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ergm 4: New Features for Analyzing Exponential-Family Random Graph Models

Pavel N. Krivitsky © University of New South Wales David R. Hunter ^(D) Penn State University

Martina Morris ⁽¹⁾ University of Washington Chad Klumb University of Washington

Abstract

The **ergm** package supports the statistical analysis and simulation of network data. It anchors the **statnet** suite of packages for network analysis in R introduced in a special issue in *Journal of Statistical Software* in 2008. This article provides an overview of the new functionality in the 2021 release of **ergm** version 4. These include more flexible handling of nodal covariates, term operators that extend and simplify model specification, new models for networks with valued edges, improved handling of constraints on the sample space of networks, and estimation with missing edge data. We also identify the new packages in the **statnet** suite that extend **ergm**'s functionality to other network data types and structural features and the robust set of online resources that support the **statnet** development process and applications.

Keywords: statnet, ERGM, exponential-family random graph models, valued networks.

1. Introduction

The statnet suite of packages for R (R Core Team 2022) was first introduced in 2008, in volume 24 of *Journal of Statistical Software*, a special issue devoted to statnet. Together, these packages, which had already gone through the maturing process of multiple releases, provided an integrated framework for the statistical analysis of network data: from data storage and manipulation, to visualization, estimation and simulation. Since that time the existing packages have undergone continual updates to improve and add capabilities, and many new packages have been added to extend the range of network data that can be modeled (e.g., dynamic, valued, sampled, multilevel). It is the ergm package, however, that provides

the statistical foundation for all of the other modeling packages in the **statnet** suite. Version 4 of **ergm**, released in 2021, is a major upgrade, representing more than a decade of changes and improvements since Hunter, Handcock, Butts, Goodreau, and Morris (2008b). This article describes many of the myriad new features available in **ergm** for more flexibly describing and analyzing exponential-family random graph models. It is a companion to Krivitsky, Hunter, Morris, and Klumb (2022), which discusses additional features and computational improvements in **ergm** version 4.

The exponential-family random graph model (ERGM) is a general statistical framework for modeling the probability of a link (or tie) between nodes in a network. It is implemented by the **ergm** package and most of its related packages in the **statnet** suite. We consider networks over a set of nodes $N = \{1, 2, ..., n\}$. If $\mathbb{Y} \subseteq N \times N$ denotes a set of potential pairwise relationships among them, in the case of a binary network the sample space \mathcal{Y} of all allowable networks can be regarded as a subset of the power set $2^{\mathbb{Y}}$ of potential relationships. More generally, if S is a (possibly multivariate) set of possible relationship values, the sample space $\mathcal{Y} \subseteq \mathbb{S}^{\mathbb{Y}}$ is a set whose elements are of the form $\{Y_{i,j} : (i,j) \in \mathbb{Y}\}$, where each $Y_{i,j}$, which we will call a dyad, maps the node pair $(i, j) \in \mathbb{Y}$ into S and denotes the value of the relationship of $(i, j) \in \mathbb{Y}$.

We begin by briefly presenting the fully general ERGM framework, referring interested readers to Schweinberger, Krivitsky, Butts, and Stewart (2020) for additional technical details. A random network **Y** is distributed according to an ERGM, written $\mathbf{Y} \sim \text{ERGM}_{\mathcal{Y},h,\boldsymbol{\eta},\mathbf{g}}(\boldsymbol{\theta})$, if

$$\mathsf{P}_{\boldsymbol{\theta},\mathcal{Y},h,\boldsymbol{\eta},\mathbf{g}}(\mathbf{Y}=\mathbf{y}) = \frac{h(\mathbf{y})\exp\{\boldsymbol{\eta}(\boldsymbol{\theta})^{\top}\mathbf{g}(\mathbf{y})\}}{\kappa_{h,\boldsymbol{\eta},\mathbf{g}}(\boldsymbol{\theta},\mathcal{Y})}, \ \mathbf{y}\in\mathcal{Y}.$$
 (1)

In (1), $\boldsymbol{\theta}$ is a *q*-dimensional parameter vector and $\boldsymbol{\eta}$ is a mapping from $\boldsymbol{\theta}$ to the *p*-vector of canonical parameters. In many cases we simply have $\boldsymbol{\eta}(\boldsymbol{\theta}) = \boldsymbol{\theta}$, an exception being when our model is curved (Hunter and Handcock 2006). The factor $h(\mathbf{y})$ is a reference measure, which is typically a constant and thus ignorable in the case of binary ERGMs. The value $\kappa_{h,\boldsymbol{\eta},\mathbf{g}}(\boldsymbol{\theta},\boldsymbol{\mathcal{Y}})$ ensures that (1) defines a legitimate probability mass function, which implies $\sum_{\mathbf{y}'\in\boldsymbol{\mathcal{Y}}} h(\mathbf{y}') \exp\{\boldsymbol{\eta}(\boldsymbol{\theta})^{\top} \mathbf{g}(\mathbf{y}')\}.$

Many of the features of **ergm** and the related packages that comprise the **statnet** suite address the statistical complications that arise from modeling network data using special cases of the ERGM in (1). For instance, the statistical framework implemented in **ergm** is computationally intensive for models that specify dyadic dependence, when $P_{\theta,\mathcal{Y},h,\eta,\mathbf{g}}(\mathbf{Y} = \mathbf{y})$ cannot be decomposed into a product of simple functions of $y_{i,j}$. In this case, the package relies on a central Markov chain Monte Carlo (MCMC) algorithm for estimation and simulation, along with maximum pseudo-likelihood estimation, contrastive divergence, and simulated annealing (SAN) in some contexts. Substantial improvements have been made to all of these algorithms, producing efficiency and speed gains of up to several orders of magnitude (Krivitsky *et al.* 2022). This article describes the most important new capabilities that have been added to **ergm** and its related packages since volume 24 of *Journal of Statistical Software* appeared in 2008. This includes both the capabilities introduced in the version 4 release itself and in releases 2.2.0–3.10.4, which postdate the *Journal of Statistical Software* volume. Versions in which each new capability was introduced can be obtained by running **news(package =** "**ergm**").

In the examples throughout the article, we assume the reader is familiar with the basic syntax and features of **ergm** included in the 2008 *Journal of Statistical Software* volume. In some The source code for the latest version of the **ergm** package (Handcock, Hunter, Butts, Goodreau, Krivitsky, and Morris 2023), along with the LICENSE information under GPL-3, is available at https://github.com/statnet/ergm. The package is also available from the Comprehensive R Archive Network (CRAN) at https://CRAN.R-project.org/package= ergm. We have included ergm 4.4.0 with this manuscript, which uses Sweave along with the knitr package (Xie 2022).

2. Extension packages in the statuet suite

The statistical models supported by the **statnet** suite have been extended by a growing number of new packages that provide additional functionality in the general ERGM framework. While the focus of this article is the base **ergm** package, in this section we provide a brief overview of the extension packages and their specific applications. Open source package development is on GitHub, accessible at https://statnet.org/. Online tutorials, found at https://statnet. org/workshops/, exist for **ergm** and many of these extension packages, and most packages also include extended vignettes. Some of the key extension packages, and the resources that support them, include:

- Building custom terms for models: One of the unique aspects of this modeling framework is that each network statistic in an ERGM requires a specialized algorithm for computing the value of the statistic from the data. The ergm package has over 150 of the most common terms encoded – see vignette("ergm-term-crossRef") or help("ergmTerm") for the full list – but the existing terms are a small subset of the possible terms one can use in an ERGM. For those who need a custom term, the package ergm.userterms (Hunter, Goodreau, and Handcock 2013) is designed to simplify the process of coding up new terms for use in ERG model specification. Online workshop materials provide an overview of the process, and demonstrate the use of this package (Hunter and Goodreau 2019).
- Modeling temporal (dynamic) network data: The statnet suite (Handcock, Hunter, Butts, Goodreau, and Morris 2008) contains several packages that provide a robust framework for storing, visualizing, describing and modeling temporal network data: The networkDynamic (Butts, Leslie-Cook, Krivitsky, and Bender-deMoll 2022) package extends network (Butts 2008a) to provide data storage and management utilities, the tsna package (Bender-deMoll and Morris 2021) extends sna (Butts 2008b) to provide descriptive statistics for network objects that change over time, the ndtv package (Bender-deMoll 2022) provides a wide range of utilities for visualizing dynamic networks and saving both static and animated output in standard formats, and tergm (Krivitsky and Handcock 2022b) extends ergm to fit the class of separable temporal ERGMs, from both sampled and fully observed network data (Krivitsky and Handcock 2014). There are two online workshops that demonstrate these tools: one that demonstrates a typical workflow from data inspection to temporal modeling (Morris and Krivitsky 2015), and another that focuses on descriptive analyses and visualization (Bender-deMoll 2016).

- Modeling valued edges: The ergm package itself contains a framework for modeling realvalued edges (see Section 6 and Section 4). Other packages provide specialized components for specific types of valued edges: ergm.count for counts (Krivitsky 2022a) and ergm.rank for ordered categories (Krivitsky 2022d). The relevant theory supporting these packages may be found in Krivitsky (2012) and Krivitsky and Butts (2017), respectively. latentnet for latent space models (Krivitsky and Handcock 2022a) also supports non-binary responses, although in a somewhat different manner (Krivitsky and Handcock 2008; Krivitsky, Handcock, Raftery, and Hoff 2009). Package vignettes and online workshop materials provide an overview of the theory, and demonstrate the use of these packages (Krivitsky and Butts 2019).
- Working with egocentrically sampled network data: In the social and health sciences, egocentrically sampled network data is the most common form of data available, because it can be collected using standard sample survey methods. The **ergm.ego** package (Krivitsky 2022b) provides methods for estimating ERGMs from egocentrically sampled network data, with a principled framework for statistical inference. The theory and an application of these methods may be found in Krivitsky and Morris (2017). Online workshop materials provide an overview of the framework and demonstrate the use of the package (Morris and Krivitsky 2019).
- Multimode, multilayer, and multilevel networks: In the social sciences, it is increasingly common to collect and fit ERGMs on data on multiple relationship types (Wang 2012; Krivitsky, Koehly, and Marcum 2020) and ensembles of networks (Slaughter and Koehly 2016). These capabilities are implemented in an extension package **ergm.multi** (Krivitsky 2022c).
- Modeling diffusion and epidemics on networks: One of the most active application areas for ERGMs and TERGMs (temporal exponential-family random graph models) is in the field of epidemic modeling. The **EpiModel** package (Jenness, Goodreau, and Morris 2018) is built on the **statnet** platform, and provides a unique set of tools for statistically principled modeling of epidemics on networks. A robust set of online training materials is available at the **EpiModel** website (https://www.epimodel.org/).

3. Enhanced handling of nodal covariates

Version 4 of **ergm** standardizes and provides greater flexibility for handling covariates used by terms in an ERGM. In particular, these covariates can be modified "on-the-fly" during model specification. A vignette called **nodal_attributes** is included in the package and illustrates some of the new capabilities.

Here, we describe some of these enhancements using **ergm**'s faux.mesa.high dataset, a simulated in-school friendship network based on data collected on 205 students. We will focus on the Grade attribute, an ordinal categorical variable with values 7 through 12 that can be accessed via the %v% operator:

```
R> data("faux.mesa.high", package = "ergm")
R> (faux.mesa.high %v% "Grade")[1:20]
[1] 7 7 11 8 10 10 8 11 9 9 9 11 9 11 8 10 10 7 10 7
```

Grade level is typical of the kind of covariate used to model selective mixing in social networks: different hypotheses lead to different model specifications. **ergm** 4 provides greater flexibility than earlier versions of **ergm** to easily define and explore different specifications.

We will sometimes call summary() and other times call ergm() to demonstrate the functionality and output below.

3.1. Transformations of covariates

It is sometimes desirable to specify a transformation of a nodal attribute as a covariate in a model term. Most ergm terms now support a new user interface, inspired by purrr (Henry and Wickham 2020), to specify transformations on one or more nodal attributes. Terms typically use this new interface via arguments called attr, attrs, by, or on; the interpretation of the argument depends on its type:

Character string: Extract the vertex attribute with this name.

- Character vector of length greater than 1: Extract the vertex attributes and paste them together, separated by dots if the term expects categorical attributes and (typically) combine into a covariate matrix if it expects quantitative attributes.
- *Function*: The function is called on the network on the left-hand side of the main ergm formula and is expected to return a vector or matrix of appropriate dimension. Shorter vectors and matrix columns will be recycled as needed.
- *Formula*: Borrowing the interface from **tidyverse** (Wickham *et al.* 2019), the expression on the right hand side of the formula is evaluated in an environment of the vertex attributes of the network, expected to return a vector or matrix of appropriate dimension. Shorter vectors and matrix columns will be recycled as needed. Within this expression, the network itself is accessible as either . or .nw.
- 'AsIs' object created by I(): Use as is, checking only for correct length and type, with optional attribute "name" providing the predictor's name.

For instance, here are three ways – as a string, formula, and function, respectively – to compute the value of

$$g(\mathbf{y}) = \sum_{(i,j) \in \mathbb{Y}} y_{i,j} (\operatorname{Grade}_i + \operatorname{Grade}_j),$$

which in an ERGM may be interpreted as the linear effect of grade on overall activity of an actor:

> nodecov.Grade nodecov.nw%v%"Grade" 3491 3491 3491

Here is a more complicated formula-based use of nodecov that defines the statistic to be

$$g(\mathbf{y}) = \sum_{(i,j)\in\mathbb{Y}} y_{i,j} \left(\frac{|\operatorname{Grade}_i - \overline{\operatorname{Grade}}|}{n} + \frac{|\operatorname{Grade}_j - \overline{\operatorname{Grade}}|}{n} \right),$$
(2)

where n is the number of nodes, i.e., the **network.size**, of the network:

```
R> summary(faux.mesa.high ~ nodecov(~ abs(Grade - mean(Grade)) /
     network.size(.)))
nodecov.abs(Grade-mean(Grade))/network.size(.)
                                      2.856514
```

Removing the absolute values from (2) gives a different result:

```
R> summary(faux.mesa.high ~ nodecov(~ (Grade - mean(Grade)) /
+
    network.size(.)))
```

```
nodecov.(Grade-mean(Grade))/network.size(.)
                                  -0.2637716
```

The non-zero output of the statistic above may be counterintuitive at first. The value of mean(Grade) is indeed equal to the mean of the faux.mesa.high %v% "Grade" vector, or 8.7317073, as we might expect. Yet for a given node *i*, the network statistic sums the value of $(\text{Grade}_i - \overline{\text{Grade}})$ not once, but rather degree(i), times, giving in a non-zero result.

Taking advantage of **nodecov**'s new ability to take matrix-valued arguments, we might also evaluate a polynomial effect of Grade, as in the following quadratic example:¹

Pr(|z|)

```
R> coef(summary(ergm(faux.mesa.high ~ edges +
     nodecov(~ cbind(Grade, Grade2 = Grade^2)))))
                 Estimate Std. Error MCMC %
                                              z value
odaoa
                8 7007063 3 508805/3
                                             2 173867 0 0133650313
```

euges	0.1291903	3.02000040	0	2.4/300/	0.0133039343
nodecov.Grade	-1.4597723	0.39614405	0	-3.684953	0.0002287445
nodecov.Grade2	0.0768836	0.02154632	0	3.568294	0.0003593133

In the code above, the column for Grade² is explicitly named Grade² whereas the row for Grade is named implicitly by R itself. Omitting the name for a row not otherwise named by R would result in a warning, as it is good practice to name all variables in the model.

Alternatively, we can use stats::poly for orthogonal polynomials. Here, the test for significance of the quadratic term is identical to the non-orthogonal example, up to rounding error (though the estimate is different given the orthogonal specification):

```
R> coef(summary(ergm(faux.mesa.high ~ edges + nodecov(~ poly(Grade, 2)))))
```

	Estimate	Std.	Error	MCMC	%	z value	Pr(> z)
edges	-4.662459	0.073	309281		0	-63.788207	0.0000000000
<pre>nodecov.poly(Grade,2).1</pre>	-1.207241	0.680	018706		0	-1.774866	0.0759199607
<pre>nodecov.poly(Grade,2).2</pre>	2.512615	0.704	16949		0	3.568196	0.0003594477

¹For this and other summaries, we omit the call information, deviances, and significance stars in the interests of space. The full summary information can be obtained by omitting **coef()** around the **summary()** call.

We can even pass a nodal covariate that is not already contained in the network object. This example randomly generates a binary-valued nodal covariate and sets its **name** attribute to be used as a label:

```
R> set.seed(123)
R> randomcov <- structure(rbinom(network.size(faux.mesa.high), 1, 0.5),
+     name = "random")
R> summary(faux.mesa.high ~ nodefactor(I(randomcov)))
nodefactor.random.1
199
```

This syntax therefore allows for simulation or estimation of models with inputs taken from arbitrary R functions or data sources, facilitating the incorporation of ERGMs into more general tool chains.

3.2. Coding categorical attributes

For model terms that use categorical attributes, **ergm** 4 has extended the methods for selecting and/or transforming levels via the use of the argument levels. Some terms, such as the **sender** and **receiver** statistics of the p_1 model (Holland and Leinhardt 1981) and the corresponding **sociality** statistics for undirected networks, treat the node labels themselves as a categorical attribute. These terms use the **nodes** argument, rather than the **levels** argument, to select a subset of the nodes.

Typically, levels or nodes has a default that is sensible for the term in question. (Information about the defaults of a term [name] may be obtained by typing help("[name]-ergmTerm") or ergmTerm?[name].) Interpretation of the possible values of the levels and nodes arguments is available by typing help(nodal_attributes). This interpretation is summarized as follows:

'AsIs' object created by I(): Use the given level, list of levels, or vector of levels as is.

Numeric or logical vector: Used for indexing of a list of all possible levels (typically, unique values of the attribute) in default order (typically lexicographic). Logical values are recycled to the length of the vector indexed. In particular, levels = TRUE retains all levels. Negative values exclude. To specify numeric or logical levels literally, wrap them in I().

NULL: Retain all possible levels; usually equivalent to passing TRUE.

Character vector: Use the given level(s) as is.

- Function: The function is called in an environment in which the network itself is accessible as .nw, the list of unique values of the attribute as . or as .levels, and the attribute vector itself as .attr. Its return value is interpreted as above.
- Formula: The expression on the right hand side of the formula is evaluated in an environment in which the network itself is accessible as .nw, the list of unique values of the attribute as . or as .levels, and the attribute vector itself as .attr. Its return value is interpreted as above.

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 - Predefined function: For convenience, a number of useful functions have been predefined. LARGEST, which refers to the most frequent category, so, say, to set such a category as the baseline, pass levels = -LARGEST. LARGEST(n) will refer to the n largest categories. SMALLEST works analogously, and ties in frequencies are broken arbitrarily.

Returning to the faux.mesa.high example, we may treat Grade as a categorical variable even though its values are numeric. We see that Grade has six levels, numbered from 7 to 12:

R> table(faux.mesa.high %v% "Grade")

7 8 9 10 11 12 62 40 42 25 24 12

We may exclude the three smallest levels or, equivalently, include levels 7, 8, and 9. Below are five of the myriad ways to do this in the context of computing basic categorical effects on node activity, implemented by nodefactor. In the second expression, I() is necessary so that 7:9 is not treated as a vector of indices.

```
R> summary(faux.mesa.high ~ nodefactor(~ Grade, levels = -SMALLEST(3)))
nodefactor.Grade.7 nodefactor.Grade.8 nodefactor.Grade.9
                                                       65
               153
                                   75
R> summary(faux.mesa.high ~ nodefactor(~ Grade, levels = I(7:9)))
nodefactor.Grade.7 nodefactor.Grade.8 nodefactor.Grade.9
               153
                                   75
                                                       65
R> summary(faux.mesa.high ~ nodefactor(~ Grade,
     levels = c("7", "8", "9")))
nodefactor.Grade.7 nodefactor.Grade.8 nodefactor.Grade.9
               153
                                   75
                                                       65
R> summary(faux.mesa.high ~ nodefactor("Grade",
     levels = function(a) a %in% 7:9))
+
nodefactor.Grade.7 nodefactor.Grade.8 nodefactor.Grade.9
               153
                                   75
                                                       65
R> summary(faux.mesa.high ~ nodefactor("Grade", levels = ~. %in% 7:9))
nodefactor.Grade.7 nodefactor.Grade.8 nodefactor.Grade.9
               153
                                   75
                                                       65
```

Any of the arguments of Section 3.1 may also be wrapped in COLLAPSE_SMALLEST(attr, n, into), a convenience function that will transform the attribute by collapsing the n least frequent categories into one, naming it according to the into argument where into must be of the same type (numeric, character, etc.) as the vertex attribute in question. Consider the Race factor of the faux.mesa.high network, where we use levels = TRUE to display all levels since the default is levels = -1:

1

Because the Hisp and NatAm categories are so much larger than the other three categories in this network, we may wish to combine the Black, White, and Other categories. The code below accomplishes this using COLLAPSE_SMALLEST while also demonstrating how to use the pipe function, %>%, from the magrittr package (Bache and Wickham 2022) for improved readability:

45

```
R> library("magrittr")
R> summary(faux.mesa.high ~ nodefactor((~ Race) %>%
+ COLLAPSE_SMALLEST(3, "BWO"), levels = TRUE))
nodefactor.Race.BWO nodefactor.Race.Hisp nodefactor.Race.NatAm
72 178 156
```

3.3. Mixing matrices

Mixing matrices, which refer to the cross-tabulation of all edges by the categorical attributes of the two nodes, are a common feature in models that seek to represent selective mixing. The mm model term, which stands for "mixing matrix", generalizes the familiar nodemix term from the original ergm implementation for this purpose. Like nodemix, mm creates statistics consisting of the cells of a matrix of counts in which the columns and rows correspond to the levels of two categorical nodal covariates. For mm, however, these covariates may or may not be the same, making it more general. We use it here to demonstrate the levels2 argument. Typing help("mm-ergmTerm") or, equivalently, ergmTerm?mm, shows that the binary-network version of the term takes the form mm(attrs, levels = NULL, levels2 = -1). The attrs argument is a two-sided formula where the left and right sides are the rows and columns, respectively, of the mixing matrix; if only a one-sided formula or attribute name is given then the rows and columns are taken to be the same. The optional levels argument can similarly be a one- or two-sided formula, and it specifies the levels of the row and column variables to keep. Finally, the optional levels2 argument may be used to select only a subset of the matrix of statistics resulting from attrs and levels.

Using this functionality, we may specify custom mixing patterns that depend upon attribute values. For instance, if we believe that the break between junior high school (grades 7–9) and

high school (grades 10–12) creates a barrier to friendships across the boundary, we can create an indicator variable $\texttt{Grade} \geq 10$, then compute a mixing matrix on that variable using mm using a single call

```
R> summary(faux.mesa.high ~ mm(~ Grade >= 10))
mm[Grade>=10=FALSE,Grade>=10=TRUE] mm[Grade>=10=TRUE,Grade>=10=TRUE]
27 43
R> summary(faux.mesa.high ~ mm(~ Grade >= 10, levels2 = NULL))
mm[Grade>=10=FALSE,Grade>=10=FALSE] mm[Grade>=10=FALSE,Grade>=10=TRUE]
133 27
mm[Grade>=10=TRUE,Grade>=10=TRUE]
43
```

The Grade >= 10 indicator variable is FALSE (for junior high school) and TRUE (for high school), and with the undirected friendships, this produces three possible combinations of the grade indicator - FALSE/FALSE, FALSE/TRUE, and TRUE/TRUE. For the default specification, levels = NULL keeps all levels of the Grade >= 10 indicator variable and levels2 = -1 eliminates the first statistic (FALSE/FALSE) in the set of 3. For the modified specification, the levels2 = NULL argument keeps all of the statistics.

We can also use the mm formula interface to filter out certain statistics from the full set of potential comparisons. An example from the nodal_attributes vignette within the ergm package using the unmodified Grade attribute defines levels2 as a one-sided formula whose right side is a function that returns TRUE or FALSE, depending on whether both elements of .levels – the list of values taken by a pair of nodes – are in the set c(7, 8). The example therefore captures mixing statistics only involving students in grades 7 or 8:

```
R> summary(faux.mesa.high ~ mm("Grade", levels2 = ~ sapply(.levels,
+ function(pair) pair[[1]] %in% c(7, 8) && pair[[2]] %in% c(7, 8))))
```

```
mm[Grade=7,Grade=7] mm[Grade=7,Grade=8] mm[Grade=8,Grade=8]
75 0 33
```

Here is an equivalent formulation using both levels and levels2 in concert:

```
R> summary(faux.mesa.high ~ mm(~ Grade, levels = TRUE ~ c("7","8"),
+ levels2 = NULL))
```

```
mm[Grade=7,Grade=7] mm[Grade=7,Grade=8] mm[Grade=8,Grade=8]
75 0 33
```

Finally, we give an example using two covariates, allowing us to capture the tendency of sets of individuals defined by values of **Grade** to mix with sets of individuals defined by values of **Race**:

```
R> summary(faux.mesa.high ~ mm(Grade >= 10 ~ Race,
+ levels = TRUE ~ c("Hisp", "NatAm", "White")))
mm[Grade>=10=TRUE,Race=Hisp] mm[Grade>=10=FALSE,Race=NatAm]
43 115
mm[Grade>=10=TRUE,Race=NatAm] mm[Grade>=10=FALSE,Race=White]
41 30
mm[Grade>=10=TRUE,Race=White]
15
```

With all values of Grade >= 10 (i.e., FALSE and TRUE) and three values of Race allowed according to the levels argument, the full mixing matrix here would include 2×3 statistics, though the default levels2 = -1 omits the first of these so there is no Grade>=10=FALSE,Race=Hisp statistic. When interpreting mixing matrix effects of this type, bear in mind that two covariates need not partition the vertex set in the same ways. Here, for instance, there can be students both above and below grade 10 with each race/ethnicity.

The nodemix term can do many of the same things that mm can do. For both terms, levels2 can take a matrix as input; in particular, for nodemix this argument can take character matrices to map multiple cells to the same statistic. For instance, in the faux.mesa.high dataset, if we want to group all sex-homophilous (male-male or female-female) ties together in the same statistic while keeping the heterophilous (male-female) ties separate, we can pass to levels2 a 2×2 matrix with matching non-blank entries along the diagonal and blanks off the diagonal:

```
R> m <- matrix(c("homophilous", "", "", "homophilous"), 2, 2)
R> summary(faux.mesa.high ~ nodemix("Sex", levels2 = m))
```

mix.Sex.homophilous	mix.Sex.F.M
132	71

4. Term operators

ergm 4 introduces a new way to augment an **ergm** function call that we call a *term operator*, or simply *operator*. In mathematics, an operator is a function, like differentiation, that takes functions as its inputs; analogously, a term operator takes one or more ERGM formulas as input and transforms them by modifying their inputs and/or outputs. Most operators therefore have a general form X(formula, ...) where X is the name of the operator, typically capitalized, formula is a one-sided formula specifying the network statistics to be evaluated, and the remaining arguments control the transformation applied to the network before formula is evaluated and/or to the transformation applied to the network statistics obtained by evaluating formula. Operators are documented alongside other terms, accessible as help("[name]-ergmTerm") or ergmTerm?[name], and we describe some frequently used operators below.

4.1. Network filters

Several operators allow the user to evaluate model terms on filtered versions of the network, i.e., on particular subsets of the existing nodes and/or edges.

Filtering edges

The operator F(formula, filter) evaluates the terms in formula on a filtered network, with filtering specified by filter. Here, filter is the right-hand side of a formula that must contain one binary dyad-independent ergm term, having exactly one statistic with a dyadwise contribution of 0 for a 0-valued dyad. That is, the term must be expressible as

$$g(\mathbf{y}) = \sum_{(i,j)\in\mathbb{Y}} f_{i,j}(y_{i,j}),\tag{3}$$

where for all possible (i, j), $f_{i,j}(0) = 0$. One may verify that condition (3) implies that an ERGM containing the single term $g(\mathbf{y})$ has the property that the dyads $Y_{i,j}$ are jointly independent, which is why such a term is called "dyad-independent". Examples of such terms include nodemix, nodematch, nodefactor, nodecov, and edgecov. Then, formula will be evaluated on a network constructed by taking \mathbf{y} and keeping only those edges for which $f_{i,j}(y_{i,j}) \neq 0$. This predicate can be modified slightly by very simple comparison or logical expressions in the filter formula. In particular, placing ! in front of the term negates it (i.e., keep (i, j) only if $f_{i,j}(y_{i,j}) = 0$) and comparison operators (==, <, etc.) allow comparing $f_{i,j}(y_{i,j})$ to values other than 0.

Sampson's Monks (Sampson 1968) can provide illustrative examples. **ergm** includes a version of these data reporting cumulative liking nominations over the three time periods Sampson asked a group of monks to identify those they liked. This directed, 18-node network is depicted in Figure 1.

```
R> set.seed(2345)
R> data("sampson", package = "ergm")
R> lab <- paste0(1:18, " ", substr(samplike %v% "group", 1, 1), ": ",
+ samplike %v% "vertex.names")
R> plot(samplike, displaylabels = TRUE, label = lab)
```

As an example of the F operator, the code below uses four different methods to summarize the number of ties between pairs of nodes in the Turks group in the samplike dataset:

```
R> summary(samplike ~ nodematch("group", diff = TRUE, levels = "Turks") +
+ F(~ nodematch("group"), ~ nodefactor("group", levels = "Turks"))
+ F(~ edges, ~ nodefactor("group", levels = "Turks") == 2)
+ F(~ edges, ~ !nodefactor(~ group != "Turks")))
nodematch.group.Turks
```

```
30
F(nodefactor("group",levels="Turks"))~nodematch.group
30
F(nodefactor("group",levels="Turks")==2)~edges
30
F(!nodefactor(~group!="Turks"))~edges
30
```

Here, the third method works because this particular $f_{i,j}(y_{i,j})$ counts how many of the two nodes *i* and *j* are **Turks**, and so equals 2 if and only if both are; and the fourth method works because the new $f_{i,j}(y_{i,j})$ is 0 only if neither *i* nor *j* is a non-**Turks** node.



Figure 1: The monks dataset, with edges indicating directed liking relationships at any of three time points and nodes numbered from 1 to 18 and with group membership as assigned by Sampson indicated by L for "Loyalists", O for "Outcasts", and T for "Young Turks".

It is also possible to filter on a quantitative variable. For instance, an alternative way to count the number of edges in faux.mesa.high that match on "Grade" is to report total edges after filtering by node pairs whose absolute difference on the "Grade" variable is less than 1:

```
R> cbind(summary(faux.mesa.high ~ nodematch("Grade") ),
+ summary(faux.mesa.high ~ F(~ edges, ~ absdiff("Grade") < 1)))</pre>
```

[,1] [,2] nodematch.Grade 163 163

While filter must be dyad-independent, formula can have dyad-dependent terms as well. For instance, we may count the transitive triples – i.e., triples (i, j, k) where $y_{i,j} = y_{j,k} = y_{i,k} = 1 - in$ the samplike network, then perform the same count on the subnetwork consisting only of those edges connecting two monks not in attendance in the minor seminary of Cloisterville before coming to the monastery:

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Treating directed networks as undirected

The operator Symmetrize(formula, rule) evaluates the terms in formula on an undirected network constructed by symmetrizing the underlying directed network according to rule. The possible values of rule, which match the terminology of the symmetrize function of the sna package, are (a) "weak", (b) "strong", (c) "upper", and (d) "lower"; for any i < j, these four values result in an undirected tie between i and j if and only if (a) either $y_{i,j}$ or $y_{j,i}$ equals 1, (b) both $y_{i,j}$ and $y_{j,i}$ equal 1, (c) $y_{i,j} = 1$, and (d) $y_{j,i} = 1$. For example, the four possible symmetrized values of the samplike ~ edges statistic are as follows:

```
R> cbind(summary(samplike ~ Symmetrize(~ edges, "weak") +
+ Symmetrize(~ edges, "strong") + Symmetrize(~ edges, "upper") +
+ Symmetrize(~ edges, "lower")))
[,1]
Symmetrize(weak)~edges 60
Symmetrize(strong)~edges 28
```

36

52

We may verify that both "weak" plus "strong" and "upper" plus "lower" yield the total number of directed edges, which in this case equals 88.

Extracting subgraphs

Symmetrize(upper)~edges

Symmetrize(lower)~edges

The operator S(formula, attrs) evaluates the terms in formula on an induced subgraph constructed from vertices identified by attrs. The attrs argument either takes a value as explained in Section 3.2 for the nodes argument or, to obtain a bipartite network, a two-sided formula with the left-hand side specifying the tails and the right-hand side specifying the heads. For instance, suppose that we wish to model the density and mutuality dynamics within the group "Young Turks" as different from those of the rest of the network:

```
R> coef(summary(ergm(samplike ~ edges + mutual +
+ S(~ edges + mutual, ~ (group == "Turks")),
+ control = snctrl(seed = 123))))
```

	Estimate	Std. Error	MCMC 2	% z	z value	Pr(> z)
edges	-2.007074	0.2377493	(0 -8.	441979	3.120095e-17
mutual	2.351613	0.4996500	(o 4.	706519	2.519819e-06
S((group=="Turks"))~edges	2.812378	0.8650057	(оз.	251282	1.148857e-03
S((group=="Turks"))~mutual	-2.165222	1.1965294	(0 -1.	809585	7.036009e-02

Thus, the density within the group is statistically significantly higher, whereas the reciprocation within the group is lower, though not statistically significantly at the 5% level.

As another example, illustrated in Figure 2, consider the directed edges from "non-Young Turks" to "Young Turks". Creating the induced subgraph from these edges results in a bipartite network – which is always taken to be undirected even though the edges were originally directed – we may count the number of four-cycles:



Figure 2: A bipartite induced subgraph between Turks (green) and Non-Turks (yellow). Edges involved in at least one undirected 4-cycle are emphasized. When directed edges from "Non-Turks" to "Turks" (black) are viewed as bipartite (undirected) edges, we obtain 4-cycles (3, 1, 18, 2), (3, 1, 8, 2), and (8, 1, 18, 2). When directed edges from "Turks" to "Non-Turks" (dotted red) are also included, we obtain the additional 4-cycles (8, 1, 18, 7) and (8, 2, 18, 7).

```
R> summary(samplike ~ S(~ cycle(4), (group != "Turks") ~ (group == "Turks")))
S((group!="Turks"),(group=="Turks"))~cycle4
```

On the other hand, if we treat the original network as undirected using Symmetrize before creating the induced bipartite subgraph, we see additional four-cycles. This example also illustrates that term operators may be nested arbitrarily:

```
R> summary(samplike ~ Symmetrize(~S(~cycle(4), (group != "Turks") ~
+ (group == "Turks")), "weak"))
Symmetrize(weak)~S((group!="Turks"),(group=="Turks"))~cycle4
```

Finally, we illustrate a common use case in which Symmetrize is used to analyze mutuality in a directed network as a function of a predictor. The faux.dixon.high dataset is a directed friendship network of seventh through twelfth graders. Suppose we wish to check how strongly the tendency toward mutuality in friendships is affected by students' closeness in grade level.

```
R> data("faux.dixon.high", package = "ergm")
R> FDHfit <- ergm(faux.dixon.high ~ edges + mutual + absdiff("grade") +
+ Symmetrize(~ absdiff("grade"), "strong"), control = snctrl(seed = 321))
R> coef(summary(FDHfit))
```

```
Estimate Std. Error MCMC %
                                                                  z value
edges
                                 -3.2468082 0.05110162
                                                             0 -63.536313
                                  3.2407587 0.12095858
                                                             0 26.792301
mutual
                                                             0 -21.223763
absdiff.grade
                                 -0.9145735 0.04309196
                                                               -2.349707
Symmetrize(strong)~absdiff.grade -0.4237874 0.18035755
                                                             0
                                      Pr(|z|)
edges
                                  0.00000e+00
mutual
                                 3.972740e-158
absdiff.grade
                                 5.762326e-100
Symmetrize(strong)~absdiff.grade 1.878819e-02
```

After correcting for the overall network density, the propensity for friendships to be reciprocated, and the predictive effect of grade difference on friendship formation, the difference in grade level has a statistically significant negative effect on the tendency to form mutual friendships (p value = 0.019).

4.2. Interaction effects

For binary ERGMs, interactions between dyad-independent ergm terms can be specified in a manner similar to lm and glm via the : and * operators. (See Section 4.1 for a definition of dyad-independent.)

Let us first consider the colon (:) operator. Generally, if term A creates p_A statistics and term B creates p_B statistics, then A:B will create $p_A \times p_B$ new statistics. If A and B are dyad-independent terms, expressed for $a = 1, \ldots, p_A$ and $b = 1, \ldots, p_B$ as

$$g_{\mathtt{A}}(\mathbf{y}) = \sum_{(i,j)\in\mathbb{Y}} x_{i,j}^{\mathtt{A}} y_{i,j} \text{ and } g_{\mathtt{B}}(\mathbf{y}) = \sum_{(i,j)\in\mathbb{Y}} x_{i,j}^{\mathtt{B}} y_{i,j}$$

for appropriate covariate matrices X^{A} and X^{B} , then the corresponding interaction term is

$$g_{\mathbf{A}:\mathbf{B}}(\mathbf{y}) = \sum_{(i,j)\in\mathbb{Y}} x_{i,j}^{\mathbf{A}} x_{i,j}^{\mathbf{B}} y_{i,j}.$$
(4)

As an example, consider the Grade and Sex effects, expressed as model terms via nodefactor, in the faux.mesa.high dataset:

```
R> summary(faux.mesa.high ~
     nodefactor("Grade"):nodefactor("Sex", levels = TRUE))
+
 nodefactor.Grade.8:nodefactor.Sex.F nodefactor.Grade.9:nodefactor.Sex.F
                                   51
                                                                         67
nodefactor.Grade.10:nodefactor.Sex.F nodefactor.Grade.11:nodefactor.Sex.F
                                   26
                                                                         60
nodefactor.Grade.12:nodefactor.Sex.F
                                      nodefactor.Grade.8:nodefactor.Sex.M
                                   30
                                                                         99
 nodefactor.Grade.9:nodefactor.Sex.M nodefactor.Grade.10:nodefactor.Sex.M
                                   63
                                                                         46
nodefactor.Grade.11:nodefactor.Sex.M nodefactor.Grade.12:nodefactor.Sex.M
                                   38
                                                                         26
```

In the call above, we deliberately include both Sex-factor levels via levels = TRUE, whereas we employ the default behavior of nodefactor for the Grade factor, which leaves out one level. Thus, the 6-level Grade factor and the 2-level Sex factor, with one level of the former omitted, produce 5×2 interaction terms in this example.

The * operator, by contrast, produces all interactions in addition to the main effects or statistics. Therefore, in the scenario described above, A * B will add $p_A + p_B + p_A \times p_B$ statistics to the model. Below, we use the default behavior of nodefactor on both the 6-level Grade factor and the 2-level Sex factor, together with an additional edges term, to produce a model with $1 + 5 + 1 + 5 \times 1$ terms:

```
R> m <- ergm(faux.mesa.high ~ edges + nodefactor("Grade") * nodefactor("Sex"))</pre>
R> print(summary(m), digits = 3)
Call:
ergm(formula = faux.mesa.high ~ edges + nodefactor("Grade") *
    nodefactor("Sex"))
Maximum Likelihood Results:
                                      Estimate Std. Error MCMC % z value
                                                               0 -17.53
edges
                                        -3.028
                                                    0.173
nodefactor.Grade.8
                                        -1.424
                                                    0.263
                                                               0
                                                                   -5.41
nodefactor.Grade.9
                                        -1.166
                                                    0.229
                                                                   -5.10
                                                               0
nodefactor.Grade.10
                                        -1.633
                                                    0.357
                                                                   -4.58
                                                               0
nodefactor.Grade.11
                                        -0.328
                                                    0.237
                                                               0
                                                                  -1.38
nodefactor.Grade.12
                                        -0.794
                                                    0.324
                                                               0
                                                                   -2.45
nodefactor.Sex.M
                                        -1.764
                                                    0.240
                                                               0
                                                                   -7.36
nodefactor.Grade.8:nodefactor.Sex.M
                                                                   6.86
                                        1.386
                                                    0.202
                                                               0
nodefactor.Grade.9:nodefactor.Sex.M
                                                                    4.79
                                        1.012
                                                    0.211
                                                               0
nodefactor.Grade.10:nodefactor.Sex.M
                                        1.347
                                                    0.264
                                                               0
                                                                    5.11
nodefactor.Grade.11:nodefactor.Sex.M
                                         0.419
                                                    0.240
                                                               0
                                                                    1.75
nodefactor.Grade.12:nodefactor.Sex.M
                                         1.059
                                                    0.290
                                                               0
                                                                    3.65
                                      Pr(|z|)
edges
                                      < 1e-04 ***
nodefactor.Grade.8
                                       < 1e-04 ***
nodefactor.Grade.9
                                       < 1e-04 ***
nodefactor.Grade.10
                                      < 1e-04 ***
nodefactor.Grade.11
                                      0.16714
nodefactor.Grade.12
                                      0.01429 *
nodefactor.Sex.M
                                      < 1e-04 ***
nodefactor.Grade.8:nodefactor.Sex.M
                                      < 1e-04 ***
nodefactor.Grade.9:nodefactor.Sex.M
                                      < 1e-04 ***
nodefactor.Grade.10:nodefactor.Sex.M < 1e-04 ***</pre>
nodefactor.Grade.11:nodefactor.Sex.M 0.08074 .
nodefactor.Grade.12:nodefactor.Sex.M 0.00026 ***
                0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Signif. codes:
     Null Deviance: 28987
                           on 20910
                                     degrees of freedom
 Residual Deviance: 2189
                           on 20898
                                     degrees of freedom
AIC: 2213 BIC: 2308 (Smaller is better. MC Std. Err. = 0)
```

Equation 4 implies that the change statistic corresponding to dyad (i, j) is given by $x_{i,j}^{A} x_{i,j}^{B}$; that is, the change statistic for the interaction is the product of the change statistics. One may define interaction change statistics for arbitrary pairs of terms similarly – that is, by taking the interaction change statistic as the product of the corresponding change statistics - though in the case of dyad-dependent terms it is unclear that a change statistic obtained as the product of change statistics corresponds to any ERGM sufficient statistic in the sense of (1). Therefore, attempting to create interactions involving dyad-dependent terms will create an error by default in **ergm**. If one wishes to create such interactions anyway, the default behavior may be changed using the **interact.dependent** term option as described in Section 8.6. Interactions involving curved ERGM terms are not supported in **ergm** 4.

Since interaction terms are defined by multiplying change statistics dyadwise and then (for dyad-independent terms) summing over all dyads, interactions of terms are not the same as products of those terms. For instance, given a nodal covariate "a", the interaction of nodecov("a") with itself is different than the effect of the square of the covariate, as we observe in the case of the wealth covariate of the (undirected) Florentine marriage dataset:

4.3. Reparametrizing the model

The term operator Sum(formulas, label) allows arbitrary linear combinations of existing statistics to be added to the model. Suppose $\mathbf{g}_1(\mathbf{y}), \ldots, \mathbf{g}_K(\mathbf{y})$ is a set of K vector-valued network statistics, each corresponding to one or more ergm terms and of arbitrary dimension. Also suppose that A_1, \ldots, A_K is a set of known constant matrices, all having the same number of rows, such that each matrix multiplication $A_k \mathbf{g}_k(\mathbf{y})$ is well-defined. Then we may define the statistic

$$\mathbf{g}_{\mathrm{Sum}}(\mathbf{y}) = \sum_{k=1}^{K} A_k \mathbf{g}_k(\mathbf{y}).$$

The first argument to Sum is a formula or a list of K formulas, each representing a vector statistic. If a formula has a left-hand side, the left-hand side will be used to define the corresponding A_k matrix: If it is a scalar or a vector, A_k will be a diagonal matrix thus multiplying each element by its corresponding element; and if it is a matrix, A_k will be used directly. When no left-hand side is given, A_k defaults to the identity matrix. To simplify this function for some common cases, if the left-hand side is "sum" or "mean", the sum (or mean) of the statistics in the formula is calculated.

As an example, consider a vector of statistics consisting of the numbers of friendship ties received by each subgroup of Sampson's monks:

```
R> summary(samplike ~ nodeifactor("group", levels = TRUE))
```

```
nodeifactor.group.Loyal nodeifactor.group.Outcasts
29 13
nodeifactor.group.Turks
46
```

We may create a single statistic equal to the friendship ties received by both groups of "non-Outcasts" by adding the first and third components of the nodefactor vector, either by left-multiplying by $\begin{bmatrix} 1 & 0 & 1 \end{bmatrix}$ or by deselecting the second component at the nodeifactor level and summing the remaining two:

```
R> summary(samplike ~
+ Sum(cbind(1, 0, 1) ~ nodeifactor("group", levels = TRUE), "nf.L_T") +
+ Sum("sum" ~ nodeifactor("group", levels = -2), "nf.L_T"))
Sum~nf.L_T Sum~nf.L_T
75 75
```

Whereas the Sum operator operates on network statistics, Parametrize(formula, params, map, gradient = NULL, minpar = -Inf, maxpar = +Inf, cov = NULL) operates on the parameters. The formula argument specifies a vector statistic $\mathbf{g}_k(\mathbf{y})$ involving one or more terms and, if curved terms are specified, a mapping $\eta_k(\boldsymbol{\theta})$. The remaining arguments follow the curved ERGM template: The params argument is a vector of names whose length determines the dimension of the parameter vector. The function map must take arguments \mathbf{x} , \mathbf{n} , and ... and map the parameter vector into the domain of η_k , transforming an ERGM term $\eta_k(\boldsymbol{\theta}_k)^{\top}\mathbf{g}_k(\mathbf{y})$ to $\eta_k(\eta_\star(\boldsymbol{\theta}_k))^{\top}\mathbf{g}_k(\mathbf{y})$, where η_\star is the function specified by map. The function gradient must take the same arguments as map and return the gradient matrix, minpar and maxpar specify the boundaries of the domain of map, and cov provides an optional argument to map. If formula is not curved, $\eta_k(\boldsymbol{\theta})$ is simply the identity function.

To simplify this function for some common special cases, if map = "rep", the parameter vector will simply be replicated to make it as long as required by $\eta_k(\theta)$, and the gradient will be evaluated automatically. Similarly, if the user is certain that map is linear or affine, the gradient will be calculated automatically if gradient = "linear" is specified.

To illustrate this, consider a simple model with the baseline edge effect and a single attractiveness effect for monks who are not "Outcasts". Following are four different ways to parameterize this model when calling the ergm function. The first two examples use the default parameterization while producing the two model statistics using different syntax:

```
R> f1 <- samplike ~ edges + nodeifactor(~ group != "Outcasts")
R> summary(f1)
```

The next two examples each define a single vector of statistics $\mathbf{g}_1(\mathbf{y})$, which we can see with the summary function. In the first example, we use Parametrize with a 3-dimensional vector

of statistics, where we specify that the new parameter will be one-dimensional (by setting **params** to be a single parameter name) and then define a map specifying that our single parameter should multiply both the first and third statistics:

```
R> f3 <- samplike ~ edges + Parametrize(~ nodeifactor("group", levels = TRUE),
+ "nf.L_T", function(x, n, ...) c(x, 0, x), gradient = "linear")
R> summary(f3)
```

nodeifactor.group.Loyal	edges
29	88
nodeifactor.group.Turks	<pre>nodeifactor.group.Outcasts</pre>
46	13

Finally, the last example defines a 2-dimensional vector of statistics and then specifies (via "rep") that the new single parameter should multiply each of these statistics:

```
R> f4 <- samplike ~ edges + Parametrize(~ nodeifactor("group", levels = -2),
+ "nf.L_T", "rep")
R> summary(f4)
```

```
edges nodeifactor.group.Loyal nodeifactor.group.Turks
88 29 46
```

All four fitted models return the same parameter estimates. Here, to save space we check only the second parameter estimates in each model, which also reveals how each example assigns parameter names:

```
R> cbind(c(coef(ergm(f1))[2], coef(ergm(f2))[2], coef(ergm(f3))[2],
+ coef(ergm(f4))[2]))
```

[,1] nodeifactor.group!="Outcasts".TRUE 0.6661217 Sum~nf.L_T 0.6661217 nf.L_T 0.6661217 nf.L_T 0.6661217

Whereas the Sum operator calculates linear combinations of network statistics, the Prod operator calculates the products of their powers. As of this writing, it is implemented for positive statistics only, by first applying the Log operator (which returns the natural logarithm, log in R, of the statistics passed to it), then the Sum operator, and finally the Exp operator (which returns the exponential function, exp in R). As a simple illustration, we may verify that the Sum and Prod operators do in fact produce network statistics as expected if we simply use each with a list of formulas having no left hand side:

```
R> summary(faux.dixon.high ~ edges + mutual +
+ Sum(list(~ edges, ~ mutual), "EdgesAndMutual")
+ Prod(list( ~ edges, ~ mutual), "EdgesAndMutual"))
```

edges mutual Sum~EdgesAndMutual 1197 219 1416 Exp~Sum~EdgesAndMutual 262143

5. Sample space constraints

In Section 1, we saw that the sample space \mathcal{Y} is a subset of the power set $2^{\mathbb{Y}}$, where \mathbb{Y} is itself a subset of all potential relationships. Many applications in fact take \mathbb{Y} to be the set of all relationships and $\mathcal{Y} = 2^{\mathbb{Y}}$, but it is sometimes desirable to restrict the sample space by placing constraints on which relationships (i, j) are allowed in \mathbb{Y} and further which networks $\mathbf{y} \in 2^{\mathbb{Y}}$ are allowed in \mathcal{Y} . As a simple example, a bipartite network allows only edges connecting nodes from one subset, or mode, to nodes from its complement. This particular constraint is so commonly used that it is hard-coded into **network** and **ergm**. As another example, consider the inverse of a bipartite setting, in which edges are only allowed *within* subsets of the node set, a situation often called a block-diagonal constraint. As still another, some applications impose a cap on the degree of any node, which constrains the sample space to include only those networks in which every node has a permitted degree.

In all of the cases above, correct statistical inference for ERGMs depends on correctly incorporating constraints into the fitting process. They are specified using the constraints argument, a one-sided formula whose terms specify the constraints on the sample space. For example, constraints = ~ edges specifies $\mathcal{Y}^{edges} = \{\mathbf{y}' \in \mathcal{Y} : |\mathbf{y}'| = |\mathbf{y}|\}$, where \mathbf{y} is the observed network, specified on the left-hand side. Some constraints, such as fixedas(y1,y0) focus on constraining \mathbb{Y} – in this case, as $\mathbb{Y}^{fixedas(y1,y0)} = \{(i,j) \in \mathbb{Y} : (i,j) \in \mathbf{y}^1 \land (i,j) \notin \mathbf{y}^0\}$ – with $\mathcal{Y} \equiv 2^{\mathbb{Y}}$.

Multiple constraints can be specified on a formula, separated by + to impose a new constraint in additional to prior or (in some instances) - to relax preceding constraints. Earlier versions of the **ergm** package implemented a number of constraints, as described for example in Section 3 of Morris, Handcock, and Hunter (2008). Since that time, many additional types of constraints and methods for imposing them have been added, some of which we describe in this section. A full list of currently implemented constraints is obtained via ?ergmConstraint, and a specific constraint [name] can be looked up with help("[name]-ergmConstraint") or ergmConstraint?[name].

5.1. Arbitrary combinations of dyad-independent constraints

In general, every combination of constraints requires a somewhat different Metropolis–Hastings proposal algorithm for efficient sampling, and so it may be impractical to support every possible combination of constraints. *Dyad-independent* constraints, which affect \mathcal{Y} only through \mathbb{Y} , and do not induce stochastic dependencies among the dyad states, are an exception. These include constraining specific dyads (such as the above-mentioned **observed** and **fixedas** constraints), dyads incident on specific actors (such as the **egocentric** constraint), and block-diagonal structure; and *any* combination of dyad-independent constraints is a dyadindependent constraint. For some such combinations, **ergm** and other packages provide optimized implementations. For the rest, **ergm** falls back to a general but efficient implementation that uses run-length encoding tools provided by package **rle** (Krivitsky 2020) to efficiently store sets of non-constrained dyads and rejection sampling to efficiently select a dyad for the proposal.

Here, we illustrate some of **ergm**'s capabilities using a dataset due to Coleman (1964) that is small enough that computational inefficiency will not present problems. These data are self-reported friendship ties among 73 boys measured at two time points during the 1957– 1958 academic year and they are included as a $2 \times 73 \times 73$ array and documented in the **sna** package. We use the Coleman data to create a **network** object with 2×73 nodes:

```
R> library("sna")
R> data("coleman", package = "sna")
R> cole <- matrix(0, 2 * 73, 2 * 73)
R> cole[1:73, 1:73] <- coleman[1,,]</pre>
R> cole[73 + (1:73), 73 + (1:73)] <- coleman[2,,]
R> diag(cole[1:73, 73 + (1:73)]) <- diag(cole[73 + (1:73), 1:73]) <- 1
R> ncole <- network(cole)</pre>
R> ncole %v% "Semester" <- rep(c("Fall", "Spring"), each = 73)</pre>
R> ncole
Network attributes:
  vertices = 146
  directed = TRUE
  hyper = FALSE
  loops = FALSE
  multiple = FALSE
  bipartite = FALSE
  total edges= 652
    missing edges= 0
    non-missing edges= 652
Vertex attribute names:
    Semester vertex.names
```

```
No edge attributes
```

By construction, the **ncole** network includes the Fall 1957 semester data and the Spring 1958 data as the upper left 73×73 and lower right 73×73 blocks, respectively. In addition, the upper right and lower left blocks indicate which nodes are the same person; that is, $y_{i,j} = 1$ whenever *i* and *j* are the same boy measured at two different times. This latter information is redundant because the ordering of the 73 boys is the same in both fall and spring, yet we include it to illustrate some techniques using entries that are not on the main block diagonal and because in principle it might not always be the case that the same individuals are observed at both time points.

5.2. Constraints via the Dyads operator

The Dyads(fix = NULL, vary = NULL) operator takes one or two ergm formulas that may contain only dyad-independent terms. For the terms in the fix formula, dyads that affect the

network statistic (i.e., have nonzero change statistic) for *any* the terms will be fixed at their current values. For the terms in the **vary** formula, only those that change *at least one* of the terms will be allowed to vary, and all others will be fixed. If both formulas are given, the dyads that vary either for one or for the other will be allowed to vary. A formula passed without an argument name will default to **fix**, for consistency with other constraints' semantics.

The key to our treatment of the ncole network using the Dyads operator is the Semester vertex attribute:

```
R> table(ncole %v% "Semester")
```

Fall Spring 73 73

In particular, the nodematch("Semester") term has a change statistic equal to one for exactly those dyads representing boys measured during the same semester, and this change statistic is zero otherwise. Therefore, in our 146-node directed network there are 146×145 , or 21,170, total dyads, of which $2 \times 73 \times 72$, or 10,512, have nonzero change statistics for nodematch("Semester"). We can easily see exactly how many total edges there are and how many of these are in the upper left or lower right blocks:

```
R> summary(ncole ~ edges + nodematch("Semester"))
```

edges nodematch.Semester 652 506

We can now calculate directly the log-odds, or logit, for both the block diagonal and the offblock diagonal subnetworks, then verify that the Dyads operator can accomplish these same calculations using a constrained ERGM. First, we fix dyads with nonzero change statistics, which yields the coefficient for block off-diagonal (non-matching) entries:

```
R> logit <- function(p) log(p / (1 - p))
R> cbind(logit((652 - 506) / (21170 - 10512)), coef(ergm(ncole ~ edges,
+ constraints = ~ Dyads(fix = ~ nodematch("Semester")))))
```

[,1] [,2] edges -4.276666 -4.276666

Next, we allow dyads with nonzero change statistics to **vary**, which yields the coefficient for block diagonal entries:

```
R> cbind(logit(506 / 10512), coef(ergm(ncole ~ edges,
+ constraints = ~ Dyads(vary = ~ nodematch("Semester")))))
        [,1] [,2]
edges -2.984404 -2.984404
```

If we remove the constraints entirely, ncole has 652 edges out of a possible 21, 170:

```
R> cbind(logit(652/21170), coef(ergm(ncole ~ edges)))
```

[,1][,2] edges -3.449013 -3.449013

A significant limitation of this specific constraint is that its initialization requires testing every possible dyad and therefore takes up time and memory in proportion to the square of the number of nodes.

5.3. Constraints via blocks

The blocks operator constrains changes to any dyads that involve certain pairs of categories defined by a particular nodal covariate. We may reproduce the examples of Section 5.2 using blocks. First, consider the full complement of statistics produced by the nodemix model term:

```
R> summary(ncole ~ nodemix("Semester", levels = TRUE, levels2 = TRUE))
    mix.Semester.Fall.Fall
                             mix.Semester.Spring.Fall
                       243
                                                    73
  mix.Semester.Fall.Spring mix.Semester.Spring.Spring
                        73
                                                   263
```

The levels = TRUE argument ensures that nodemix considers every value of "group" in constructing a mixing matrix of possible dyad combinations. The levels2 = TRUE argument ensures that, from the full complement of such possible combinations, every one is included as a statistic. By default, levels = TRUE whereas levels 2 = -1, since we frequently want to exclude at least one possible mixing combination to avoid collinearity in a model that also includes the edges term.

We may now use levels2 in conjunction with blocks to select exactly which of the nodemix combinations should be constrained as fixed to reproduce the examples of Section 5.2. First, we fix all dyads where the group values match:

```
R> coef(ergm(ncole ~ edges,
    constraints = ~ blocks("Semester", levels2 = c(1, 4))))
+
    edges
-4.276666
```

Second, we fix the dyads where group values do not match:

```
R> coef(ergm(ncole ~ edges,
+
     constraints = ~blocks("Semester", levels2 = c(2, 3))))
    edges
-2.984404
```

Additional examples using levels2, among other nodal attribute features, are contained in the nodal_attributes vignette within the ergm package.

5.4. Additional constraints

Multiple different constraints on the sample space of possible networks, as defined by the values of certain network statistics, may be implemented beyond those discussed already in this section. The bd constraint, for instance, may be used to enforce a maximum allowable degree for any node, via the maxout argument. A comprehensive list of available constraints is available via ?ergmConstraint. The handling of various constraints by MCMC proposals in the ergm package is addressed in Krivitsky *et al.* (2022).

6. Modeling networks with valued edges

Starting with version 3.1, the **ergm** package can handle some types of networks whose ties are not merely binary, indicating presence or absence, but may have nonzero values other than unity. For example, the value of a tie might represent a count, such as the number of times a particular relationship has occurred; or it might represent an ordinal variable, if node i ranks a subset of its neighbors. Valued ties can increase complexity relative to binary ties in, for example, specifying the model and ensuring that the chosen statistics are meaningful for the types of edge values being modeled. Whether the scale of measurement of tie values is ordinal, interval, or ratio, it becomes necessary to specify the distribution of these values and to create functions to aggregate these values into ERGM statistics.

In the ergm(), simulate(), and summary() functions, the valued mode is typically activated by passing a response argument, giving the name of the edge attribute containing the value of the response. Non-edges are assumed to have value 0. The argument may also be a formula whose right-hand side is an expression in terms of the edge attributes that evaluates to the response value and whose left-hand side, if present, gives the name to be used. If it evaluates to a logical (TRUE/FALSE) value (e.g., response = threeContacts ~ (contacts >= 3)), a binary ERGM is used.

6.1. Reference specification

Krivitsky (2012) pointed out that sufficient statistics alone do not suffice to specify an ERGM on a network whose relations are valued. Consider a simple ERGM of the form

$$\mathsf{P}(\mathbf{Y} = \mathbf{y}; \theta) \propto h(\mathbf{y}) \exp\left(\theta \sum_{(i,j) \in \mathbb{Y}} y_{i,j}\right),$$

where $y_{i,j} \in \{0, 1, ...\}$ is an unbounded count. If $h(\mathbf{y})$ is any constant, then $Y_{i,j} \stackrel{\text{i.i.d.}}{\sim} \text{Geometric}[p = 1 - \exp(\theta)]$. On the other hand, if $h(\mathbf{y}) = 1/\prod_{(i,j)\in\mathbb{Y}} y_{i,j}!$, then $Y_{i,j} \stackrel{\text{i.i.d.}}{\sim} \text{Poisson}[\mu = \exp(\theta_k)]$. For this reason, Krivitsky (2012) called a distribution with $h(\mathbf{y}) = 1$ and a sample space of nonnegative integers a *Geometric-reference ERGM* and one with $h(\mathbf{y}) = 1/\prod_{(i,j)\in\mathbb{Y}} y_{i,j}!$ a *Poisson-reference ERGM*.

For ergm(), simulate(), and other functions, reference distributions are specified with a reference argument, which is a one-sided formula with one term. The ergm package allows

Unif (a, b) and DiscUnif (a, b) references, specifying $h(\mathbf{y}) = 1$, the former on a dyad space $y_{i,j} \in [a, b]$, the latter on $y_{i,j} \in \{a, a+1, \ldots, b\}$. A companion package, ergm.count, allows the additional references Poisson and Geometric, described above, as well as Binomial(trials) for $h(\mathbf{y}) = \prod_{(i,j) \in \mathbb{Y}} {n_{\text{trials}} \choose y_{i,j}}$ in the case $y_{i,j} \in \{0, \ldots, n_{\text{trials}}\}$. For rank-order relational data, a CompleteOrder reference distribution is implemented in the ergm.rank package for situations where rankings are complete. Where ties are permitted, DiscUnif() can be used as a reference. See Krivitsky and Butts (2019) for further details on both the ergm.count and ergm.rank packages, and their vignettes.

Reference distributions are explained in more detail in Section 3 of Krivitsky and Butts (2019). This reference also illustrates how the **network** package may be used to visualize some kinds of valued networks (Section 2) and even how the **latentnet** package can handle latent-space models with valued ties (Section 4). Online help on the reference distributions that are implemented by all packages currently loaded in an R session can be obtained by typing help("ergm-references").

6.2. Dyad-independent statistics

As in Section 4.1, a component of the vector $\mathbf{g}(\mathbf{y})$ is called a dyad-independent statistic if, when one builds an ERGM using it as the *only* model statistic, the joint distribution (1) of the network factors into the product of its marginal dyad distributions. That is, the univariate version of (1) may be written

$$\mathsf{P}(\mathbf{Y} = \mathbf{y}; \theta) = \prod_{(i,j) \in \mathbb{Y}} \mathsf{P}(Y_{i,j} = y_{i,j}) = \frac{h(\mathbf{y})}{\kappa_{h,\eta,g}(\theta, \mathcal{Y})} \prod_{(i,j) \in \mathbb{Y}} \exp\{\eta(\theta)g_{i,j}(\mathbf{y})\}$$

for $\mathbf{y} \in \mathcal{Y}$ and for some appropriately chosen $g_{i,j}(\mathbf{y})$. Equation 6.1 shows that the sum of the values $y_{i,j}$, which implies $g_{i,j}(\mathbf{y}) = y_{i,j}$, is one such example. Another example is the sum of the nonzero indicators that arises if we define $g_{i,j}(\mathbf{y}) = \mathbb{I}\{y_{i,j} > 0\}$. Each of these basic dyad-independent statistics is implemented in **ergm**:

- sum(pow = 1) Sum of edge values: This is simply the summation of edge values. For most valued ERGMs, this is the natural intercept term. In particular, for reference distributions such as Poisson and Binomial, using this term produces intercept effects of Poisson log-linear and binomial logistic regressions, respectively. Optionally, the dyad values can be raised to a power before being summed.
- **nonzero** Number of nonzero edge values: This term counts nonzero edge values. It can be used to model zero-inflation that is common in networks: It is often the case that a network is sparse but has edges with relatively high weights when they are present.

Binary ERGM statistics cannot be used directly for valued networks nor vice versa, but most dyad-independent binary ERGM statistics have been generalized by imposing a covariate on one of the two above forms. They have the same arguments as their binary ERGM counterparts, with an additional argument: form, which has two possible values: "sum" (the default) and "nonzero". The former creates a statistic of the form $\sum_{(i,j)\in\mathbb{Y}} x_{i,j}y_{i,j}$, where $y_{i,j}$ is the value of dyad (i, j) and $x_{i,j}$ is the term's covariate associated with it. The latter computes a sum of indicator variables, one for each dyad, indicating whether the corresponding edge has a nonzero value. When form = "sum" is used, typically a GLM-like effect results, whereas

form = "nonzero" can be used to model sparsity effects (Krivitsky 2012). Krivitsky and Butts (2019) gives an example of the form argument with the nodematch term.

Other terms that control a dyad's distribution are atleast(threshold = 0), atmost(threshold = 0), equalto(value = 0, tolerance = 0), greaterthan(threshold = 0), ininterval(lower = -Inf, upper = +Inf, open = c(TRUE, TRUE)), and smallerthan(threshold = 0). Each of these terms counts the dyad values that satisfy the criterion identified by its name.

6.3. Mutuality

The binary mutual term in ergm counts the number of pairs of mutual ties. Its valued counterpart is mutual(form), which permits the following values of form. For each of these, a higher coefficient will tend to increase the similarity of reciprocating dyad values.

- "product" Sum of products of reciprocating edge values: This is the most direct generalization. However, for a Poisson-reference ERGM in particular, a positive coefficient on this term produces an infinite normalizing constant and therefore lies outside the parameter space.
- "geometric" Sum of geometric mean of reciprocating edge values: This form solves the product form's problem by taking a square root of the product. It can be viewed as the uncentered covariance of variance-stabilized counts.
- "min" *Minimum of reciprocating edge values*: This effect is, perhaps, the easiest to interpret, at the cost of statistical power.
- "nabsdiff" Absolute difference of reciprocating edge values: This effect is more symmetrical than min.

We refer the reader to Krivitsky (2012) for a further discussion of the effects.

6.4. Actor heterogeneity

Different actors may have different overall propensities to interact. This has been modeled using random effects, as in the p_2 model, and using degeneracy-prone terms like k-star counts. For valued ERGMs, the following term, also introduced by Krivitsky (2012) and discussed in more detail there, models actor heterogeneity:

nodesqrtcovar(center, transform) Covariance between $y_{i,j}$ incident on same actor: The default transform = "sqrt" will take a square root of dyad values before calculating, and the default center = TRUE will center the transformed values around their global mean, gaining stability at the cost of locality.

6.5. Triadic effects

To generalize the notion of triadic closure, ergm implements very flexible transitiveweights(twopath, combine, affect) and similar cyclicalweights statistics.

The transitive weight statistic has the general form

$$g_{\boldsymbol{v}}(\mathbf{y}) = \sum_{(i,j)\in\mathbb{Y}} v_{\text{affect}}\left(y_{i,j}, v_{\text{combine}}\left(v_{2\text{-path}}(\mathbf{y}_{i,k}, \mathbf{y}_{k,j})_{k\in N\setminus\{i,j\}}\right)\right),$$

which can be customized by varying three functions:

- $v_{2\text{-path}}$: Given $\mathbf{y}_{i,k}$ and $\mathbf{y}_{k,j}$, what is the strength of the two-path they form? The options are "min", to take the minimum of the two-path's constituent values, and "geomean", to take their geometric mean, gaining statistical power at a greater risk of model instability.
- v_{combine} : Given the strengths of the two-paths $\mathbf{y}_{i \to k \to j}$ for all $k \neq i, j$, what is the combined strength of these two-paths between i and j? The choices are "max", for the strength of the strongest of the two-paths – analogous to transitiveties or gwesp(0) binary ERGM effects – and "sum", the sum of the path strengths. The latter choice is better able to detect effects but is more subject to degeneracy; it is analogous to triangles.
- v_{affect} : Given the combined strength of the two-paths between *i* and *j*, how should they affect $Y_{i,j}$? The choices are "min", the minimum of the combined strength and the focus two-path, and "geomean", again more able to detect effects but more likely to cause degeneracy.

Usage of the transitiveweights and cyclicalweights terms is illustrated in Section 3.1 of Krivitsky and Butts (2019).

6.6. Using binary ERGM terms in valued ERGMs

ergm also allows general binary terms to be passed to valued models. The mechanism that allows this is the term operator B(formula, form), which is further described in the **ergm** online help under help("B-ergmTerm") or the shorthand ergmTerm?B. Here, formula is a one-sided formula whose right hand side contains the binary ergm terms to be used. Allowable values of the form argument are form = "sum" and form = "nonzero", which have the effects described in Section 6.2, with form = "sum" only valid for dyad-independent formula terms; or a one-sided formula may be passed to form, containing one *valued* ergm term, with the following properties:

- dyadic independence;
- dyadwise contribution of either 0 or 1;
- dyadwise contribution of 0 for a 0-valued dyad.

That is, it must be expressible as

$$g(y) = \sum_{(i,j) \in \mathbb{Y}} g_{i,j}(y_{i,j}),$$

where for all $i, j, and \mathbf{y}, g_{i,j}(y_{i,j}) \in \{0,1\}$ and $g_{i,j}(0) \equiv 0$. Such terms include nonzero, ininterval(), atleast(), atmost(), greaterthan(), lessthan(), and equalto(). The operator will then construct a binary network \mathbf{y}^{B} such that $y_{i,j}^{\mathrm{B}} = 1$ if and only if $g_{i,j}(y_{i,j}) = 1$, and evaluate the binary terms in formula on it.

6.7. Modeling ordinal values using binary term operators

To illustrate the use of binary ergm terms on a valued network as described above, we construct an example that uses the B (for "binary") operator. The code snippet below gives an example of a valued ergm that uses the DiscUnif, or discrete uniform, reference distribution, which is included in the ergm package itself; that is, there is no need to load the ergm.count or ergm.rank packages to run the following example. The example fits a multinomial logistic regression model that assumes that the edge values are independent of one another and take ordinal values that have the same interpretation for each dyad. (In general, rating and ranking data may not allow edge values to be compared across egos (Krivitsky and Butts 2017); the ergm.rank package contains terms that remain valid in this more complex setting.) Models for independently observed ordinal random variables have a long history in the statistical literature; relevant references specific to network models include Robins, Pattison, and Wasserman (1999) and, in a Bayesian framework, Caimo and Gollini (2020).

First, we build a valued network by pooling the three binary friendship nomination networks due to Sampson (1968), exactly as in Section 2.1 of Krivitsky and Butts (2019).

We will use the B operator to construct new statistics consisting of the number of edges with value k or higher, where k is 1, 2, or 3.

Since there are 18×17 , or 306, possible edges, the summary statistics above tell us that the valued network we have constructed has 30 edges with value 3, 50 - 30 = 20 edges with value 2, 88 - 50 = 38 edges with value 1, and the remaining 218 edges with value 0. The ERGM with these statistics has independent edges, where the probabilities an edge takes the values 0, 1, 2, or 3 are given by 1/D, $\exp\{\theta_1\}/D$, $\exp\{\theta_1 + \theta_2\}/D$, and $\exp\{\theta_1 + \theta_2 + \theta_3\}/D$, respectively, where

$$D = 1 + \exp\{\theta_1\} + \exp\{\theta_1 + \theta_2\} + \exp\{\theta_1 + \theta_2 + \theta_3\}.$$

We may verify that ergm's stochastic fitting algorithm obtains maximum likelihood estimates (MLEs) very close to the exact values:

```
R> mod <- ergm(samplk.tot ~ B(~ edges, ~ atleast(1)) +
+ B(~ edges, ~ atleast(2)) +
+ B(~ edges, ~ atleast(3)), response = "nominations",
+ reference = ~ DiscUnif(0, 3), control = snctrl(seed = 123))
R> coef(mod)
```

This example could have used the equalto terms in place of all the atleast terms above. Then, the estimated proportions would have been proportional to 1, $\exp\{\theta_1\}$, $\exp\{\theta_2\}$, and $\exp\{\theta_3\}$ instead of 1, $\exp\{\theta_1\}$, $\exp\{\theta_1 + \theta_2\}$, and $\exp\{\theta_1 + \theta_2 + \theta_3\}$. Such a model does not assume ordinality of the edge values, so it could be used for a multinomial logit model in which the edges take categorical non-ordered values.

7. Estimation in the presence of missing edge data

It is quite common that network data are incomplete in various ways. The **ergm** package includes the capability to handle missing edge data, whereas other types of missingness such as missing nodal information are not addressed. Early versions of **ergm** allowed the R object NA to be treated as though it were a regular value of a nodal covariate; however, since this behavior can lead to misleading results, more recent **ergm** packages return an error when a nodal covariate with missing values is used in an **ergm** term.

Handcock and Gile (2010) formulated a framework for modeling networks with missing edges and expressed the log-likelihood as

$$\ell(\boldsymbol{\theta}) = \log \mathsf{P}(\mathbf{Y} \in \mathcal{Y}(\mathbf{y}^{\text{obs}}); \boldsymbol{\theta}) = \log \sum_{\mathbf{y}' \in \mathcal{Y}(\mathbf{y}^{\text{obs}})} \mathsf{P}(\mathbf{Y} = \mathbf{y}'; \boldsymbol{\theta}),$$
(5)

where $\mathcal{Y}(\mathbf{y}^{\text{obs}})$ is defined as the set of networks whose partial observation could have produced \mathbf{y}^{obs} : essentially, all of the ways to impute the missing ties in \mathbf{y}^{obs} . (When there are no missing ties in \mathbf{y}^{obs} , $\mathcal{Y}(\mathbf{y}^{\text{obs}})$ contains only \mathbf{y}^{obs} .) They then proposed to maximize this likelihood by taking advantage of the fact that, if

$$\kappa_{\mathcal{Y}'}(\boldsymbol{\theta}) \stackrel{\text{def}}{=} \sum_{\mathbf{y}' \in \mathcal{Y}'} h(\mathbf{y}') \exp\{\boldsymbol{\eta}(\boldsymbol{\theta})^\top \mathbf{g}(\mathbf{y}')\},\$$

the log-likelihood can be expressed as $\ell(\boldsymbol{\theta}) = \log \kappa_{\mathcal{Y}(\mathbf{y}^{\text{obs}})}(\boldsymbol{\theta}) - \log \kappa_{\mathcal{Y}}(\boldsymbol{\theta})$, resulting in the score equation

$$\boldsymbol{\nabla}_{\boldsymbol{\theta}} \ell(\hat{\boldsymbol{\theta}}) = \boldsymbol{\eta}'(\hat{\boldsymbol{\theta}})^{\top} [\mathsf{E}_{\mathcal{Y}(\mathbf{y}^{\mathrm{obs}})} \{ \mathbf{g}(\mathbf{Y}); \hat{\boldsymbol{\theta}} \} - \mathsf{E}_{\mathcal{Y}} \{ \mathbf{g}(\mathbf{Y}); \hat{\boldsymbol{\theta}} \}] = \mathbf{0},$$

with MCMLE (Markov chain maximum likelihood estimate) approximation also possible for the first term by fixing a particular θ^t and drawing a sample from $\text{ERGM}_{\mathcal{Y}(\mathbf{y}^{\text{obs}})}(\theta^t)$ as explained in Section 3 of Krivitsky *et al.* (2022). The **ergm** package invokes the above approach automatically when a network has missing edge variables. The simplest way to encode a missing edge is to set its value to NA. The **network** package natively supports missing edge variables coded in this way, and **network** objects with missingness are thus handled without additional intervention. **ergm**'s methods for assessing goodness of fit of a model by comparing observed values of certain network statistics to the distribution of their simulated values under the model (Hunter, Goodreau, and Handcock 2008a, Hunter *et al.* (2008b)) have also been adapted to missing edge data: the (unavailable) observed values of the statistics of interest $t(\mathbf{y})$ are replaced by their conditional expectations $\mathsf{E}_{\mathcal{V}(\mathbf{y}^{\mathrm{obs}})}\{t(\mathbf{Y}); \hat{\boldsymbol{\theta}}\}.$

Here we fit a simple model with edges, mutuality (reciprocated dyads), transitive ties, and cyclical ties to the Sampson Monks dataset depicted in Figure 1. For the sake of comparison, we first fit the model assuming no missing edge data, which may be quickly verified using the output of the print(samplike) command:

```
R> print(samplike)
```

```
Network attributes:
  vertices = 18
  directed = TRUE
  hyper = FALSE
  loops = FALSE
  multiple = FALSE
  total edges= 88
    missing edges= 0
    non-missing edges= 88
 Vertex attribute names:
    cloisterville group vertex.names
 Edge attribute names:
    nominations
R> summary(full.fit <- ergm(samplike ~ edges + mutual + transitiveties +
     cyclicalties, eval.loglik = TRUE), control = snctrl(seed = 321))
+
Call:
ergm(formula = samplike ~ edges + mutual + transitiveties + cyclicalties,
    eval.loglik = TRUE)
Monte Carlo Maximum Likelihood Results:
               Estimate Std. Error MCMC \% z value Pr(>|z|)
                            0.3745
                                         0 -5.172
                                                     <1e-04 ***
edges
                -1.9372
mutual
                 2.4684
                            0.4467
                                         0
                                             5.525
                                                     <1e-04 ***
                            0.3063
                                                     0.0786 .
transitiveties
                 0.5387
                                         0
                                             1.759
```

-0.4543

cyclicalties

0.2522

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

0 -1.802

0.0716 .

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Null Deviance: 424.2 on 306 degrees of freedom Residual Deviance: 329.0 on 302 degrees of freedom

AIC: 337 BIC: 351.9 (Smaller is better. MC Std. Err. = 0.624)

Now, suppose that Monk #1 (John Bosco) refused to respond during all three waves, rendering his replies missing:

```
R> samplike1 <- samplike
R> samplike1[1, ] <- NA
R> print(samplike1)
 Network attributes:
  vertices = 18
  directed = TRUE
  hyper = FALSE
  loops = FALSE
  multiple = FALSE
  total edges= 99
    missing edges= 17
    non-missing edges= 82
 Vertex attribute names:
    cloisterville group vertex.names
 Edge attribute names:
    nominations
```

-0.2741

cyclicalties

If we pass this modified object to ergm, it will automatically calculate the MLE under the assumption that the monk's refusal is unrelated to his choice of relations, i.e., that the data are ignorably missing with respect to the specified model:

```
R> summary(m1.fit <- ergm(samplike1 ~ edges + mutual + transitiveties +
     cyclicalties, eval.loglik = TRUE), control = snctrl(seed = 321))
+
Call:
ergm(formula = samplike1 ~ edges + mutual + transitiveties +
   cyclicalties, eval.loglik = TRUE)
Monte Carlo Maximum Likelihood Results:
              Estimate Std. Error MCMC % z value Pr(>|z|)
edges
               -2.0324
                         0.3847 0 -5.283
                                                  <1e-04 ***
                           0.4672
                                         5.143
                                                  <1e-04 ***
mutual
                2.4025
                                      0
transitiveties
                0.4631
                           0.4190
                                      0
                                           1.105
                                                   0.269
```

0.3806

0 -0.720

0.471

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Null Deviance: 400.6 on 289 degrees of freedom
Residual Deviance: 313.4 on 285 degrees of freedom
AIC: 321.4 BIC: 336 (Smaller is better. MC Std. Err. = 0.5569)

The degrees of freedom associated with the missing data fit have decreased because unobserved dyads do not carry information. For details regarding the ignorability assumption for edge variables, see Handcock and Gile (2010).

The estimation approach above can be extended to other types of incomplete network observation. Karwa, Krivitsky, and Slavković (2017) applied it to fit arbitrary ERGMs to networks whose dyad values had been stochastically perturbed – ties added and removed at random, with known probabilities – in order to preserve privacy. Another use case is multiple imputation for networks with missing data, in which multiple random versions of the full network are constructed by randomly inserting values for unobserved dyads according to probabilities that are determined based on, say, some type of logistic regression model. These mechanisms may be invoked by passing an obs.constraints formula, specifying how the network of interest was observed. Of particular interest are the following constraints:

observed: Restricts the proposal to changing only those dyads that are recorded as missing.

- egocentric(attr = NULL, direction = c("both", "out", "in")): Restricts the proposal to changing only those dyads that would not be observed in an egocentric sample. That is, dyads cannot be modified that are incident on vertices for which attribute specification attr has value TRUE or, if attr is NULL, the vertex attribute "na" has value FALSE. For directed networks, direction == "out" only preserves the out-dyads of those actors, and direction == "in" preserves their in-dyads.
- dyadnoise(p01, p10): Unlike the others, this is a soft constraint to adjust the sampled distribution for dyad-level noise with known perturbation probabilities, which can arise in a variety of contexts (Karwa *et al.* 2017). It is assumed that the observed LHS (left-hand side) network is a noisy observation of some unobserved true network, with p01 giving the dyadwise probability of erroneously observing a tie where the true network had a non-tie and p10 giving the dyadwise probability of erroneously observing a nontie where the true network had a tie. p01 and p10 can be either both be scalars or both be adjacency matrices of the same dimension as that of the LHS network giving these probabilities.

We may use the obs.constraints argument to re-fit the model above:

```
R> samplike2 <- samplike
R> samplike2[1,] <- 0
R> samplike2 %v% "responded" <- rep(c(FALSE,TRUE),c(1,17))
R> print(samplike2)
Network attributes:
  vertices = 18
```

```
directed = TRUE
  hyper = FALSE
  loops = FALSE
  multiple = FALSE
  total edges= 82
    missing edges= 0
    non-missing edges= 82
 Vertex attribute names:
    cloisterville group responded vertex.names
 Edge attribute names:
    nominations
R> summary(m2.fit <- ergm(samplike2 ~ edges + mutual + transitiveties +
     cyclicalties, obs.constraints = ~ egocentric(~ responded, "out"),
     control = snctrl(seed = 123)))
Call:
ergm(formula = samplike2 ~ edges + mutual + transitiveties +
    cyclicalties, obs.constraints = ~egocentric(~responded, "out"),
    control = snctrl(seed = 123))
Monte Carlo Maximum Likelihood Results:
               Estimate Std. Error MCMC % z value Pr(>|z|)
                                       0 -5.196
edges
                -2.0090 0.3867
                                                    <1e-04 ***
mutual
                 2.3890
                          0.4764
                                        0
                                            5.015
                                                    <1e-04 ***
                           0.4353
                                       0 1.011
                                                     0.312
transitiveties 0.4401
cyclicalties
               -0.2660
                            0.3918
                                        0 -0.679
                                                     0.497
___
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
     Null Deviance: 400.6 on 289
                                   degrees of freedom
 Residual Deviance: 313.9 on 285
                                   degrees of freedom
AIC: 321.9 BIC: 336.6 (Smaller is better. MC Std. Err. = 0.4579)
Finally, since the observational process can be viewed as a part of the network dataset, we
may specify it using the %ergmlhs% operation, giving a third way to fit the model above:
R> samplike2 %ergmlhs% "obs.constraints" <- ~ egocentric(~ responded, "out")</pre>
R> summary(m3.fit <- ergm(samplike2 ~ edges + mutual + transitiveties +
+
     cyclicalties), control = snctrl(seed = 231) )
Call:
ergm(formula = samplike2 ~ edges + mutual + transitiveties +
```

```
cyclicalties)
```

Monte Carlo Maximum Likelihood Results:

Estimate Std. Error MCMC % z value Pr(>|z|)edges -2.0288 0.3945 0 -5.142 <1e-04 *** 0.4694 5.123 <1e-04 *** mutual 2.4047 0 0.246 0.4685 0.4034 0 1.161 transitiveties cyclicalties -0.28440.3660 0 -0.777 0.437 ___ Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 Null Deviance: 400.6 on 289 degrees of freedom Residual Deviance: 313.1 on 285 degrees of freedom AIC: 321.1 BIC: 335.8 (Smaller is better. MC Std. Err. = 0.4385)

8. Other enhancements

We close this paper by highlighting a number of miscellaneous enhancements to the ergm package since the Hunter *et al.* (2008b) article.

8.1. Exact calculations for small networks

For small networks, it is possible to obtain full enumeration of all possible network statistic vectors over the entire sample space of possible networks. This enumeration enables exact calculations of such quantities as the log-likelihood function, the MLE, or the normalizing constant. If we consider only binary networks on an unconstrained sample space, the total number of networks is $2^{n(n-1)/2}$ for undirected networks and $2^{n(n-1)}$ for directed networks, which imposes a practical limit of n = 8 nodes in the undirected case or n = 6 in the directed case unless the user wants to compute for a long time, and the functions described in this section return an error for larger networks than these unless the **force = TRUE** option is invoked.

The ergm.allstats function, added to the ergm more than a decade ago in version 2.4, performs an efficient, "brute-force" tabulation of all possible network statistic vectors for an arbitrary ERGM by visiting every possible network. The ergm.exact function uses ergm.allstats to calculate exact likelihood values. Due to the computationally intractable normalizing constant $\kappa_{h,\eta,\mathbf{g}}(\boldsymbol{\theta},\mathcal{Y})$ of (1), except in the case of dyadic independence models, ergm.exact and ergm.allstats may only be used for small networks. In a test, the code below took about 254 times as long on a 9-node network as it did on an 8-node network, which is not surprising because the 9-node sample space has 2^{36-28} , or 256, times as many networks.

user system elapsed 46.288 0.061 46.391

Naturally, many networks of interest are too large to utilize ergm.allstats and ergm.exact. Yet calculations on small networks can still provide useful test cases; for instance, see Schmid and Hunter (2020) or Vega Yon, Slaughter, and de la Haye (2021).

8.2. Estimation based only on sufficient statistics

In exponential family parlance, $\mathbf{g}(\mathbf{y}^{\text{obs}})$ is often called the vector of sufficient statistics. Since the likelihood function of (5) depends on \mathbf{y}^{obs} only via these sufficient statistics, it is not actually necessary to observe \mathbf{y}^{obs} in order to calculate an MLE. The MLE-finding algorithm in **ergm** exploits this fact by implementing the idea of Hummel, Hunter, and Handcock (2012) to replace $\mathbf{g}(\mathbf{y}^{\text{obs}})$ by a vector of statistics that is closer to the sample mean generated by a current fixed, known parameter value. Maximizing the resulting version of the loglikelihood function yields a parameter value which may then be used to generate a new random sample of networks, and the process is repeated to give a sequence of parameter values approaching the desired MLE.

In some applications, such as when data are egocentrically sampled, it is possible to observe or estimate the vector $\mathbf{g}(\mathbf{y}^{\text{obs}})$ of statistics that would in principle have been observed in the network, even if other information about the network itself is absent. Estimation may still proceed by passing a target.stats argument containing a vector of network statistics. For example, we may reproduce (up to the stochasticity of the fitting algorithm) the analysis of the full.fit example in Section 7 by passing the vector of statistics on the samplike network via target.stats even though the network used in the ergm function call has no edges at all:

```
R> ts <- summary(samplike ~ edges + mutual + transitiveties + cyclicalties)
R> emptynw <- network.initialize(network.size(samplike), directed = TRUE)
R> ts.fit <- ergm(emptynw ~ edges + mutual + transitiveties + cyclicalties,
+ target.stats = ts, control = snctrl(seed = 123))
R> rbind(coef(full.fit), coef(ts.fit))
```

```
edges mutual transitiveties cyclicalties
[1,] -1.937163 2.468433 0.5387231 -0.4542983
[2,] -1.911295 2.459711 0.5375529 -0.4642011
```

8.3. Predicting individual edge probabilities

The predict method, which may be called on either formula or ergm objects, calculates model-predicted conditional or unconditional edge probabilities for dyads in a binary network. In the conditional case, we require not only a fitted ERGM but also a full network. For every possible *i* and *j*, the model-based conditional probability that $Y_{ij} = 1$, given the status of all other edges in the full network, is easily calculated based on (1). Indeed, this is exactly what the ergmMPLE function does in order to calculate an MPLE (maximum pseudo-likelihood estimator) (see Krivitsky *et al.* 2022, Section 3.1). Thus, when conditional = TRUE, the predict method produces exact calculations for any model.

By contrast, setting conditional = FALSE always results in simulation-based estimates of the edge probabilities – despite the fact that for any dyad-independent model, edges are independent of one another. This independence means that conditional and unconditional probabilities coincide, so exact unconditional probability calculations are possible as explained in the previous paragraph. On the other hand, for dyad-dependent models, it is generally computationally intractable to calculate exact unconditional edge probabilities, so only simulation-based estimates are possible.

The difference between conditional = TRUE and conditional = FALSE is best illustrated by a very simple dyad-independent model. Here, we consider **ergm**'s **g4** network with 4 nodes and 5 directed ties. We add a simple nodal covariate that indicates the first node, then fit a two-term dyad-independence model:

```
R> data("g4", package = "ergm")
R> g4 %v% "First" <- c(TRUE, FALSE, FALSE, FALSE)
R> SimpleERGM <- ergm(g4 ~ edges + nodecov("First"))</pre>
R> as.matrix(g4)
   V1 V2 V3 V4
V1
    0
       1
          1
             1
          0
V2
   0
       0
             0
VЗ
       0
          0
             0
    1
V4
   0
       0
          1
             0
```

Our model estimates one edge probability for node 1 and a second edge probability for all other nodes. The adjacency matrix above makes clear that 4 of the 6 possible edges incident on node 1 are present, while only 1 of the remaining 6 possible edges is present. This makes the exact edge probabilities according to this maximum likelihood-fitted model easy to calculate, and they coincide with those obtained using predict with conditional = TRUE:

```
R> predict(SimpleERGM, conditional = TRUE, output = "matrix")
          V1
                     V2
                               V3
                                          V4
V1 0.0000000 0.6666667 0.6666667 0.6666667
V2 0.6666667 0.0000000 0.1666667 0.1666667
V3 0.6666667 0.1666667 0.0000000 0.1666667
V4 0.6666667 0.1666667 0.1666667 0.0000000
On the other hand, conditional = FALSE forces a simulation-based estimate of the uncon-
ditional probabilities:
R> set.seed(123)
R> predict(SimpleERGM, conditional = FALSE, output = "matrix", nsim = 1000)
      V1
            V2
                   V3
                         V4
```

V1 0.000 0.673 0.649 0.677 V2 0.662 0.000 0.178 0.154 V3 0.683 0.165 0.000 0.185 V4 0.641 0.173 0.173 0.000

8.4. Flattened control arguments via a single list

Many of the core functions of **ergm** and related packages have **control** arguments that control various aspects of their working. Within just **ergm**, for instance, the functions **ergm**, **simulate** (for simulating a random network from a Markov chain with a specified ERGM as its stationary distribution), and **san** (for creating a network whose statistics match a given set of values) all require various control parameters. Packages such as **ergm.ego** include additional core functions like **ergm.ego** requiring control parameters. Moreover, it is not unusual that, say, a call to **ergm** will invoke **simulate** and possibly **san** implicitly. This means that a single **ergm** (or **ergm.ego**) call could have multiple lists of control parameters, sometimes passed as nested lists. **ergm** 4 implements a method that flattens these nested lists, allowing users to enter all control parameters in a single list. Furthermore, this method allows for the usual tab-completion of available arguments when using most R environments.

The key to entering control arguments for all of the various functions requiring them is the single function snctrl(), which is shorthand for "StatNet ConTRoL". The snctrl() function is used as the single value of the control argument in a function such as ergm. For instance, if we wish to force Monte-Carlo-based estimation in a simple ERGM that could be estimated exactly – because it is a dyadic independence model in which the pseudo-likelihood is the same as the likelihood – we might type

```
R> coef(ergm(g4 ~ edges, control = snctrl(force.main = TRUE, seed = 321)))
edges
```

-0.349256

If the code above is entered in RStudio, then pressing the tab key after typing ...control = snctrl(will reveal the various possible control parameters, including force.main. Additional illustrations of this method of entering control parameters are in Krivitsky *et al.* (2022).

ergm 4 is backwards-compatible with the previous method of passing control parameters via control.ergm, control.simulate, control.san, and others.

8.5. Improved help for model terms, constraints, and reference measures

As alluded to at several points earlier in this article, online help for model terms, which include term operators, may be obtained by typing either help("[name]-ergmTerm") or the shorthand version ergmTerm?[name], where [name] is the name of the term or operator. A full list of terms is available via ?ergmTerm, indexed by type and keywords. This list is updated dynamically as extension packages are loaded and unloaded. Similarly, help on sample space constraints or reference measures may be obtained by typing ?ergmConstraint or ?ergmReference, respectively. Available keywords and their meanings can be obtained by typing ?ergmKeywords. When using RStudio, it is possible to press the tab key after starting a line with ?ergm to view the wide range of possible help options beginning with the letters ergm.

8.6. Setting package options

ergm 4 has a number of options that affect ERGM estimation as well as the behavior of some terms, explained below as global options and term options, respectively. A current list of available options may be obtained via help("ergm-options") or the shorthand options?ergm.

Global options

A number of **ergm** behaviors can be set globally using the familiar **options()** command. For example, whether **ergm()** and similar functions evaluate the likelihood of the fitted model – a very computationally intensive process, particularly for valued networks – by default is controlled by option **ergm.eval.loglik**, which itself defaults to **TRUE**. Running

R> options(ergm.eval.loglik = FALSE)

instructs ergm() to skip likelihood calculation unless overridden in the call via ergm(..., eval.loglik = TRUE).

Other global options currently implemented are

- ergm.loglik.warn_dyads: Whether log-likelihood evaluation should issue a warning when the effective number of dyads that can vary in the sample space is poorly defined, such as if the degree sequence is constrained.
- ergm.cluster.retries: ergm's parallel routines implement rudimentary fault-tolerance. This option controls the number of retries for a cluster call before giving up.

ergm.term: This allows the default term options list, described below, to be set globally.

Term options

ergm 4 implements an interface for setting certain options for ERGM term behavior. The global setting is controlled via options(ergm.term = list(...)) where ... are key-value pairs specifying the options. Individual options can be overwritten on an ad hoc basis within a function call. For functions that have a control argument, such as ergm() and simulate(), this is done via a term.options control parameter, and for those that do not, such as summary(), it is done by passing the options directly or by passing a term.options argument with the list.

Options used as of this writing include:

- **version**: A string that can be interpreted as an R package version. If set, the term will attempt to emulate its behavior as it was that version of **ergm**. Not all past version behaviors are available.
- gw.cutoff: In geometrically weighted terms (gwesp, gwdegree, etc.) the highest number of shared partners, degrees, etc. for which to compute the statistic. This usually defaults to 30.
- cache.sp: Whether the gwesp, dgwesp, and similar terms should use a cache for the dyadwise number of shared partners. This usually improves performance significantly and therefore defaults to TRUE, but it can be disabled.
- interact.dependent: How to handle attempts to use interaction terms : and * with dyaddependent terms. Possible values are "error" (the default), "message", "warning", and "silent". Each of the last three will allow such terms, defined as described in Section 4.2 via their change statistics.

9. Discussion

Since version 2.1 of the **ergm** package was released concurrently with Hunter *et al.* (2008b), the package has undergone substantial changes. This paper describes the changes that are most likely to be of general interest, including – but not limited to – those that are new with the release of major version 4 (Handcock *et al.* 2023). Development of **ergm** and the growing list of related packages, many of which are described in Section 2 of this article, is ongoing. Thus, while this article describes many new features, it represents a snapshot of the evolving code comprising the **statnet** suite of packages for R (R Core Team 2022).

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Affiliation:

David R. Hunter Department of Statistics Pennsylvania State University University Park, PA 16802, United States of America E-mail: dhunter@stat.psu.edu URL: https://personal.psu.edu/drh20/

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