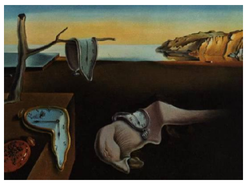

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ergm.graphlets: A Package for ERG Modeling Based on Graphlet Statistics

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Abstract

Exponential-family random graph models are probabilistic network models that are parametrized by sufficient statistics based on structural (i.e., graph-theoretic) properties. The **ergm** package for the R statistical computing environment is a collection of tools for the analysis of network data within an exponential-family random graph model framework. Many different network properties can be employed as sufficient statistics for exponential-family random graph models by using the model terms defined in the **ergm** package; this functionality can be expanded by the creation of packages that code for additional network statistics. Here, our focus is on the addition of statistics based on graphlets. Graphlets are classes of small, connected, induced subgraphs that can be used to describe the topological structure of a network. We introduce an R package called **ergm.graphlets** that enables the use of graphlet properties of a network within the **ergm** package of R. The **ergm.graphlets** package provides a complete list of model terms that allows to incorporate statistics of any 2-, 3-, 4- and 5-node graphlets into exponential-family random graph models. The new model terms of the **ergm.graphlets** package enable both exponential-family random graph modeling of global structural properties and investigation of relationships between node attributes (i.e., covariates) and local topologies around nodes.

Keywords: graphlet, graphlet degree, subgraph, exponential-family random graph model, **ergm**, **statnet**, R.

1. Introduction

Networks are widely used representations of complex, relational systems from different domains such as biology, sociology, economics, and technology. A *network* (or *graph*) consists of *nodes* (or *vertices*) that represent the objects of the complex system and *edges* that represent the relationships between the objects. For example, in a friendship network, the nodes correspond to people, and an edge is drawn between two people if they are friends with each other (illustrated example in Figure 1). Networks can be further enriched with node attributes that describe various categorical features (e.g., the gender of the people in the friendship network) or numeric features (e.g., the age of the people in the friendship network) of the nodes.

Understanding the processes underlying the formation of edges in a network is one of the main challenges in network modeling. Various network models describe different rules for formation of edges; e.g., Erdös-Rényi random graph models (also known as Bernoulli graphs; Erdös and Rényi 1959), so-called "scale-free" models (Barabási and Albert 1999), geometric models (Penrose 2003), and stickiness-index-based models (Pržulj and Higham 2006). Recent work on the statistical modeling of networks has focused on the use of discrete exponential families as general representations for these and other graph distributions. Exponential-family random graph models (ERG models or ERGMs, also known as "p*" models) are probabilistic network models that are parametrized in terms of sufficient statistics based on various topological properties (Holland and Leinhardt 1981; Pattison and Wasserman 1999; Robins, Pattison, Kalish, and Lusher 2007). In ERGMs, the conditional probability of the existence of an edge given the rest of the graph is determined by the effect that the edge has on the values of these statistics (and hence topology) which are conventionally called model *terms*. Using suitable model terms, ERGMs enable statistical investigation of the importance of different structural properties on the formation of edges. For example, for a friendship network, ERGMs can answer questions such as: Are the chances of a friendship tie between two persons enhanced by having a friend in common? Is this effect stronger than would be expected due to clustering on observed characteristics (e.g., gender)? Does this effect differ based on the gender or race of the common friend? Etc.

The **ergm** package (Hunter, Handcock, Butts, Goodreau, and Morris 2008b; Handcock, Hunter, Butts, Goodreau, Krivitsky, and Morris 2014) for the R statistical computing environment (R Core Team 2015) provides a set of tools for analyzing networks within an ERGM framework. The **ergm** package allows the users to define ERGMs based on a wide range of network properties, fit ERGMs to observed networks using likelihood-based methods, simulate networks from an ERGM, perform graphical goodness-of-fit tests of the type described by Hunter, Goodreau, and Handcock (2008a) and Handcock, Hunter, Butts, Goodreau, and Morris (2003). The **ergm** package itself provides a large but limited number of model terms. Custom model terms can be introduced into the **ergm** package using the **ergm.userterms** package (Handcock, Hunter, Butts, Goodreau, and Morris 2013).

Using the functionality of the **ergm.userterms** package, we introduce a new R package called **ergm.graphlets** that enables defining ERGMs based on induced subgraph (also known as *graphlet*) properties of networks. The **ergm.graphlets** package provide model terms for an extended list of subgraph properties that capture all connected, undirected, induced subgraph patterns of size 2, 3, 4 and 5. Furthermore, the terms of the **ergm.graphlets** package differ from the available subgraph property terms of the **ergm** package as only "induced" subgraph patterns are taken into account; when evaluating a subgraph induced on a set of nodes, all

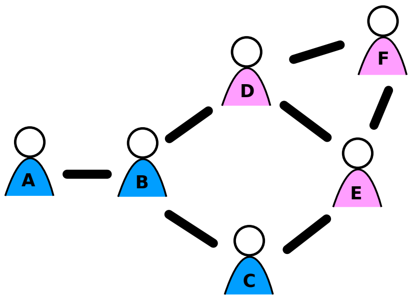


Figure 1: A hypothetical friendship network where nodes correspond to people and edges are drawn between nodes if they are friends with each other. The node colors correspond to gender (e.g., blue = male).

edges connecting the chosen set of nodes are considered.

In the remainder of this article, we proceed as follows. First, we provide some background information on various network properties, graphlets and ERGMs (Section 2). Second, we provide detailed explanations of the new model terms of the **ergm.graphlets** package in Section 3. Third, we illustrate the ERG modeling process with the new model terms on two real-world networks in Section 4. Finally, we conclude by providing a brief summary and discussing the future directions in Section 5.

2. Background

In this section, we provide a brief introduction to the graph-theoretic definitions, network properties, graphlets and exponential-family random graph models.

2.1. Definitions, network properties and graphlets

A *network* (or graph) is represented as $G = (V, E)$ where V is the set of nodes and E is the set of edges of graph G. Edges are represented by pairs of nodes, and represent ties; two node joined by an edge are said to be *adjacent*. A network G' is a *subgraph* of a network G if its nodes and edges are subsets of the nodes and edges of G. A subgraph G' is *induced* if it contains all the edges that appear between its nodes in its originating network G. Different subgraphs of a network can have very different configurations, such as a triangle, k-star, or k-cycle. A *triangle* is a complete network of three nodes (i.e., where each pair of nodes is adjacent). A *k-star* is a network of $k+1$ nodes where some node is adjacent to all other nodes. A *k-cycle* is a network of k nodes such that there exists an ordering of the nodes $v_1, v_2, \ldots, v_k$ such that each node is adjacent to the node immediately before and after it, and the first node is adjacent to the last.

For understanding complex systems, analyzing the topological properties of their network representations is crucial. Many such properties have been defined and found to be useful in various substantive contexts. The degree distribution (i.e., the distribution of the number of neighbors each node has), clustering coefficient (a measure of the tendency of edges to be contained in triangles), and diameter (i.e., the length of the maximum shortest path between any two nodes in the network) are among the most well-known examples of structural properties (Wasserman and Faust 1994; Newman 2010). Recent work has identified many useful properties based on graphlets. *Graphlets* are isomorphic equivalence classes of small, connected induced subgraphs within a larger network (Pržulj, Corneil, and Jurisica 2004). The set of possible graphlets of a given order (number of nodes) can be enumerated, and we depict the set of 2- to 5-node graphlets in Figure 2. A range of different structural properties can be defined by reference to graphlets. The most basic graphlet properties – *graphlet counts* – are defined as the number of times that each graphlet appears in a given network. E.g., for the friendship network in Figure 1: the count of G_0 is the number of edges in the network, 7; the count of G_1 is the number of induced two-path subgraphs, 8; the count of G_2 is the number of triangles, 1, etc. More refined network properties can be defined by considering the symmetries (i.e., automorphisms) within the graphlets (Milenković and Pržulj 2008). Two nodes within a network are said to belong to the same *automorphism orbit* (or *automorphic equivalence class*) if there exists a relabeling of nodes in the graph that exchanges the two nodes while preserving the graph's adjacency structure (Wasserman and Faust 1994). Applying this notion to each 2- to 5-node graphlet yields 73 equivalence classes (i.e., *orbits*), as illustrated in Figure 2. Each orbit reflects a distinct way of participating in a graphlet structure, and counts of orbit memberships provide a node-level indicator of structural position. The *graphlet degree* of a node is the number of graphlets that the node touches at a given orbit; this generalizes the conventional notion of *degree*, which is the size of a node's neighborhood (in graphlet terms, the number of type 0 orbits that it occupies). The computation of the 73 graphlet degrees for node A in the friendship network is illustrated in Figure 3. The vector containing the 73 graphlet degrees of a node, named the *graphlet degree vector (GDV)*, provides a detailed description of network structure local to a node. Finally, the third set of graphlet properties considered here summarizes the node-level graphlet degrees by considering their distribution over the whole network. A generalization of the degree distribution, the *graphlet degree distribution* of an orbit corresponds to the distribution of the corresponding graphlet degrees of all nodes in the network (with the conventional degree distribution being the graphlet degree distribution of orbit 0). The topology of a network can be richly described with the 73 graphlet degree distributions associated with each of the 2- to 5-node graphlet automorphism orbits.

2.2. Exponential-family random graph modeling

Exponential-family random graph models (ERGMs) are probabilistic network models parametrized by sufficient statistics based on different network properties. ERGMs are specified via three elements: a vector of terms (sufficient statistics or functions thereof); a vector of real-valued parameters; and a support (often chosen to be the set of all graphs or digraphs of a given order; Kolaczyk 2009; Hunter *et al.* 2008b).[1] Sufficient statistics for an ERGM can be functions representing any topological properties of the network (and, optionally, covariates), e.g., the number of edges, the degree distribution, the number of triangles, the number of k-stars, or the number of k-cycles. In general, few constraints on model terms are required; any real-valued functions are permissible, so long as they are finite and (for identifiable models) affinely independent on the support. Model terms can also relate node or edge attributes with their topological properties, e.g., the correlation between a node's attribute value and its degree. Readers can refer to Morris, Handcock, and Hunter (2008) for a summary of model

[1]Technically, a *reference measure* is also required; for unvalued graphs on finite support, this can be taken without loss of generality to be the counting measure (Krivitsky 2012).

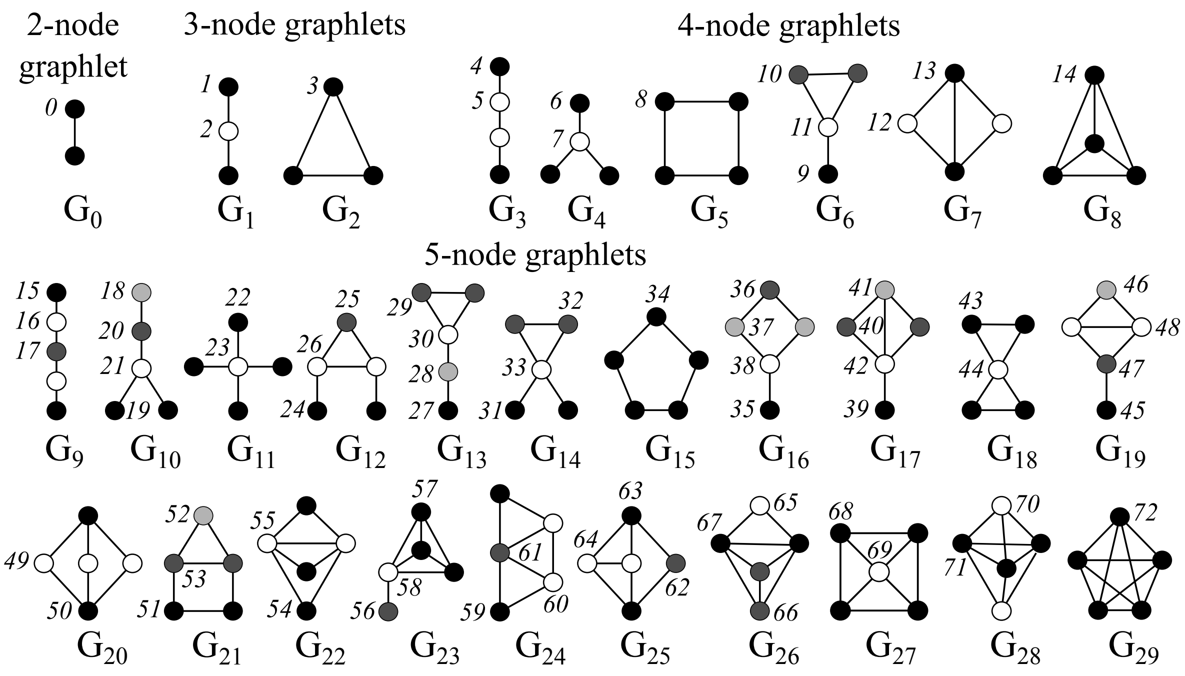
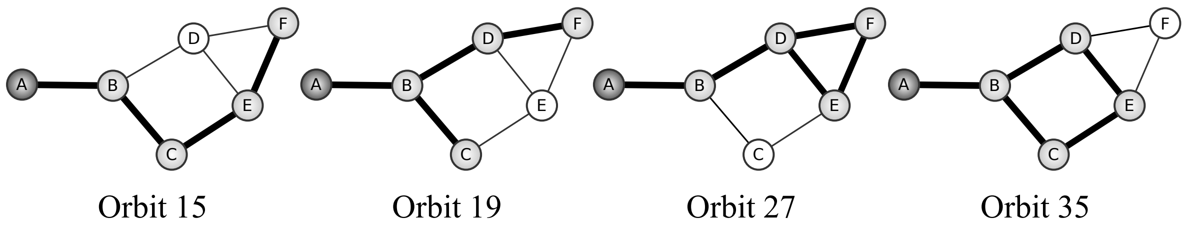


Figure 2: All 2-, 3-, 4- and 5-node graphlets, G_0, G_1, …, G_{29}, and their automorphism orbits, 0, 1, 2, …, 72. (Pržulj 2007)



Orbit	0	1	2...3	4	5	6	7...14	15	16...18	19	20...26	27	28...34	35	36...72
GDV(A)	1	2	0...0	3	0	1	0...0	1	0...0	1	0...0	1	0...0	1	0...0

Figure 3: Computation of the graphlet degree vector (GDV) of node A in the friendship network in Figure 1. The number of graphlets that node A touches at orbit i is the ith element of the GDV (Milenković and Pržulj 2008).

terms that are available in the **ergm** package.

ERGMs may be more formally summarized as follows. Let $\mathbf{Y}$ be a random variable that represents the n-by-n adjacency matrix of an unweighted, loopless (no self-edges), undirected network with n nodes. $\mathbf{Y}$ can have $2^{\binom{n}{2}}$ different values (configurations), where each value represents a different network having n nodes. The number of configurations arises from the fact that there are $\binom{n}{2}$ dyads in an order-n graph, each of which may here take two distinct states. The set of all possible configurations forms the *support* for $\mathbf{Y}$, denoted here by $\mathcal{Y}$. Any element of $\mathcal{Y}$ is a potential *realization* of $\mathbf{Y}$ and is represented by $\mathbf{y}$. An ERGM describes the probability of observing a realization, $\mathbf{y}$, as a function of a vector of sufficient statistics. The probability of observing a realization is expressed in ERGM form per Equation 1:

$$\mathsf{P}_{\theta,\mathcal{Y}}(\mathbf{Y}=\mathbf{y}|\theta,t)=\frac{\exp\{\theta^\top t(\mathbf{y})\}}{\sum_{z\in\mathcal{Y}}\exp\{\theta^\top t(z)\}},\mathbf{y}\in\mathcal{Y}, \tag{1}$$

where θ is the vector of model coefficients (i.e., the weights for the model terms) and t is the vector of sufficient statistics (i.e., model terms corresponding to network properties of interest; Frank and Strauss 1986; Wasserman and Pattison 1996). A generalization of the above to more general cases (e.g., graphs with loops, digraphs, etc.) is immediate given an alternative choice of $\mathcal{Y}$; extension to valued graphs is treated by Krivitsky (2012). Since any probability mass function for $\mathbf{Y}$ on finite $\mathcal{Y}$ can be written in this form, ERGMs are a fully general representation for random graphs of finite order.

In an inferential context, ERG models for an observed network, $\mathbf{y}$, are typically fit by estimating the model coefficients, θ, that maximize the conditional probability, $\mathsf{P}_{\theta,\mathcal{Y}}(\mathbf{Y}=\mathbf{y}|\theta,t)$ for some selected t (with statistics being chosen based on a combination of exploratory analysis and prior theory). The most common approaches to estimation are currently maximum pseudo-likelihood estimation (MPLE, generally avoided except as an approximation) and maximum likelihood estimation (MLE, implemented via one of several techniques). Since the computation of the normalizing factor (i.e., denominator) in Equation 1 is intractable, current MLE methods do not directly compute the normalizing factor, but instead, use Markov chain Monte Carlo (MCMC) algorithms to perturb the edge states of the networks one-by-one and estimate the model parameters based on the change statistics of these edge flips (for details, see Handcock *et al.* 2014). One consequence of this is that the model statistics themselves need never be directly computed: for most purposes, only the change scores of edge flips are directly necessary. This approach yields substantial savings in the computational time required for estimating the model parameters.

The **ergm** package also employs this approach for estimating the model parameters of an ERGM. For this reason, when defining new model terms with the **ergm.userterms** package, users need to focus on identifying efficient ways of computing the change statistics of the new model terms. For example, for defining "the number of edges" term, the implementation should return $+1$ when a new edge is added into the network and -1 when an edge is removed. Since these change statistics computations are likely to be performed millions of times during a typical MCMC run for parameter estimation, the computation of the change statistics should be time-optimized.

3. The ergm.graphlets package

We define graphlet statistics for ERGMs by introducing the **ergm.graphlets** package (Yaveroglu, Fitzhugh, Kurant, Markopoulou, Przulj, and Butts 2015) that is built upon the **ergm.userterms** package. The **ergm.graphlets** package is available from the Comprehensive R Archive Network (CRAN) at http://CRAN.R-project.org/package=ergm.graphlets. To install and load **ergm.graphlets**, type the following in R prompt:

```
R> install.packages("ergm.graphlets")
R> library("ergm.graphlets")
```

The **ergm.graphlets** package is open-source and released under GPL-2 and higher. The **ergm.graphlets** package introduces four graphlet based ERG modeling terms into the **ergm** package for R. These model terms are summarized as follows:

1. *Graphlet counts* – `graphletCount(g)`*:*

   Statistics for the number of times that a graphlet appears in a network can be included in an ERGM by using the `graphletCount` term. The question that the change score function of this term answers is: how does the number of graphlets of type G_i change when an edge is flipped in the network? This term has an optional argument, g. g is a vector of distinct integers representing the list of graphlets to be evaluated during the estimation of model coefficients (see Figure 2 for the list of graphlets). When this argument is not provided, all graphlets are evaluated by default. The term adds one network statistic to the model for each element in g. This term is defined for the 30 graphlets with up to 5 nodes. Therefore, g accepts values between 0 and 29.

   The `graphletCount` term shows similarity with some terms of the **ergm** package, e.g., `cycle`, `edges`, `kstar`, `threepath`, `triangle`, `twopath`. The major difference between these existing **ergm** terms and the `graphletCount` term is that the existing terms consider arbitrary subgraphs, while `graphletCount` enforces the subgraphs to be induced. For example, `graphletCount` does not count the two-path subgraphs in a three node subgraph forming a triangle, while the `twopath` term counts three different two paths in a triangle subgraph. A closer parallel is the `triadcensus` term, which counts induced subgraphs on three nodes; note, however, that the triad census includes all isomorphism classes of order 3, while the order 3 graphlets consist only of the classes corresponding to connected graphs. Thus, while there is overlap between some quantities computed by `graphletCount` and some existing **ergm** terms, the two are on the whole distinct.

2. *Graphlet orbit covariance* – `grorbitCov(attrname, grorbit)`*:*

   The correlation between a node's graphlet degree and a numeric attribute value can be included into an ERGM by using the `grorbitCov` term. The question that the change score function of this term answers is: what is the change in covariance between a vector of node attributes and graphlet degrees (for a given orbit) when an edge is changed? This term has two arguments: `attrname` and `grorbit`. The `attrname` is a character vector giving the name of a numeric node attribute. The optional `grorbit` argument is a vector of distinct integers representing the list of graphlet orbits to include into the ERGM model (see Figure 2 for the list of graphlet orbits). When `grorbit` is not provided, all graphlet orbits are evaluated by default. The term adds one network statistic to the model for each element in `grorbit`. Each term is equal to the sum given in Equation 2:

   $$grorbitCov(G, i, X) = \sum_{v \in V} GD_i(G, v) * X_v, \qquad (2)$$

   where X is the vector of node attribute values, i is the queried graphlet orbit and $GD_i(G, v)$ is the number of graphlets that touch node v at orbit i. This term is defined for the 73 orbits corresponding to graphlets with up to 5 nodes. Therefore, `grorbit` accepts values between 0 and 72.

   The `grorbitCov` term can be viewed as an extension of the the `nodecov` term in the **ergm** package to higher-order structures. In fact, the `nodecov` term is a special case of `grorbitCov` where the `grorbit` argument is set to 0.

3. *Graphlet orbit factor* – `grorbitFactor(attrname, grorbit, base)`*:*

   The `grorbitFactor` term adds a relationship between graphlet degrees and a categorical node attribute into an ERGM. The question that the change score function of this term answers is: what is the change in the total graphlet degree (for a given orbit) for those nodes with a given attribute value, for a particular edge change? This term has three arguments: `attrname`; `grorbit`; and `base`. `attrname` is a character vector giving the name of a categorical node attribute. The optional `grorbit` argument is a vector of distinct integers representing the list of graphlet orbits to include into the model (see Figure 2 for the list of graphlet orbits). When `grorbit` is not provided, all graphlet orbits are evaluated by default. The optional `base` argument is a vector of distinct integers representing the list of categories in `attrname` that are going to be omitted. When this argument is set to 0, all categories are evaluated. Otherwise, the attribute values are sorted lexicographically and the attributes that are indexed by the `base` value(s) are omitted. For example, if the “fruit” attribute has values “orange”, “apple”, “banana” and “pear”, `grorbitFactor("fruit", 0, 2:3)` will ignore the “banana” and “orange ” factors and evaluate the “apple” and “pear” factors. When the `base` argument is not provided, the argument is set to 1 by default. The `grorbitFactor` term adds $a * |$`grorbit`$|$ terms into the model where a represents the number of attribute values that are evaluated in the model and $|$`grorbit`$|$ is the number of graphlet orbits to be evaluated in the model. Each term is equal to the sum in Equation 3:

   $$\mathit{grorbitFactor}(G, i, X_c) = \sum_{v \in V, \mathit{category}(v) = X_c} GD_i(G, v), \tag{3}$$

   where X_c is the category of the term, i is the queried graphlet orbit, $\mathit{category}(v)$ is the category that node v belongs to, and $GD_i(G, v)$ is the number of graphlets that touch node v at graphlet orbit i. This term is defined for the 73 graphlet orbits corresponding to graphlets with up to 5 nodes. Therefore, `grorbit` accepts values between 0 and 72.

   The `grorbitFactor` term extends the `nodefactor` term in the **ergm** package. In fact, the `nodefactor` term is a special case of `grorbitFactor` where the `grorbit` argument is set to 0.

4. *Graphlet degree distribution* – `grorbitDist(grorbit, d)`*:*

   The graphlet degree distributions of different graphlet orbits can be included into the ERGM by using the `grorbitDist` term. The question that the change score function of this term answers is: how do the number of nodes having graphlet degree n for orbit i change when an edge is flipped? This term has two arguments: `grorbit` and `d`. The `grorbit` argument is a vector of distinct integers representing the list of graphlet orbits to include into the model (see Figure 2 for the list of graphlet orbits). The `d` argument is a vector of distinct integers. This terms adds one network statistic to the model for each pairwise combination of the arguments in `grorbit` and `d` vectors. The statistic for the combination of (i, j) is equal to the number of nodes in the network that have graphlet degree j for orbit i. This term is defined for the 15 graphlet orbits corresponding to graphlets with up to 4 nodes. Therefore, `grorbit` accepts values between 0 and 14. Graphlets of size 5 are omitted for this term because of the high computational complexity of the change score computation of the term.

The `grorbitDist` term extends the `degree` term in the **ergm** package. In fact, the `degree` term is a special case of `grorbitDist` where the `grorbit` argument is set to 0. However, the `grorbitDist` function does not support the filtering functionalities of the `degree` term that are defined with the `by` and `homophily` arguments.

For detailed explanations and algorithmic details on the implementation of the new terms of the **ergm.graphlets** package, please refer to Appendix A.

4. Illustration: ERGMs with graphlet terms

In this section, we illustrate the use of terms from the **ergm.graphlets** package with two examples, one from the social sciences (Figure 4A) and one from the biological sciences (Figure 4B).

4.1. Lake Pomona emergent multi-organizational network (EMON)

Our first example comes from Drabek, Tamminga, Kilijanek, and Adams (1981)'s set of inter-organizational communication networks in the context of search and rescue operations. The setting for our example is the immediate aftermath of the capsizing of the Showboat Whippoorwill following its contact with a tornado near the southern shore of Lake Pomona, due south of Topeka, Kansas (Drabek *et al.* 1981). Sixty passengers and crew were stranded in the lake, prompting the immediate response of the twenty organizations whose communication ties compose our network. We use the `grOrbitFactor` and `grOrbitCov` terms of the **ergm.graphlets** package to analyze the patterns of brokerage (i.e., mediator nodes that bridge two nodes that are not directly connected as described by Gould and Fernandez 1989) in the organizational search and rescue network. Previous studies of brokerage have been limited

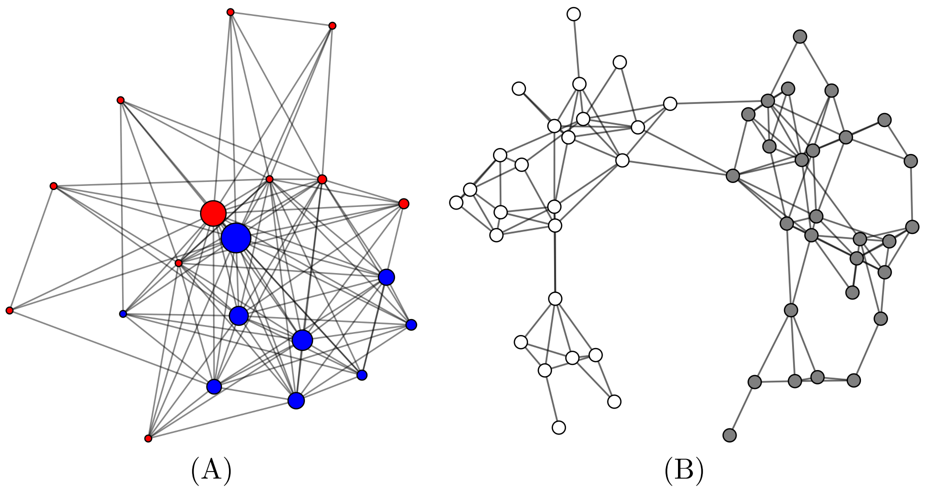


Figure 4: (A) Lake Pomona emergent multi-organizational network (EMON) tasked with a search and rescue operation. Node size is scaled by command rank score and nodes are colored by whether they had permanent headquarters situated locally (red) or non-locally (blue). (B) Network representation of the protein structure of the two matriptase-BPTI complexes. Secondary structure elements are shaded by the complex to which they belong.

to the use of marginal tests to determine whether levels of brokerage exceed what we would expect by some baseline (Gould and Fernandez 1989; Marcum, Bevc, and Butts 2012; Lind, Tirado, Butts, and Petrescu-Prahova 2008; Spiro, Acton, and Butts 2013). The introduction of these graphlet terms enables us to examine brokerage using conditional tests in which we can identify entities' propensities to occupy brokerage roles independent of confounding factors such as degree.

Although Drabek's *emon* dataset is originally represented as a digraph, informants were asked to report on communication between organizations (without regard to directionality) and the relation is thus inherently undirected. We symmetrize the original *emon* network via union rule (Krackhardt 1987), treating a tie as present if an informant from either involved organization reports it. We include the command rank score, location and sponsorship node attributes of the original network with our undirected version. *Command rank score* is a rating of each organization's prominence in the network's chain of command, as reported by informants from all organizations participating in the search and rescue effort. When ranking those with the strongest position in the chain of command, informants were limited to the six organizations present from the early phase of the response. As a result, some organizations were not ranked and have been coded "NA" in the *emon* data. For our example, we assume those who were not ranked have the lowest possible command rank score (arriving later and being more marginal to the unfolding response) and assign them a score of 0. The *location* of each group's headquarters was also recorded; organizations were situated locally or non-locally in the Lake Pomona response. Finally, we include the *sponsorship level* of each organization: city, county, state, federal, or private. The resulting undirected network can be readily loaded from the **ergm.graphlets** package by typing:

```
R> data("emon3", package = "ergm.graphlets")
```

We illustrate the network in Figure 4A. Our network resembles a core-periphery structure with the core primarily composed of non-local organizations and organizations with high command rank scores.

In our ERGM model for the *emon* network, we begin with an `edge` term for the total number of edges (baseline density). We use dyadic independence terms (i.e., `nodefactor` and `nodecov`) for sponsorship level and command rank score. One might expect organizations at different sponsorship levels to be involved with more or fewer communication partnerships than organizations from a different sponsorship; likewise, an organization's command rank score may be associated with its propensity to be involved in more communication partnerships. Finally, we include terms related to graphlet structure. Graphlet G_6, which involves brokerage between a dyad and a pendant, is a natural choice given the core-periphery structure of the graph, and we include all its orbits (i.e., 9, 10, and 11) into our model. We incorporate the location covariate into the term to evaluate whether an organization's location is associated with its propensity to occupy these specific orbits. The results will demonstrate whether the location of an organization in this type of subgraph is associated with its role as a pendant (orbit 9), member of a dyad with ties to a broker (orbit 10), or broker between the pendant and the dyad (orbit 11). We model the network as shown below:

```
R> emon.ergm <- ergm(emon.3 ~ edges + nodefactor("Sponsorship") +
+    nodecov("Command.Rank.Score") + grorbitFactor("Location", 9:11),
+    control = control.ergm(seed = 1, MCMC.samplesize = 50000,
+    MCMC.interval = 100000, MCMC.burnin = 50000, parallel = 60))
```

```
Iteration 1 of at most 20:
Loading required package: rlecuyer
Convergence test P-value: 0e+00
The log-likelihood improved by 0.6982
Iteration 2 of at most 20:
Convergence test P-value: 0e+00
The log-likelihood improved by 0.1079
...
Iteration 9 of at most 20:
Convergence test P-value: 9e-01
Convergence detected. Stopping.
The log-likelihood improved by < 0.0001

This model was fit using MCMC.  To examine model diagnostics and check
for degeneracy, use the mcmc.diagnostics() function.
```

Before examining the coefficients we examine the MCMC diagnostics to ensure the estimation process did not exhibit any peculiar behavior (Hunter *et al.* 2008a). This model appears to have converged properly.

A summary of the model object reproduces the original formula for the model, the coefficients, deviance measures, and measures of the goodness of fit.

```
R> summary(emon.ergm)

==========================
Summary of model fit
==========================

Formula:   emon.3 ~ edges + nodefactor("Sponsorship") +
nodecov("Command.Rank.Score") + grorbitFactor("Location", c(9:11))

Iterations:  20

Monte Carlo MLE Results:
                                 Estimate Std. Error MCMC %  p-value
edges                           -2.450670   0.688351      9 0.000473 ***
nodefactor.Sponsorship.County   -0.437354   0.319080      3 0.172175
nodefactor.Sponsorship.Federal -0.581708   0.606596      5 0.338852
nodefactor.Sponsorship.Private -0.041876   0.188267      1 0.824230
nodefactor.Sponsorship.State    -1.326516   0.785447      1 0.092967 .
nodecov.Command.Rank.Score       0.333315   0.075229      5  < 1e-04 ***
grorbitFactor.orb_9.attr_NL      0.009319   0.020540      0 0.650596
grorbitFactor.orb_10.attr_NL    -0.018051   0.014288      2 0.208081
grorbitFactor.orb_11.attr_NL     0.158800   0.031310      7  < 1e-04 ***
---

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

```
     Null Deviance: 263.4  on 190  degrees of freedom
 Residual Deviance: 144.8  on 181  degrees of freedom

AIC: 162.8    BIC: 192    (Smaller is better.)
```

The results show significant effects for our `edge` term, command rank score, and non-local organizations' occupation of orbit 11. The results show a strong, positive association between an organization's command rank score and its odds of forming a tie. Most relevant to our interests, we find that one of the automorphism orbit terms is significant. Specifically, we find a positive, significant association between an organization's being non-local (NL) and its propensity to occupy a brokerage role between a pendant and a dyad (orbit 11). Substantively, this demonstrates that non-local organizations tend to occupy this specific structure of extended brokerage in which an organization occupies a brokerage position between one organization and a pair of connected organizations. Interestingly, location is not related to occupancy of orbit 9 (a brokered pendant) or orbit 10 (a brokered cluster), which tells us that non-local organizations engaging in brokerage are not preferentially brokering between a local "core" and a non-local periphery. The role of the non-local organizations in brokerage for this response is thus richer than might be imagined at first blush.

We use the `gof` command to examine model adequacy. While the AIC and BIC demonstrate substantial improvements over a baseline model, the `gof` command measures demonstrate how well networks simulated from our model reproduce statistics from the original network. We examine the model's reproduction of four statistics: geodesic distance, degree distribution, edgewise shared partner distribution, and the triad census. We demonstrate below how we produce plots to examine these measures of fit.

```
R> EMONgof <- gof(emon.ergm, GOF = ~ degree + distance + espartners +
+    triadcensus)
R> par(mfrow = c(2, 2))
R> plot(EMONgof)
```

The plots are illustrated in Figure 5. As there are no clear discrepancies between the model-simulated networks and the original network, we find the model to be an adequate fit.

The graphlet orbit terms enable us to link local position to covariates in a model-based framework. As demonstrated, this is a useful tool for modeling brokerage, as we are able to link an entity's covariates to its propensity to occupy a specific brokerage role, whether it is a traditional (i.e., `twopath`) brokerage role or an extended brokerage role (e.g., orbit 11 in our model). Beyond brokerage, these techniques can extend to any particular automorphism orbit contained within a graphlet: pendants, clique members, or other nodes whose position may be linked to some categorical or continuous variable. Being able to incorporate these covariate-driven graphlet terms into a model-based framework will enhance our ability to understand which factors are associated with nodes' occupation of local positions within graphlets.

4.2. Protein secondary structure network

The past decade has seen a surge of interest in identifying network motifs (i.e., subgraphs that are overrepresented or underrepresented in a network, relative to chance; Milo, Shen-Orr,

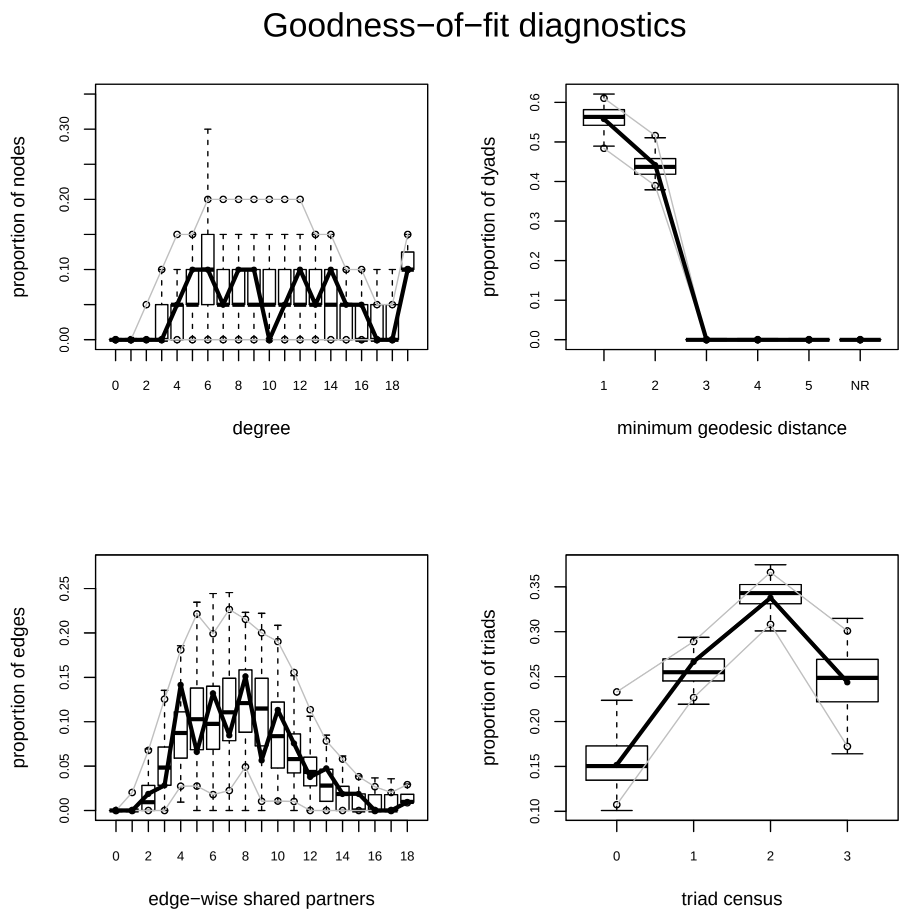


Figure 5: The solid black line in each plot represents the Lake Pomona EMON's observed statistics. The box plots illustrate the statistics for our simulated networks, as produced by the MLE.

Itzkovitz, Kashtan, Chklovskii, and Alon 2002; Milo *et al.* 2004). Typically, scholars have used marginal tests to identify how frequently these subgraphs occur relative to some baseline. In these types of tests the observed network is compared to a set of randomized networks that hold constant some statistic of the original network, often the degree distribution. While these types of marginal tests have been employed by networks scholars for decades (see, e.g., Wasserman and Faust 1994; Butts 2008, for reviews), a model-based approach allows us to examine the likelihood of observing these subgraphs, conditioned on a variety of parameters (e.g., degree, triadic closure, covariates, etc.). This is particularly important where the method of data collection itself may bias structure in particular ways; failure to account for these effects may result in spurious findings. We use the `graphletCount` terms to examine patterns of biological network motifs in an ERGM framework, while controlling for artifacts of the data collection process.

We analyse the the protein structure network of a matriptase-aprotinin complex (PDB ID: 1eaw; Friedrich *et al.* 2002) whose nodes are secondary structure elements (specifically, α helices and β sheets) which are "tied" if the distance between them is smaller than 10

Angstroms (Å) (Milo *et al.* 2004)[2]. Milo *et al.* (2004) examine the overrepresentation and underrepresentation of subgraphs in this network, by comparison to uniform random graphs conditional on the degree distribution. They find that subgraphs in the form of graphlets G_3 and G_4 are underrepresented while subgraphs in the form of G_6, G_7, and G_8 are over-represented. We will determine whether these results hold in a model-based framework that allows us to account for potentially confounding degree, transitivity, and mixing effects, some of which represent artifacts of the data collection process.

Before modeling the protein structure network, it is important to consider how this network was obtained. Although Milo *et al.* (2004) do not report on the content of the structure[3], Friedrich *et al.* (2002) note that the asymmetric unit of the crystal structure (from which the network is constructed) contains two biological assemblies, each of which is a complex of two proteins (the catalytic domain of matriptase/MT-SP1 and a bovine pancreatic trypsin inhibitor/BPTI). The presence of multiple copies of a biologically relevant complex within a crystal structure is a common artifact of the crystallization process, and indeed the same system could potentially have been observed with more or fewer complexes in the asymmetric unit. This is of considerable importance for modeling the resulting network, as we would typically expect far more adjacencies within complexes than between them; failure to control for this effect may lead to very misleading conclusions. Indeed, as shown in Figure 4B, the network is dominated by two dense subgraphs corresponding to the two complexes, with very few ties spanning these subgraphs. To account for this, we create vertex attributes based on biological assembly membership as reconstructed from information in the Protein Data Bank (Friedrich *et al.* 2002), with polypeptide chains A and B of the structure belonging to assembly 1, and chains C and D belonging to assembly 2. By incorporating these attributes into the model, we are much better able to account for the patterns of clustering in the network than we would be if we neglected the data collection process. The protein structure network containing the assembly membership node attributes can be readily loaded by typing:

```
R> data("spi", package = "ergm.graphlets")
```

We begin by setting up our ERGM with an `edges` term, a dyadic independence term, and several dyadic dependence terms, including our graphlet terms. Because we observe very little tie formation across the sets of chains associated with each complex, we include a homophily term for protein assembly in our model. Additionally, we include a within-assembly triadic closure term (i.e., closure of triads where all members belong to the same assembly). We also include a degree term, as the original paper was concerned with graphlet counts net of the degree distribution. Of principal interest is our `graphletCount` term, which includes graphlets G_3, G_4, G_6, G_7, and G_8, the same set Milo *et al.* (2004) find to occur at greater or lesser levels than chance.

Our first model includes all terms described above. To speed up model fit, one may omit the "control" arguments, although the resulting standard errors (and accordingly, p values) will be larger than what we report.

[2]This protein structure network can be obtained from: `http://www.weizmann.ac.il/mcb/UriAlon/Papers/networkMotifs/1eawInter_st.txt`.

[3]The structure is not described in the paper, and is (inaccurately) summarized in the supplemental materials only as "a serine protease inhibitor" (Table S1). In fact, the structure contains two assemblies, each of which is a complex of one domain of a serine protease (MT-SP1) with an inhibitor (BPTI).

```
R> spi.ergm.34678 <- ergm(spi ~ edges + nodematch("Assembly") +
+    triangle("Assembly") + gwdegree(0.5, fixed = TRUE) +
+    graphletCount(c(3, 4, 6, 7, 8)), control = control.ergm(seed = 1,
+    MCMC.samplesize = 500000, MCMC.interval = 75000, MCMC.burnin = 300000,
+    parallel = 60))

Iteration 1 of at most 20:
Loading required package: rlecuyer
Convergence test P-value: 0e+00
The log-likelihood improved by 0.3676
Iteration 2 of at most 20:
Convergence test P-value: 0e+00
The log-likelihood improved by 0.06913
...
Iteration 10 of at most 20:
Convergence test P-value: 8.3e-01
Convergence detected. Stopping.
The log-likelihood improved by < 0.0001

This model was fit using MCMC.  To examine model diagnostics and
check for degeneracy, use the mcmc.diagnostics() function.

R> summary(spi.ergm.34678)

==========================
Summary of model fit
==========================

Formula:   spi ~ edges + nodematch("Assembly") + triangle("Assembly") +
gwdegree(0.5, fixed = T) + graphletCount(c(3, 4, 6, 7, 8))

Iterations:  20

Monte Carlo MLE Results:
                  Estimate Std. Error MCMC %  p-value
edges             -6.42760    1.22926     12  < 1e-04 ***
nodematch.Assembly  2.48031    0.74204      6 0.000852 ***
triangle.Assembly   3.87343    0.67331      1  < 1e-04 ***
gwdegree            2.40227    1.51019      5 0.111906
graphlet.3.Count    0.04962    0.02964      7 0.094298 .
graphlet.4.Count   -0.03917    0.05467      1 0.473841
graphlet.6.Count   -0.15361    0.04993      0 0.002137 **
graphlet.7.Count   -0.47295    0.17782      0 0.007910 **
graphlet.8.Count   -2.49869    0.72543      0 0.000590 ***
---

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

```
     Null Deviance: 1910.3  on 1378  degrees of freedom
 Residual Deviance:  593.9  on 1369  degrees of freedom

AIC: 611.9    BIC: 658.9    (Smaller is better.)
```

Our model finds a significant, positive effect for within-assembly homophily, a positive effect for triadic closure within complexes, and a propensity for the graph to be biased against formation of graphlets G_6, G_7, and G_8, assuming all other terms are held constant. We find no significant results for graphlets G_3 and G_4.

We proceed to remove the non-significant terms to see if that improves model fit. AIC suffers slightly if we remove G_3 from the model (AIC: 612.97), while BIC improves (654.8). Both improve if we keep G_3 and remove G_4 (AIC: 610.73, BIC: 652.56). We find the best fit by removing both G_3 and G_4 (AIC: 610.7, BIC: 647.3). Accordingly, we fit our final model as follows.

```
R> spi.ergm.all <- ergm(spi ~ edges + nodematch("Assembly") +
+    triangle("Assembly") + gwdegree(0.5, fixed = TRUE) +
+    graphletCount(c(6, 7, 8)), control = control.ergm(seed = 1,
+    MCMC.samplesize = 15000, MCMC.interval = 2000, MCMC.burnin = 15000))

Iteration 1 of at most 20:
Convergence test P-value: 0e+00
The log-likelihood improved by 0.2026
Iteration 2 of at most 20:
Convergence test P-value: 0e+00
The log-likelihood improved by 0.05503
...
Iteration 8 of at most 20:
Convergence test P-value: 9.7e-01
Convergence detected. Stopping.
The log-likelihood improved by < 0.0001

This model was fit using MCMC.  To examine model diagnostics
and check for degeneracy, use the mcmc.diagnostics() function.

R> summary(spi.ergm.all)

==========================
Summary of model fit
==========================
Formula:   spi ~ edges + nodematch("Assembly") + triangle("Assembly") +
 gwdegree(0.5, fixed = T) + graphletCount(c(6, 7, 8))

Iterations:  20
```

```
Monte Carlo MLE Results:
                   Estimate Std. Error MCMC %  p-value
edges              -4.80106    0.73658      8  < 1e-04 ***
nodematch.Assembly  2.11636    0.66232      5 0.001428 **
triangle.Assembly   3.27864    0.53805      0  < 1e-04 ***
gwdegree            1.12902    1.21795      1 0.354095
graphlet.6.Count   -0.12037    0.04122      2 0.003560 **
graphlet.7.Count   -0.46225    0.16905      0 0.006330 **
graphlet.8.Count   -2.31074    0.68949      0 0.000826 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

     Null Deviance: 1910.3  on 1378  degrees of freedom
 Residual Deviance:  596.7  on 1371  degrees of freedom

AIC: 610.7    BIC: 647.3    (Smaller is better.)
```

Once again we find positive, significant effects for homophily within complexes and triadic closure within complexes. Controlling for this, we find negative, significant effects for graphlet terms G_6, G_7, and G_8.

Our final model appears to have converged without any notable issues (Hunter *et al.* 2008a). We now assess model adequacy. As Figure 6 indicates, our model closely approximates the observed network; our simulated networks show no clear deviations from the observed statistics on degree, geodesic distance, shared partners, or the triad census.

It is interesting to compare the results of our joint, multivariate analysis with the marginal tests conducted by Milo *et al.* (2004). Milo *et al.* (2004) find that the network overrepresents graphlets G_6, G_7, and G_8 and underrepresents G_3 and G_4. After controlling for other factors (particularly clustering within each complex), we find no evidence of additional underrepresentation or overrepresentation of G_3 or G_4; further, we actually find that the network appears biased *against* formation of graphlets G_6, G_7, and G_8, once other terms are accounted for. The discrepancy here is due to the use of marginal tests by Milo *et al.* (2004). To determine whether a graphlet occurs more or less often relative to chance, they compare the number of observed graphlets to the number observed in a set of random graphs conditioned on the degree distribution (a form of *conditional uniform graph test*). For this protein structure network, such random graphs bear little resemblance to the data in question (Figure 7), and in particular do not include effects related to the fact that the structure is a composite of two distinct complexes. While this does not make the results of such tests wrong per se, it does render them unable to distinguish between structural biases arising from simple features arising from the data collection process, and those arising from more subtle and informative biochemical mechanisms. The marginal approach is also unable to unravel the joint influence of multiple biases simultaneously; because graphlet structures are dependent upon one another, over- or underrepresentation of multiple graphlets (relative to a uniform baseline) may actually be the result of biases to a smaller number of features. Such complexities are difficult to unravel using marginal tests, and are more flexibly handled via the ERGM framework.

Our analysis underscores the fact that one can obtain misleading conclusions when trying to use marginal tests to assess graphlet counts, particularly when the baseline distribution being

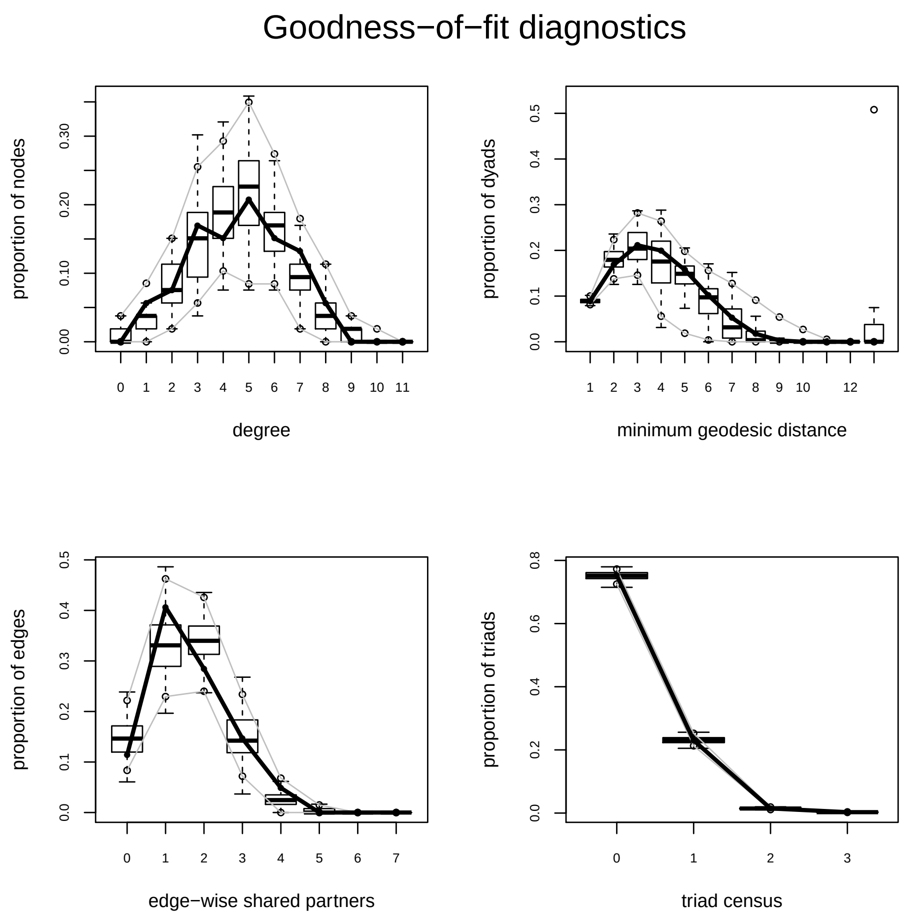


Figure 6: The solid black line in each plot represents the protein network's observed statistics. The box plots illustrate the statistics for our simulated networks, as produced by the MLE.

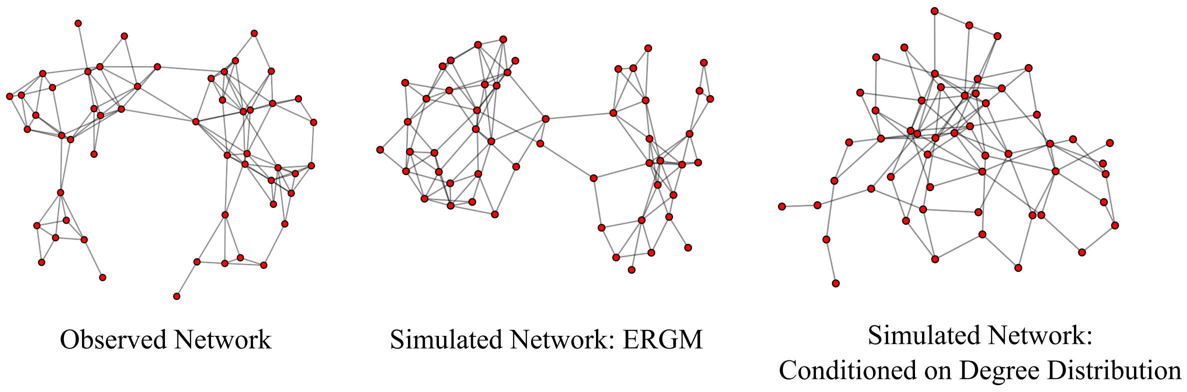


Figure 7: Observed protein network (left), typical protein network simulated by our final model (middle), and typical random graph produced by holding constant the observed network's degree distribution (right).

employed does not incorporate extremely basic features of the system being studied. While inference for complex, highly dependent systems is difficult under the best of conditions, the generative nature of the ERGM framework allows us to assess the adequacy of our models by comparison to features of the original data; given that we have identified a model that is both sensible and that successfully regenerates the important properties of the observed network, we have a stronger basis for subsequent investigation than would be obtained from simple rejection of a null hypothesis.

By using an ERGM approach and incorporating our graphlet terms, we are able to produce more sophisticated models of protein networks that include not only network motifs but also other important biological and/or chemical properties of the system in question. Scholars in a variety of biological sub-disciplines have begun to use ERGMs to model many different types of networks, including protein-protein interaction networks (Bulashevska, Bulashevska, and Eils 2010; Clark, Dannenfelser, Tan, Komosinski, and Ma'ayan 2012), neural networks (Hinne, Heskes, Beckmann, and van Gerven 2013; Simpson, Hayasaka, and Laurienti 2011; Simpson, Moussa, and Laurienti 2012), and metabolic networks (Saul and Filkov 2007). Introducing the tools from the **ergm.graphlets** package to the network community should enhance the field's ability to model graphlet counts in the context of network motifs or any other application where one is interested in counts of small, undirected, induced subgraphs.

5. Discussion

The **ergm.graphlets** package introduces four new terms into the **ergm** package which enable ERG modeling using the graphlet properties of a network. The `graphletCount` term enables defining ERGMs based on the number of graphlets in the network. `grorbitCov` term uses the relation between a numeric node attribute with a specific structural feature in order to introduce node attribute relations into a model. The `grorbitFactor` term is similar to the `grorbitCov` term except that it relates categorical node attributes with graphlet degrees. The `grorbitDist` term uses the graphlet degree distribution for ERG modeling. The `graphletCount`, `grorbitCov` and `grorbitFactor` terms are defined for graphlets with 2, 3, 4 and 5 nodes. Because of the computational complexity issues, `grorbitDist` is not defined for 5 node graphlets.

Model degeneracy, instability, and sensitivity are currently important challenges for modeling within the ERGM framework (Handcock 2003; Schweinberger 2011). For some combinations of model terms, the MCMC procedure may fail to converge within a reasonable number of iterations: this is generally because the graph distribution associated with the specified model family is ill-behaved. Like most dependence terms, the terms in the **ergm.graphlets** package sometimes suffer from these instability issues, depending on the modeled network and the other terms in the ERGM. Typically, degeneracy problems are currently handled either by using user-selected terms whose effects partially cancel (e.g., using sparse graphlets and complete graphlets together) or using curved exponential family models (Hunter and Handcock 2006; Butts 2011; Schweinberger 2011) that systematically combine large numbers of terms in a manner that balances their total effect. The former technique requires having an intuition about the structure of the data and a number of trials with different combinations of terms under this intuition. It can be hard to identify the best terms for generating an ERGM model and there is currently no general solution that works well in all settings. Our experience suggests that graphlet terms for which the change score is non-zero for most of the steps in the MCMC procedure are good terms to start the modeling process with. For example, it is not reasonable to model a sparse network using dense graphlets, as the change score will be 0 for most of the MCMC steps. In this respect, the graphlet terms that are expected to be overrepresented in the network can also be good candidate terms to start ERG modeling. Using terms of the same graphlet size together usually improves the convergence of the MCMC process, since smaller graphlets might already be contained in a number of larger graphlets and this causes dependency issues among model terms. We have also observed that the MCMC procedure converges faster when graphlets containing closed-loop structures (e.g., triangles, cycles) are excluded from the model definition: This is mainly because of the instability of these terms, as explained in Schweinberger (2011). As more data sets are subjected to analysis using ERGMs (and models with graphlet terms in particular), better heuristics are likely to emerge.

Past work with partial (i.e., non-induced) subgraph terms has suggested that curved exponential family models can also be used for improving degeneracy issues. In curved exponential families, the parameters associated with model statistics are constrained to lie on a non-linear surface of reduced dimension, forcing them to remain in a fixed relationship with one another; this can be helpful when dealing with intrinsically correlated graph statistics, as very precise weighting may be needed to avoid the degenerate regime. Examples of curved terms include the `gwdegree`, `gwdsp`, and `gwesp` terms of the **ergm** package, as well as the closely related *alternating k-star* and *alternating path* statistics of Snijders, Pattison, Robins, and Handcock (2006). Because graphlet statistics do not "nest" in the same way as partial subgraph statistics, they may benefit from novel formal development. On the other hand, some ideas used in existing curved families – e.g., geometrically weighted degree distributions – could potentially be applied to graphlet degrees in a relatively straightforward manner. This would seem to be a promising direction for future research.

When the over- or underrepresentation of a specific graphlet statistic is of particular interest but inclusion of this statistic into one's model proves difficult, another alternative is the use of a simplified model omitting the statistic as a reference distribution against which to test the observed graphlet statistic. Specifically, let t' be the statistic of interest, and let t be the vector of statistics in the best-fitting model without t'. A test of the hypothesis that the parameter θ' associated with the joint model $(t' \cup t, \theta' \cup \theta)$ is non-zero can be conducted by examining the quantiles of $t'(y)$ in the distribution of $t(Y)$, where $Y \sim \mathrm{ERG}(\hat{\theta}, t)$ and $\hat{\theta}$ is the MLE of θ given y. This approach (which was one motivation for the original development of ERGMs) is described in more detail by Holland and Leinhardt (1981).

Although we have tried to minimize the complexity of the change score computation, there is still room for improving the graphlet counting process. We apply a brute-force algorithm, which tries to minimize the number of computations: this gives an exact solution. Further gains in efficiency may be possible. These improvements would enable the implementation of `grorbitDist` for graphlets with 5 nodes. The model coefficients for terms related with larger graphlets would also be estimated more quickly with these improvements.

In addition to their inferential value, we note that the terms in the **ergm.graphlets** package can be used for evaluating the goodness-of-fit of an ERGM model estimate based on other (non-graphlet terms). When a model (with or without graphlet related terms) is estimated, the quality of this model in explaining the structure of the data in terms of graphlet properties of the network can be assessed by simulating new networks from the model and using the `summary` function to compute the graphlet counts and graphlet degree distributions. The graphlet properties of the network can be compared with these simulation results to evaluate whether the structure of the network fits to the structure described by the model. An example that describes how this test can be performed is explained in Goodreau, Handcock, Hunter, Butts, and Morris (2008).

In conclusion, the **ergm.graphlets** package extends the functionality of the **ergm** package by incorporating graphlet statistics. The new terms are of particular utility when modeling processes such as brokerage, functional mediation, or other phenomena that depend not only on the edges that are present within a graph, but also on those that are absent. Such processes are common in both social and biological systems, and the ability to capture them is an important goal of modern network analysis.

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A. Algorithms and implementation

The terms in the **ergm.graphlets** package are implemented using the **ergm.userterms** package (Handcock *et al.* 2013). The **ergm.userterms** package enables users to introduce new model terms into the **ergm** package by implementing C code which calculates the change statistics of the new term. For the **ergm.graphlets** package, the change score function should answer the question: how do the graphlet counts in the network and graphlet degrees of the nodes change when an edge is flipped in the network? This question can be answered efficiently by *touching* the graphlets on the flipped edge and counting only the graphlets that are going to be affected by the edge flip. For this purpose, we identify all *edge automorphism orbits* in graphlets with 2, 3, 4 and 5 nodes. The 69 different edge automorphism orbits are in Figure 8 (Solava, Michaels, and Milenkoviċ 2012). In this section, we use *node orbits* for graphlet orbits that are provided in Figure 2 and *edge orbits* for edge automorphism orbits in Figure 8 for clarity.

We apply a brute-force search algorithm for computing the change score for graphlet terms. For each flipped edge, the edge orbits that are related with the queried graphlet are mapped on the flipped edge and the neighborhood of that edge is searched for nodes that complete the graphlet. For each node combination that completes the graphlet, the count of the affected graphlets is incremented by one. For identifying the change in the count of a specific graphlet, the computation is performed only for relevant edge orbits. The relations among graphlets and edge orbits are summarized in Table 1. For example, the change score for the counts of graphlet G_{11} and G_{12} can be calculated by counting $E_{19}, E_{20}, E_{21}, E_{22}, E_{27}, E_{36}, E_{40}, E_{48}$. After counting these edge orbits, the change score for G_{11} is equal to $(E_{19} - E_{27})$ and the change score for G_{12} is equal to $(E_{20} + E_{21} + E_{22} - E_{36} - E_{40} - E_{48})$ where E_x represents the number of graphlets counted by placing edge orbit x on the flipped edge. By counting the graphlet change scores based on edge orbits, we do not only restrict the counting process to graphlets that are affected from the edge flip, but also avoid repeated counting of the same edge orbit for different graphlet counts. For instance, E_3 affects the count of G_2 positively and the count of G_1 negatively. With our implementation, the number of graphlets affected by E_3 is counted only once, and this change score is computed for identifying the changes in the counts of both G_1 and G_2. The edge orbit based counting procedure is applied for computing the change scores for all the terms in the **ergm.graphlets** package.

The computational complexity of this approach is dependent on the average degree (and therefore the density) of the modelled network. The *average degree* of a network is defined as the average number of ties that a node has in the network. The *density* of a network is defined as $\frac{|E|}{\binom{|N|}{2}}$ where $|E|$ is the number of edges and $|N|$ is the number of nodes in the graph. In the average case, the computational complexity of the change counting procedure is $O(d^2)$ where d represents the average degree of a node. The worst case scenario occurs when searching for graphlet G_9 in a clique. In this case, the computational complexity of the function is $O(n^3)$ where n is the number of nodes in the network. But this situation occurs very rarely as most real-world networks are sparse.

The four terms in the **ergm.graphlets** package are all implemented using edge orbits. However, the computation of the change scores differ slightly from each other depending on the way that the graphlet counts contribute to change statistics for these terms. The computation of the four terms in the **ergm.graphlets** package are explained as follows:

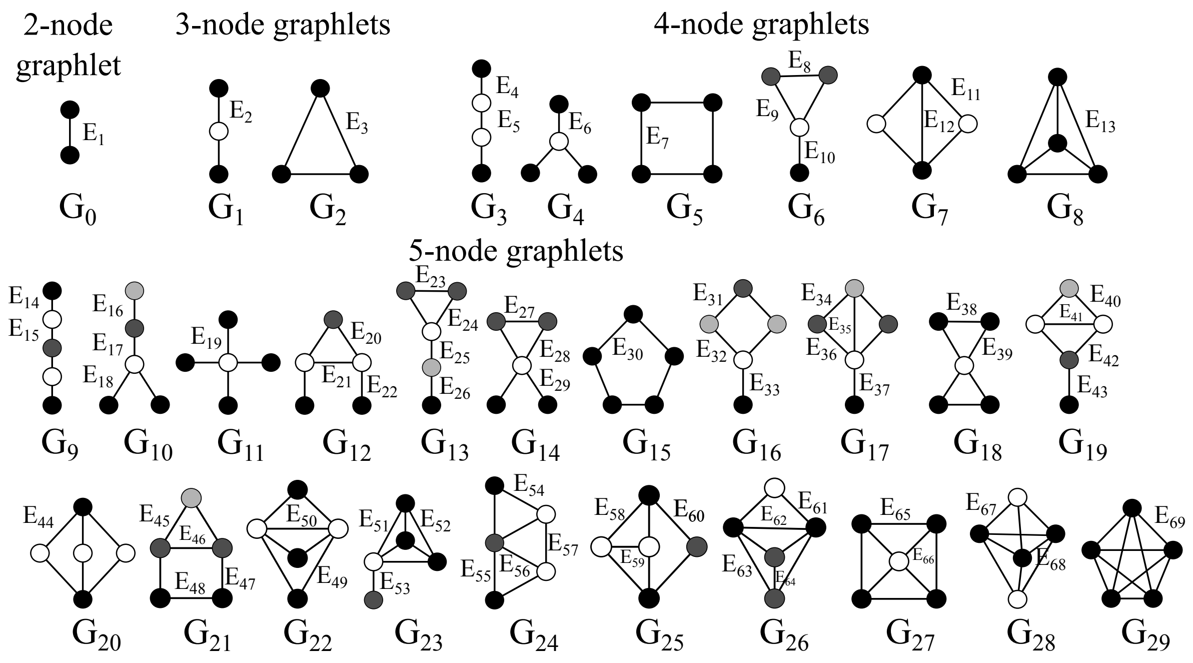
2-node graphlet
3-node graphlets
4-node graphlets
5-node graphlets
G0 G1 G2 G3 G4 G5 G6 G7 G8
G9 G10 G11 G12 G13 G14 G15 G16 G17 G18 G19
G20 G21 G22 G23 G24 G25 G26 G27 G28 G29
E1 E2 E3 E4 E5 E6 E7 E8 E9 E10 E11 E12 E13
E14 E15 E16 E17 E18 E19 E20 E21 E22 E23 E24 E25 E26 E27 E28 E29 E30 E31 E32 E33 E34 E35 E36 E37 E38 E39 E40 E41 E42 E43
E44 E45 E46 E47 E48 E49 E50 E51 E52 E53 E54 E55 E56 E57 E58 E59 E60 E61 E62 E63 E64 E65 E66 E67 E68 E69

Figure 8: The edge automorphism orbits in 2-, 3-, 4- and 5-node graphlets. Adapted from Solava *et al.* (2012).

	Edge automorphism			Edge automorphism	
Graphlet	Positive	Negative	Graphlet	Positive	Negative
G_0	E_1	–	**G_{15}**	E_{30}	E_{46}
G_1	E_2	E_3	**G_{16}**	E_{31}, E_{32}, E_{33}	E_{35}, E_{41}, E_{44}, E_{45}
G_2	E_3	–	**G_{17}**	E_{34}, E_{35}, E_{36}, E_{37}	E_{49}, E_{52}, E_{54}
G_3	E_4, E_5	E_7, E_9	**G_{18}**	E_{38}, E_{39}	E_{57}
G_4	E_6	E_8	**G_{19}**	E_{40}, E_{41}, E_{42}, E_{43}	E_{51}, E_{55}, E_{60}
G_5	E_7	E_{12}	**G_{20}**	E_{44}	E_{50}, E_{59}
G_6	E_8, E_9, E_{10}	E_{11}	**G_{21}**	E_{45}, E_{46}, E_{47}, E_{48}	E_{56}, E_{58}
G_7	E_{11}, E_{12}	E_{13}	**G_{22}**	E_{49}, E_{50}	E_{64}
G_8	E_{13}	–	**G_{23}**	E_{51}, E_{52}, E_{53}	E_{61}
G_9	E_{14}, E_{15}	E_{21}, E_{24}, E_{30}, E_{32}	**G_{24}**	E_{54}, E_{55}, E_{56}, E_{57}	E_{63}, E_{65}
G_{10}	E_{16}, E_{17}, E_{18}	E_{20}, E_{23}, E_{28}, E_{31}	**G_{25}**	E_{58}, E_{59}, E_{60}	E_{62}, E_{66}
G_{11}	E_{19}	E_{27}	**G_{26}**	E_{61}, E_{62}, E_{63}, E_{64}	E_{67}
G_{12}	E_{20}, E_{21}, E_{22}	E_{36}, E_{40}, E_{48}	**G_{27}**	E_{65}, E_{66}	E_{68}
G_{13}	E_{23}, E_{24}, E_{25}, E_{26}	E_{39}, E_{42}, E_{47}	**G_{28}**	E_{67}, E_{68}	E_{69}
G_{14}	E_{27}, E_{28}, E_{29}	E_{34}, E_{38}	**G_{29}**	E_{69}	–

Table 1: The relations between graphlet types and edge automorphism orbits. The "Positive" columns list the edge automorphism orbits that increase the graphlet count, and the "Negative" columns list the edge automorphism orbits that decrease the graphlet count when an edge is added.

1. `graphletCount(g)`: The counting procedure is based on identification of graphlets. Therefore, each identified graphlet directly increments (or decrements) the change score for the related graphlet by 1. The change score for this term is computed by counting all edge orbits that are associated with the graphlets provided in argument g. When all required edge orbits are counted, these counts are summed to get the overall change in

the number of graphlets. For example, the change score for graphlet G_{12} is equal to the summation of $(E_{20} + E_{21} + E_{22} - E_{36} - E_{40} - E_{48})$ where E_x represents the number of graphlets that touch the flipped edge on edge orbit x.

2. `grorbitCov(attrname, grorbit)`: This term relates a numeric node attribute with the graphlet degrees of the nodes according to Equation 2 as explained in Section 3. The change score of this term depends on the graphlet degrees. Therefore, for each identified graphlet, the nodes of this graphlet are associated with the node orbits that they correspond to. Let us say that a graphlet of type G_4 is identified for the subgraph of nodes a, b, c, d, when the edge $(a,\ b)$ is added into network. The identified subgraph is in Figure 9. Then the change score for node orbit 6 is incremented by $X_b + X_c + X_d$, and the change score for node orbit 7 is incremented by X_a, where X is the attribute vector keeping the attribute values for all nodes. The same logic applies when an edge is removed from the network. The final change score is obtained by summing these values for all edge orbits that are related with the graphlet that the query node orbit belongs to.

3. `grorbitFactor(attrname, grorbit, base)`: This term relates a categorical attribute with the graphlet degrees of the nodes according to Equation 3 as explained in Section 3. The change score of this term depends on the graphlet degrees. When the flip of an edge affects a node orbit, the change score that relates the category of the affected node with the node orbit is incremented (or decremented) by 1. Let us say a graphlet of type G_4 is identified for the subgraph of nodes a, b, c, d, when an edge $(a,\ b)$ is added into the network. The identified subgraph is in Figure 9. Nodes a and b belong to "Category 1", c and d belong to "Category 2". In this scenario, the change score for "Node Orbit 7, Category 1" and "Node Orbit 6, Category 1" will increase by 1 with the contribution of nodes a and b. The change score for "Node Orbit 6, Category 2" will increase by 2 because of the nodes c and d. The same logic applies when an edge is removed from the network. The final change score is obtained by summing these values for all edge orbits that are related with the graphlet that the query node orbit belongs to.

4. `grorbitDist(grorbit, d)`: This term identifies the change in the graphlet degree distribution of a node orbit when an edge is flipped during the MCMC process, as explained in Section 3. The change score computation for this term is slightly different from the other terms, as graphlet degrees for all nodes in the network are required for the computation. In order to reduce the computational complexity of the problem, we compute the graphlet signatures of all nodes at the beginning of the MCMC procedure. During the execution of the MCMC procedure, we update these signatures using the change scores. The computation of the changes in graphlet degrees of the nodes is performed similar to the algorithm applied for the other terms. However, as graphlets can convert to each other with the addition or removal of edges, the counting procedure should be applied for all edge orbits. Therefore, it is not possible to restrict the counting procedure to edge orbits that are related with the query node orbits. For these reasons, the computational complexity of this term is higher than the other terms in the **ergm.graphlets** package. We implement the `grorbitDist` term only for graphlets with 2, 3, and 4 nodes, because of the high computational complexity of the computation of change score for graphlets with 5 nodes.

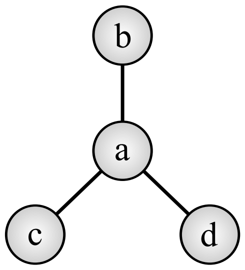

Figure 9: The subgraph that is used for illustrating the change statistics computation for the `grorbitCov` and `grorbitFac` terms.

We first test the correctness of the terms in the **ergm.graphlets** by using the `summary` function. The `summary` function computes the statistics for the provided terms. If the change score function is implemented correctly, the `summary` function produces the actual value of the term statistic for the provided network. In this respect, we validated the correctness of the `graphletCount` term by running:

```
R> summary(ntwk ~ graphletCount)
```

The output of the `summary` function was exactly the same as the graphlet counts produced by the graphlet counting implementation of Pržulj (2007). Evaluating the correctness of the `grorbitCov` term is slightly different from `graphletCount` as it is related with a node attribute value. To test the correctness of this term, we first created a dummy node attribute that is named "dummy". This node attribute has value 1 for all nodes in the network. We validated the correctness of `gorbitCov` by running:

```
R> summary(ntwk ~ grorbitCov("dummy"))
```

The output of the `summary` function was exactly the same with the sum of the graphlet degrees of all nodes for all node orbits. We repeated this test with weighted attribute values, e.g., when all attribute values are set to 2. The correctness of the results is also validated for this case. The validation for the `grorbitFactor` term is similar to the `grorbitCov` term. We assigned the same value for the category attribute, named "dummy", of all nodes and called the `summary` function as:

```
R> summary(ntwk ~ grorbitFactor("dummy", 0:72, 0))
```

This call correctly returns the sum of graphlet degrees of all terms. When the category value is changed to another value, the output of the call does not change. Finally, for validating the `grorbitDist` term, we called the `summary` function as:

```
R> summary(ntwk ~ grorbitDist(0:14, 0:10))
```

This call produces the correct graphlet degree distributions for all node orbits as validated in comparison with the output of the implementation of Pržulj (2007).

We also validated the correctness of our implementation by performing simulations on ERGMs that contain graphlet terms. In these tests, we defined ERGMs containing an `edge` term and a graphlet term. We manually set the model coefficient for the graphlet related term to various positive and negative values. We simulated 30 networks from each of these ERGMs. With these simulations, we validated that positive coefficients promote the count of the related graphlet in the simulated networks. The count of related graphlet increases up to a certain coefficient value. After this threshold, the simulated networks contain the maximum possible number of related graphlets in the simulated networks. Similarly, negative coefficients have an effect of suppressing the appearance of the graphlet in the simulated networks. As the coefficient value gets closer to 0, the suppressing effect disappears. The range where the graphlet counts increase with the coefficient depends on the coefficients of the other terms in the ERGM.

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