{Var}”.

```r
library("simcausal")
D <- DAG.empty() +
  network("net", netfun = "rnet.gnp", p = 0.1) +
  node("Var", distr = "rbern", prob = 0.5)
```

\textsuperscript{2}Note that the network generator \text{rnet.gnp} is provided as part of the \text{simcausal} package. It uses the \text{igraph} \text{R} package function \text{sample.gnp} to sample a network graph and then converts its output into the \text{simcausal} network matrix representation. See \text{?rnet.gnp} for additional information.
Next, we define a new node, named “Var.F1”, as the value of Var for the first friend of each observation \(i = 1, \ldots, N\). We do this by defining a node with a constant (degenerate) distribution, \texttt{distr="rconst"}, and indexing the first friend of each observation with the expression “Var[[1]]”, as shown in the following example:

\[
D <- D + \text{node}("Var.F1", \texttt{distr = "rconst"}, \texttt{const = Var[[1]]})
\]

Suppose we now wish to list the Var values among the first 4 friends from each set \(F_i\). This can be accomplished by defining a single multivariate node and using the expression “Var[[1:4]]”, as shown next:

\[
D <- D + \text{node}(\texttt{paste0("Var.F",1:4)}, \texttt{distr = "rconst"}, \texttt{const = Var[[1:4]]})
\]

As our final example, we define a new degenerate node, named “mean.F1to4”, as the mean of Var amongst the first 4 friends, for each \(i = 1, \ldots, N\). We also define a new Bernoulli node, named “Var.F1to4”, for which the \(i\)-specific probability of success is also given as the mean of Var amongst the first 4 friends in \(F_i\). The data for the variables defined thus far can now be simulated by simply calling the functions \texttt{set.DAG} and \texttt{sim} in sequence and specifying the desired sample size \(N\) with the argument “n”.

\[
D <- D + \\
\text{node("mean.F1to4", \texttt{distr = "rconst"}, \texttt{const = mean(Var[[1:4]], na.rm=TRUE)}) +} \\
\text{node("Var.F1to4", \texttt{distr = "rbern"}, \texttt{prob = mean(Var[[1:4]], na.rm=TRUE)})}
\]

\[
D <- \text{set.DAG}(D, \texttt{n.test = 200}) \\
\text{\texttt{sim}(D, n = 50)}
\]

In summary, for a given indexing vector \texttt{indx}, the network-indexing expression, such as “Var[[indx]]”, will evaluate to a matrix with \(N\) rows and the number of columns determined by the length of \texttt{indx}. We note that indexing variable \texttt{indx} can be a non-negative integer-valued vector, with values starting from 0 and bounded above by a special reserved constant named “\texttt{Kmax}”. That is, the variable \texttt{Kmax} can be used for finding out the maximal friend index for any given network, as we demonstrate in examples in following sections. In addition, one can use 0 as part of the same friend indexing vector, where the expression “Var[[0]]” is equivalent to using “Var”. This provides a convenient syntax for indexing the actual Var value of observation \(i\) along with the Var values of \(i\)’s friends, for example, allowing the expressions such as “\texttt{sum(Var[[0:Kmax]])}”. Furthermore, for a specific observation \(i\), the expression “Var[[k]]” will evaluate to a missing value (i.e., “NA”) whenever \(i\) has fewer than \(k\) friends. This default behavior can be also altered by passing a special named argument “\texttt{replaceNAw0=TRUE}” to the corresponding \texttt{node()} call, in which case all of such missing (NA) values are automatically replaced with 0 values. In addition, any node expression can reference a special reserved variable “\texttt{nF}”, which is a vector of length \(n\) and it stores the total number of friends for observation \(j\) in its \(j\)th entry.

Finally, we note that any function that defines a network-indexing node summary can be similarly applied as a summary of a time-varying node and vice-versa. For example, for a time varying node “Var.t”, the expression “\texttt{sum(Var.t[t_indx])}” is analogous to our previous example of the network summary “\texttt{sum(Var[[indx]])}”, except that in the former case we are summing the values of a time-varying node Var.t for time-points defined by the indexing vector \texttt{t_indx}. We also provide some additional examples of such network summaries in the following sections. For more in-depth description of this functionality we refer to Sofrygin et al., Section 2.3. “Specifying a structural equation model”. Furthermore, both of these indexing operators, i.e., the time indexing operator “[...]” and the network indexing operator “[[...]]”, can be combined to form a single summary applied to a time-varying node, as we demonstrate in Section ??.

4 Simulation Study Comparing Performance of Dependent-Data Estimators

The simulation study described here is a simplified version of a hypothetical observational study that might have been conducted to evaluate the social influence of healthy living on personal long term health status.
We assumed that this study collected data on an interconnected community of \( N \) individuals. For each individual \( i \), we would have measured their social network \( F_i \), baseline covariates \( W_i \), an exposure \( A_i \) and a binary outcome \( Y_i \). The exposure was assessed as a continuous physical activity index and the outcome indicated if the person was obese after some follow-up period. We evaluated the average-causal effect of a stochastic intervention that intervened only on some members of the community by shifting their observed physical activity level by some known constant \( shift > 0 \), while keeping the exposures of others unchanged. More precisely, such stochastic intervention for each unit \( i \) can be defined by a function \( \delta(A_i, W_i) \) that assigns the new (intervened) exposure to either \( A_i + shift \) or \( A_i \), depending on the covariate values \( W_i \). Such interventions have been described in the past (Müñoz and van der Laan, 2012) and they arise naturally in settings with continuous exposures where it is not feasible to intervene on every member of the population. For example, in our hypothetical study it might be infeasible to increase the level of physical activity for an individual with a pre-existing medical condition who is above a certain age. Therefore, as an alternative, we may consider a dynamic interventions that does not intervene on such community members, as determined by the pre-specified function \( \delta(A_i, W_i) \). This in turn allows us to define the types of causal parameters which are less likely to violate the positivity assumption (Robins, 1999) (also known as the assumption of experimental treatment assignment (ETA) (Neugebauer and van der Laan, 2005)).

In our simulation, we start by sampling a network graph for \( N \) units (nodes) according to the “small-world” model (Watts and Strogatz, 1998), along with three unit-specific baseline covariates,

\[
W_i = (W_i(1), W_i(2), W_i(3)),
\]

for \( i = 1, \ldots, N \), where \( W_i(1) \) is a categorical risk factor, and \( (W_i(2), W_i(3)) \) are binary confounders. The unit-specific exposure \( A_i \) is then simulated conditionally on \( W_i \) as normal with mean \( \mu(W_i) = 0.58 * W_i(2) + 0.35 * W_i(3) \) and standard deviation \( \sigma^2 = 1 \). We also let the conditional density of \( A_i \) given \( W_i \) to be denoted as \( g_0(a|w) \). We denote the intervened exposure on \( i \) as \( A_i^\ast \), with its corresponding conditional density denoted as \( g^\ast \). We set \( A_i^\ast \) to \( A_i + shift \), for some known constant \( shift > 0 \), only if the following condition holds:

\[
A_i - \mu(W_i) \leq \frac{\log(trunc)}{shift} + \frac{shift}{2} \tag{3}
\]
or known truncation constant \( trunc > 0 \), and otherwise, the intervention keeps the observed exposure \( A_i \) unchanged. Note that the above inequality in 3 is equivalent to the following condition

\[
\frac{g_0(A_i - shift|W_i)}{g_0(A_i|W_i)} \leq trunc, \tag{4}
\]

due to the fact that \( g_0 \) is a normal density. Thus, by picking small enough values of \( trunc \) and \( shift \), we can define interventions that shift the observed values of \( A_i \) by \( shift \), for observations that satisfy the inequality 3. By defining our intervention \( g^\ast \) in this manner we thus avoid interventions that result in large values of \( (g^\ast/g_0)(A_i|W_i) \), which reduces the risk of violating the positivity assumption.

Finally, the binary outcome \( Y_i \) is simulated as dependent on all three of \( i \)'s baseline covariates in \( W_i \), \( i \)'s exposure \( A_i \), as well as the baseline covariate values and exposures of \( i \)'s friends. In particular, we assume that the probability of success for each binary outcome \( Y_i \) is logit-linear function of the summary measures \((W_i^s, A_i^s)\), which are defined as

\[
W_i^s := \left( W_i, \frac{1}{|F_i|} \sum_{j \in F_i} W_j(1), \sum_{j \in F_i} W_j(2), \sum_{j \in F_i} W_j(3) \right) \text{ and } A_i^s := (A_i, \sum_{j \in F_i} A_j).
\]

Our target causal quantity is then defined as the sample-average of \( N \) \( i \)-specific expected counterfactual outcomes \( Y_i^\ast \), under stochastic intervention \( g^\ast \), for \( i = 1, \ldots, N \). These counterfactual outcomes are generated by modifying the observed data-generating distribution, which consists of replacing the structural equation for generating \( N \) observed exposures \( A_i \) with a new structural equation that defines the intervened exposures \( A_i^\ast \), for \( i = 1, \ldots, N \). The outcomes \( Y_i^\ast \), for \( i = 1, \ldots, N \) can then be sampled from such a modified data-generating
distribution. Note that we are using the new notation $Y^*_i$ to denote the fact that the conditional distribution of the observed data $(W_i, A_i, Y_i)$ has been modified by replacing $g_0$ with the intervention $g^*$. We denote this causal quantity as $\psi_0$ and define it as:

$$\psi_0 := E \left( \frac{1}{N} \sum_{i=1}^{N} Y^*_i \right).$$

### 4.1 Specifying the network distribution and the structural equation model for dependent data

As noted, for this simulation the network graph is sampled according to the small-world network model (Watts and Strogatz, 1998). We will use the network generator function "rnet.SmWorld", which is provided by the simcausal package. This function serves as a wrapper for the function sample_smallworld of the igraph R package (Csardi and Nepusz, 2006), which performs the actual sampling of an undirected network graph. The nodes of the graph returned by the sample_smallworld function are treated as individual observations and are indexed as $i = 1, \ldots, N$. An undirected edge between two nodes $i$ and $j$ is interpreted as two directed edges, meaning that unit $j$ is a friend of unit $i$ and vice versa. In terms of our notation, this means that $j \in F_i$ and $i \in F_j$. The resulting network object produced by the igraph package is then converted into its simcausal network representation, where each friend set $F_i$ is determined according to the above described rule. We remind the reader that simcausal represents the network as a matrix with $N$ rows, each row $i$ representing the set of friends $F_i$ (social connections of unit $i$), where each $F_i$ may be padded with extra NAs to make sure all $F_i$ have the same length.

We proceed by first instantiating an empty DAG object, which is assigned to variable “D” below. We will use this DAG object to define the network distribution, as well as to encode the unit-specific distribution of the data. As a next step, we register the network generator function (rnet.SmWorld), making it a part of the object D. This will allow us to: (a) generate a specific network, and (b) use this network as a way to connect nodes defined within the same DAG object D. Specifically, as we show in the following code snippet, we add a network to the object D by using syntax “D <- network()”. The name of the network generator is passed on to the network() call with an argument “netfun”. The network() call also requires a “name” argument (first argument), which specifies a name of a particular network. The function network allows passing any number of additional arguments, which will be passed to the underlying network generator function (e.g., arguments dim, nei and p in the example below). These additional arguments allow the user to further parametrize the distribution of the network graph.

```r
D <- DAG.empty()
D <- D + network("Net", netfun = "rnet.SmWorld", dim = 1, nei = 3, p = 0.3)
```

Next, we define a 3-dimensional IID covariate $W = (W(1), W(2), W(3))$, where $W(1)$ is a categorical node “W1”, $W(2)$ is a binary node “W2” and $W(3)$ is a binary node “W3”, as shown below:

```r
D <- D +
    node("W1", distr = "rcat.b0", probs = c(0.0494, 0.1823, 0.2806, 0.2680, 0.1651, 0.0546)) +
    node("W2", distr = "rbern", prob = plogis(-0.2 + W1/3)) +
    node("W3", distr = "rbern", prob = 0.6)
```

In our next step, we define the conditional distribution of a continuous exposure $A_i$ (node “A.obs”), which is sampled as normal, with its mean given by a linear combination of $W_i(2)$ and $W_i(3)$ (nodes “W2” and “W3”) and the standard deviation of 1. The following example also defines another node named “A”, which is set equal to A.obs. The node A plays no role in the definition of our observed data generating process. However, it will be utilized when we define our intervention $g^*$ in Section 4.3. By intervening on A, instead of A.obs, we will be able to define an intervention that is itself a function of the observed exposure values stored in A.obs.

---

3The actual value of the name argument of network() function becomes only relevant when the user wants to either over-write the existing network or define several different networks within the same DAG object.
D <- D +
node("A.obs", distr = "rnorm", mean = 0.58 * W2 + 0.33 * W3, sd = 1)+
node("A", distr = "rconst", const = A.obs)

Finally, for each unit $i = 1, \ldots, N$, we model the conditional probability of success for the binary outcome $Y_i$ (node “Y”) as a logit-linear function of the earlier described summary measures $(W^*_i, A^*_i)$. These summaries include $(W_i, A_i)$, as well as the covariate summaries of units in $F_i$ (i.e., variables measured on friends of unit $i$). In more detail, for each unit $i$, these network summaries include the average of $W_j(1)$ and the sum of the exposures $A_j$ among all units $j$ that are friends with $i$ (i.e., $j \in F_i$).

D <- D +
node("Y", distr = "rbern",
prob = plogis(5 + -0.5*W1 - 0.58*W2 - 0.33*W3 +
-1.5*ifelse(nF > 0, sum(W1[[1:Kmax]])/nF, 0) +
-1.4*sum(W2[[1:Kmax]]) + 2.1*sum(W3[[1:Kmax]]) +
+0.35*A + 0.15*sum(A[[1:Kmax]])
),
replaceNAw0 = TRUE)
Dset <- set.DAG(D, n.test = 200)

Note that the above object Dset has saved the described data-generating distribution, which includes the definition of the network and that of unit-specific data. In other words, Dset object saves all the information that is needed in order to be able to simulate: (1) the network graph on $N$ units, and (2) the observations $(W_i, A_i, Y_i)$, for $i = 1, \ldots, N$. Also note that such unit-specific data may or may not be dependent (i.e., it may or may not use the network structure), depending on a particular SEM parameterization selected by the user.

4.2 Simulating network and observed data

In our next code example we simulate the observed data on $N$ units from the distribution specified in the above object Dset. This is accomplished by calling the function sim, where the total number of units $N$ is specified with the argument n. This example saves the resulting data frame with observations $(W_i, A_i, Y_i)$, for $i = 1, \ldots, N$, as an object named “datO”. The network matrix and the vector counting the number of friends for each unit are saved as objects named “NetInd_mat” and “nF”, respectively.

nsamp <- 100
datO <- sim(Dset, n = nsamp, rndseed = 54321)
NetInd_mat <- attributes(datO)$netind_cl$NetInd
nF <- attributes(datO)$netind_cl$nF

The plot.igraph function in igraph package can be used for visualizing such simulated network. However, the network ID matrix NetInd_mat needs to be first converted back into its original igraph object representation (g), as we show below.

library("igraph")
g <- sparseAdjMat.to.igraph(NetInd.to.sparseAdjMat(NetInd_mat, nF = nF))

We can now apply the plot.igraph function of the igraph package to visualize the simulated network structure stored in the object g, as shown in Figure 2.
4.3 Defining interventions, simulating counterfactual data and evaluating the true value of the causal quantity

Our next goal is to evaluate the true value of the causal parameter $\psi_0$ under intervention $g^*$ via Monte-Carlo simulation that samples from the distribution of the counterfactual outcomes $Y_i^*$, for $i = 1, \ldots, N$. This process consists of two stages. First, as we show in the following code snippet, the intervention of interest is defined by modifying some of the nodes of the observed data-generating distribution. This is accomplished by calling the function `action` and adding the result of this call to the previously defined DAG object `Dset`. The resulting modified structural equation model defines the distribution of the counterfactual data, which includes the counterfactual outcome. Importantly, each action-specific counterfactual distribution is saved within the same object, along with the observed data generating distribution, allowing the user to define any number of such interventions. Below we define an intervention named “$g_{\text{star}}$” by providing a new definition of the exposure node $A$. This intervention is defined according to our previously described stochastic intervention $g^*$, using the assignment criteria in equation 3. Note that the definition of $g^*$ requires the input of the observed unit-specific exposures, and in our current example these exposure values were defined in node $A_{\text{obs}}$.

```r
Dset <- Dset +
  action("gstar",
    nodes = node("A", distr = "rconst",
      const = ifelse(A.obs - (0.58*W2 + 0.33*W3) > (log(trunc)/shift + shift/2),
        A.obs,
        A.obs + shift)),
    trunc = 1, shift = 0.3)
```
Second, we perform Monte-Carlo simulation by sampling from this newly defined counterfactual distribution defined by action $g_{star}$ and generate the counterfactual data, as shown in the following code example. We do this by calling the function `sim` and specifying the name of the previously defined action with an argument actions. That is, the procedure in `sim` first samples the network of size $N = 500$, proceeded by sampling of the counterfactual data. Note that our target causal quantity $\psi_0$ is defined conditionally on the network sample size $N$, namely, as an average of $N$ expected counterfactual outcomes. This implies that the true value of $\psi_0$ is allowed to change as the network’s sample size changes. Therefore, in the following evaluation of $\psi_0$ we use fixed sample size ($N = 500$), which allows us to obtain Monte-Carlo estimates of true causal quantity $\psi_0 := E[1/N \sum_{i=1}^{N} Y_i^*]$. In particular, a single Monte-Carlo simulation step consists of sampling $N$ counterfactual outcomes $Y_i^*$ and then taking the empirical mean of these outcomes over 500 observations, thus yielding a single estimate of $\psi_0$. By taking the mean over 10,000 of such Monte-Carlo estimates we can obtain a very close approximation of $\psi_0$. This causal parameter now defines our gold standard: the quantity which we may use for evaluating and comparing the performance of different statistical methods. One possible application of such causal parameters is exhibited in the following section.

```r
require("doParallel")
registerDoParallel(cores = detectCores())
networksize <- 500
nsims_psi0 <- 10000
psi0_reps <- foreach(i.sim = seq(nsims_psi0), .combine = "c") %dopar% {
  dat_gstar <- sim(Dset, actions="gstar", n = networksize)[["gstar"]]
  psi0 <- mean(dat_gstar[["Y"]])
}
psi0 <- mean(psi0_reps)
print(psi0)
## [1] 0.743815
```

### 4.4 Case study: comparing performance of dependent-data estimators

We describe one possible application for the `simcausal` package by conducting a simulation study that compares the performance of the three dependent-data estimators implemented in `tmlenet` R package (Sofrygin and van der Laan, 2015). The data is simulated according to the above described data generating distribution. The estimation procedures implemented in `tmlenet` have been previously described in Sofrygin and van der Laan (2016). In particular, `tmlenet` package implements three dependent-data estimators: Target Maximum Likelihood Estimator (TMLE), the Inverse Probability Weighted Estimator (IPW) and the G-computation substitution estimator (GCOMP). Our intervention of interest and the corresponding target causal quantity were introduced in the previous section. We will now use this target causal quantity as our gold standard, namely, it is the quantity that will generally remain known in a real data-generating process. Our simulation study hence uses this gold standard as a mean of comparing the finite sample performance of these three dependent-data estimators over iterated samples of hypothetical observed data. For additional details on these estimators we refer to (Sofrygin and van der Laan, 2016).

As our first step, we simulate the observed data, as shown below, for 500 units.

```r
datO <- sim(Dset, n = 500)
net_obj <- attributes(datO)[["netind_cl"]]
NetInd_mat <- net_obj[["NetInd"]]
nF <- net_obj[["nF"]]
Kmax <- net_obj[["Kmax"]]
```

As our next step, we define the input parameters for the `tmlenet()` estimation function, as shown in the following code snippets. In particular, we define the observed-data baseline summary measures $W_i^*$ by calling
the `tmlenet` function “`def_sW`”, as shown below. We also define the exposure summary measures $A_s^i$ by calling the `tmlenet` function “`def_sA`”, as shown below. The summary measures defined by `def_sW` and `def_sA` will be utilized by `tmlenet` for constructing estimators of $\psi_0$. Note that the functions `def_sW` and `def_sA` use syntax that is nearly identical to the previously described `simcausal` syntax for specifying the same network-based summaries.

```r
require("tmlenet")
def.sW <- def_sW(W1, W2, W3) +
def.sW(meanW1 = ifelse(nF > 0, sum(W1[[1:Kmax]])/nF, 0), replaceNAw0 = TRUE) +
def.sW(sumW2 = sum(W2[[1:Kmax]]), replaceNAw0 = TRUE) +
def.sW(sumW3 = sum(W3[[1:Kmax]]), replaceNAw0 = TRUE)
def.sA <- def_sA(A, sumA = sum(A[[1:Kmax]]), replaceNAw0 = TRUE)
```

In the following example we define the intervention of interest by calling the `tmlenet` function “`def_new_sA`”.

```r
trunct <- 1; shift <- 0.5
newA.gstar <- def_new_sA(A = ifelse(A - (0.58*W2 + 0.33*W3) > (log(trunct)/shift + shift/2), A, A + shift))
```

In our following example we define the regression formulas, where the regression defined by the variable “`Qform`” is used for modeling the conditional outcome $Y_i$ given the previously defined summary measures $(W_s^i, A_s^i)$ and the regression in “`hform`” is used for modeling the conditional probabilities of the observed exposure summaries $A_s^i$ given the observed baseline summaries $W_s^i$, namely, `hform` describes the model for $P(A_s^i | W_s^i)$. We also call `tmlenet_options` to specify additional tuning parameters for the `tmlenet`. In particular, we specify the parameter “`bin.method`”, which defines the method for discretizing continuous variables in $A_s^i$ (those variables are detected automatically by `tmlenet`). Furthermore, we specify the parameter “`maxNperBin`”, which defines the maximum number of bins (cutoff intervals) when performing such discretization (see `?tmlenet_options` for additional details and for other optional tuning parameters available in `tmlenet`).

```r
Qform <- "Y ~ A + sumA + meanW1 + sumW2 + sumW3 + W1 + W2 + W3"
hform <- "A + sumA ~ meanW1 + sumW2 + sumW3 + W1 + W2 + W3"
tmlenet_options(bin.method = "equal.mass", maxNperBin = 50)
```

Finally, we call the estimation routine `tmlenet()`, as shown below, where we pass all of the above-defined variables, including the previously simulated dependent data `datO`, as well as the network matrix `NetInd_mat`. Furthermore, we specify some optional parameters by using the argument `optPars`. In particular, by passing a list with `bootstrap.var = TRUE`, we request that the TMLE inference is performed with parametric bootstrap (along with two standard approaches described below). Finally, the argument `n.bootstrap` controls the number of the parametric bootstrap samples (higher number will lead to more precise bootstrap variance estimates, but will significantly increase the computation time).

```r
res <- tmlenet(data = datO, sW = def.sW, sA = def.sA,
                Kmax = Kmax, NETIDmat = NetInd_mat,
                intervene1.sA = newA.gstar ,
                Qform = Qform, hform.g0 = hform,
                optPars = list(bootstrap.var = TRUE, n.bootstrap = 100))
```

The above function call returns a list containing the estimates of the parameter $\psi_0$, where $\psi_0$ is defined as the sample-average of the expected counterfactual outcomes under the intervention specified in `newA.gstar`. The table of estimates consists of the TMLE, IPW and GCOMP and it can be obtained by running the following code (output not shown):
The `tmlenet` function also returns the corresponding 95% confidence intervals (CIs) for the TMLE and IPW under the list item named "IC.CIs". Note that these CIs are based on the variance estimates of the influence curves that also adjusts for the network-based dependence among the units, as described in Sofrygin and van der Laan (2016). These CIs can be printed by running the following code (output not shown):

```r
res["EY_gstar1"][["IC.CIs"]]
```

Furthermore, an alternative estimate of the 95% CI for the TMLE can be obtained via the parametric bootstrap approach. This approach also estimates the TMLE variance in the presence of network-based dependence among units. However, in small samples the parametric bootstrap can achieve better performance (better nominal coverage), compared to the above described influence curve-based variance estimate of the TMLE. The corresponding CI for the parametric bootstrap is stored under the list item named "boot.CIs" and it can be obtained by running the following code (output not shown):

```r
res["EY_gstar1"][["boot.CIs"]]
```

Finally, one can also obtain the 95% CIs for the TMLE and IPW based on the approach that estimates the variance of corresponding influence curves assuming the observed units are IID. One would expect that such IID-based CIs are going to be overly optimistic (too narrow) when, in fact, the units are dependent. Thus, this approach will generally result in CIs with inadequate coverage, as is also demonstrated by our simulation study below. Finally, these IID-based 95% CIs can be obtained by running the following code (output not shown):

```r
res["EY_gstar1"][["iid.CIs"]]
```

Our simulation study repeated the above described estimation procedure 5,000 times, each time using a newly sampled dataset of 500 network-dependent observations. The corresponding R code for this simulation study can be found in Supplementary Materials. We evaluated the absolute bias, the mean-squared error (MSE) and the variance of the above described three estimators, with results presented in Table 1 (all performance metrics were multiplied by 10). In addition, we evaluated the mean of the TMLE variance estimate based on the parametric bootstrap procedure, along with its corresponding 95% CI, as reported in columns “BOOT.VAR” and “BOOT.CI.cover” of Table 2. We also evaluated the mean of the TMLE variance estimate which adjusted for the dependence among units based on the estimated variance of the efficient influence curve and the coverage of its corresponding 95% CI, as reported in columns “DEP.VAR” and “DEP.CI.cover” in Table 2. Finally, we evaluated the mean of the TMLE variance estimate which completely ignored the network information and assumed units are IID, along with its corresponding 95% CI, as reported in columns “IID.VAR” and “IID.CI.cover” of Table 2. As expected, the IID-based variance estimator resulted in 95% CIs that had inadequate coverage, compared to the coverage probabilities of 0.935 and 0.924 for the parametric bootstrap and the influence curve-based CIs, respectively.

| Estimator | Bias10 | MSE10   | Variance10 |
|-----------|--------|---------|------------|
| TMLE      | 0.0042 | 0.01371 | 0.01372    |
| IPW       | 0.0183 | 0.01724 | 0.01721    |
| GCOMP     | 0.0019 | 0.01278 | 0.01278    |

Table 1: Performance of the three dependent data estimators across 5,000 simulations, each simulation consisted of $N = 500$ network-dependent units. The reported bias, mean squared error (MSE) and variance are multiplied by 10.
Table 2: Monte-Carlo approximated mean of the TMLE variance based on parametric bootstrap ('BOOT.VAR'), dependent data ('DEP.VAR'), TMLE variance estimator for IID data ('IID.VAR'), the coverage of the 95% CI for parametric bootstrap variance ('BOOT.CI.cover'), dependent data variance ('DEP.CI.cover') and IID variance ('IID.CI.cover') estimates across 5,000 simulations, each simulation consisting of \( N = 500 \) network-dependent units.

4.5 Case study: the effect of network dependence on TMLE inference

We also conducted a simulation study where we varied the strength of the effect of the above defined baseline network summaries \( ((1/|F_i|) \sum_{j \in F_i} W_{ij}(1), \sum_{j \in F_i} W_{ij}(2), \sum_{j \in F_i} W_{ij}(3)) \) on the outcome \( Y_i \) of each unit \( i \). In particular, we considered 9 data-generating scenarios, where in each scenario these three network summaries had different coefficient values in the formula that defines the distribution of the node \( Y \). The first simulation (Scenario 1) was based on a data-generating distribution with coefficient values of (-0.5, -0.4, -0.1), thus, resulting in the following definition of node \( Y \):

```r
node("Y", distr = "rbern",
    prob = plogis(5 + -0.5*W1 - 0.58*W2 - 0.33*W3 +
        -0.5*ifelse(nF > 0, sum(W1[[1:Kmax]])/nF, 0) +
        -0.4*sum(W2[[1:Kmax]]) + -0.1*sum(W3[[1:Kmax]]) +
        +0.35*A + 0.15*sum(A[[1:Kmax]])
),
    replaceNAw0 = TRUE)
```

The last simulation (Scenario 9) used the coefficient values of (-1.5, -1.4, 2.1), i.e., the values used in the original definition of node \( Y \), as defined above in Section 4.1. Finally, the simulation scenarios in between (Scenario 2 - Scenario 8) set these coefficient values at equally spaced intervals between those used in Scenario 1 and Scenario 9. Thus, the outcome \( Y_i \) in Scenario 1 could be described as being the least dependent on the baseline covariate values of \( i \)’s friends (baseline network summaries), while the simulations in Scenario 2 to 9 progressively increase the strength of this dependence. We also kept the intervention and the parameter of interest unchanged from the previous simulation. Furthermore, we assessed the effects of varying the strength of this relationship on TMLE inference, as shown in Table 3. As expected, the coverage probability of the IID-based 95% CIs that ignore between-unit dependence (column “IID.CI.cover”) decreases as we continue to increase the dependence of each \( Y_i \) on the baseline covariates of \( i \)’s friends.
### Table 3: The effect of network dependence on inference across 5,000 simulations, each simulation consisting of $N = 500$ dependent units. The results are ordered by increasing strength of network dependence of $Y_i$ on the baseline covariates of $i$’s friends. The first row corresponds with a simulation that has the least dependence, with subsequent rows ordered by the increasing amount of the dependence.

| Scenarios | sims     | BOOT.VAR | DEP.VAR | IID.VAR | BOOT.CL.cover | DEP.CL.cover | IID.CL.cover |
|-----------|----------|----------|---------|---------|--------------|--------------|--------------|
| Scenario 1 | 0.000954 | 0.000858 | 0.000689 | 0.934   | 0.901        | 0.878        |
| Scenario 2 | 0.000706 | 0.000642 | 0.000503 | 0.930   | 0.894        | 0.875        |
| Scenario 3 | 0.000773 | 0.000703 | 0.000499 | 0.936   | 0.909        | 0.866        |
| Scenario 4 | 0.000660 | 0.000548 | 0.000370 | 0.938   | 0.911        | 0.859        |
| Scenario 5 | 0.000682 | 0.000626 | 0.000387 | 0.935   | 0.913        | 0.844        |
| Scenario 6 | 0.000767 | 0.000712 | 0.000402 | 0.939   | 0.916        | 0.827        |
| Scenario 7 | 0.000750 | 0.000694 | 0.000367 | 0.937   | 0.913        | 0.814        |
| Scenario 8 | 0.001231 | 0.001152 | 0.000498 | 0.935   | 0.924        | 0.769        |
| Scenario 9 | 0.001353 | 0.001275 | 0.000508 | 0.938   | 0.925        | 0.747        |

#### 5 Discussion

We described how the **simcausal** R package can facilitate the conduct of network-based simulation studies in causal inference research, specifically allowing one to model data with known network and known functional form of dependence among units. We also described how the package can be used for simulations with longitudinal data structures. We described how the **simcausal** R package allows creating a wide range of artificial datasets often encountered in public health applications of causal inference methods. In particular, this includes simulations of causal mechanisms of interference or spillover. To simplify the specification of such models we implemented a novel R syntax which allows for a concise and intuitive expression of complex functional dependencies for a large number of nodes. We also demonstrated how this syntax can be used for simplifying the specification and simulation of complex network-based summaries of the data. Moreover, we argued that such complex simulations are often necessary when one tries to conduct a realistic simulation study that attempts to replicate a large variety of scenarios one might expect to see from a true data-generating process. We also note that our package can work in conjunction with other network simulation tools, as we demonstrated with the example of the **igraph** R package that was used to sample the actual networks. In addition, the **simcausal** package allows the user to specify and simulate counterfactual data under various interventions (e.g., static, dynamic, deterministic, or stochastic). These interventions may represent exposures to treatment regimens, the occurrence or non-occurrence of right-censoring events, or of specific monitoring events. These simulations provide practical settings with the types of data generating distributions which might be used for validation, testing and comparison of statistical methods for causal inference. To the best of our knowledge there are no other tools which implement the specific type of functionality afforded by the network-based syntax that is implemented in **simcausal** and is described in this article.

One of the distinguishing features of **simcausal** is that it allows the user to define and compute various causal target parameters, such as, the treatment-specific counterfactual mean, that can then serve as the model-free gold standard. That is, the causal parameter is always the same functional of the counterfactual data distribution, regardless of the user-selected parameterization of the structural equation model. For example, the gold standard defined in this manner provides an objective measure of bias that does not depend on the modeling assumptions of a specific statistical method. Coupled with a wide variety of possible data generating distributions that may be specified in **simcausal**, this package provides statisticians with a powerful tool for testing the validity and accuracy of various statistical methods. For example, one may use our package for validating an implementation of a novel statistical method, using the simulated data with the known truth (the true value of the causal parameter), prior to applying such an algorithm to real data, in which this truth is unknown. As another example, one may use **simcausal** to simulate data from a variety of data-generating distributions and conduct a simulation study comparing the properties of different methods.
statistical procedures (e.g., bias, mean-squared error (MSE), asymptotic confidence interval coverage) against the user-selected causal parameter. We emphasize that the main purpose of our package is not to assess the impact of real-life interventions, but rather to test the validity and performance of statistical methods, which can then be applied to real datasets. Moreover, we demonstrated that the simcausal R package is a flexible tool that enables easier communication of assumptions between various practitioners and thus helps improve the transparency about the assumptions of different statistical methods.

We also note that the implementation of additional features in future releases of the simcausal package should further expand its utility for methods research. Among such possible improvements is to allow interventions on the network structure and provide a unified interface for changes to friend structure as part of the intervention. Future work will also focus on modeling the changes in network structure over time, for example, by providing an interface for specifying a time-varying analogs of the network function, modeling the probability of forming a new tie or removing a certain friend over time and allowing one to sample new networks conditional on the previously sampled networks.

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