Statistical Models for Degree Distributions of Networks

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Abstract

We define and study the statistical models in exponential family form whose sufficient statistics are the degree distributions and the bi-degree distributions of undirected labelled simple graphs. Graphs that are constrained by the joint degree distributions are called dK-graphs in the computer science literature and this paper attempts to provide the first statistically grounded analysis of this type of models. In addition to formalizing these models, we provide some preliminary results for the parameter estimation and the asymptotic behaviour of the model for degree distribution, and discuss the parameter estimation for the model for bi-degree distribution.

1 Introduction and background

Introduction. Exponential random graph models (ERGMs) form a flexible and powerful family of statistical models for network data, used in variety of fields and especially in the social scenes; see [17] and other papers within the same special issue. These models are of exponential family form with proposed sufficient statistics that can range from the number of edges of the network [9] to the number of k-stars, or other graphical features of networks; see for example [12] [10].

While ERGMs can be specified using any network statistics, it has been long known that node degrees and statistics thereof have great expressive power in representing and modeling networks, perhaps more than most network statistics. See, e.g., [15] and [11]. Some of the recent literature on ERGMs have focussed on the properties of the beta model, for which the degree sequence of a network is the sufficient statistic and postulates independent edges; see [2], [7], and [16]. In this paper we consider instead the less studied class of ERGMs whose sufficient statistics are derived from the joint degree distribution of the nodes, for which the assumption of dyadic independence no longer holds.

This work is motivated in great part by the desire to describe the statistical properties of a class of network statistics known as dK-graphs, originally proposed by [13]. dK-graphs were originally formulated as a means to capture increasingly refined properties of networks in a hierarchical manner based on higher order interactions among node degrees (see, e.g., [8]). Despite the significant appeal of dK graphs as summary statistics of networks and their ability to capture stochastic dependencies among noes (see, in particular, [18]), to the best of our knowledge, the statistical properties of such statistics have not been investigated. The purpose of this paper is to uninitiate such study and to offer some preliminary but non-trivial results that
highlight the complexity and modeling power of these statistics. Like it is often the case with ERGMs relying on network statistics that are not based on dyadic independence, the theoretical analysis is particularly challenging.

**Contributions.** This paper contains the following contributions. We formally define ERGMs based on $dK$ sequences of different dimensions. For the 1K and 2K models, we derive conditions for the existence of the MLE of the model parameter and, therefore, for their estimability. We consider the general case of $m \geq 1$ i.i.d observations, which in particular includes the more interesting and common case of $m = 1$ observed network. We are concerned with the asymptotic behavior of the above model and compare it specifically to the behavior of the dense Erdős-Rényi model. We show that the 1K model is in fact radically different from the Erdős-Rényi model, an appealing feature that many ERGMs do not always possess, as demonstrated by $\S$. Finally, we define the ERGM with bi-degree distribution and provide ideas and conjectures for further work for such models.

**Basic definitions and concepts.** We denote the set of simple, undirected, labeled graphs with $n$ nodes by $\mathcal{G}_n$. If in an iid sample there is at least one observation of each members of $\mathcal{G}_n$, a natural estimation of the probability of observing $g \in \mathcal{G}_n$ is the ratio of the number of observations of $g$ to the total number of observations. However, in most practical cases, there are considerably fewer observations than this, and in the most common case, there is only one observation available.

For the above purpose, we propose a family of ERGMs in order to extract as much information as possible on the (joint) degrees of nodes of the few available observations. More precisely, the sufficient statistics of a model in this family are scaled forms of the number of induced connected subgraphs with a specific number of nodes with the same degree sequence. We call such subgraphs configurations. For example, for one-node configurations of the graph $g$ with $n$ nodes, that is, nodes of $g$, the sufficient statistics are the number of nodes with degrees $(0, \ldots, n - 1)$, denoted by $n^{(1)}(g) = (n_0(g), n_1(g), \ldots, n_{n-1}(g))$; and for two-node configurations of $g$, that is, edges of $g$, the sufficient statistics are the number of edges with degrees $((1, 1), (1, 2), \ldots, (n-2, n-1), (n-1, n-1))$, denoted by $n^{(2)}(g) = (n_{11}(g), n_{12}(g), \ldots, n_{n-1,n-1}(g))$, whose components are indexed lexicographically. The three-node configurations of $g$ are triangles (i.e., complete subgraphs with three nodes) and 2-stars (i.e., subgraphs with three nodes, in which a node is connected to two non-adjacent nodes) of $g$, and so on. For example, in the graph $g$ in Figure 1, $n^{(1)}(g) = (n_0(g), n_1(g), n_2(g), n_3(g)) = (0, 1, 2, 1)$ and $n^{(2)}(g) = (n_{11}(g), n_{12}(g), n_{13}(g), n_{22}(g), n_{23}(g), n_{33}(g)) = (0, 0, 1, 1, 2, 0)$.

![Figure 1: Graph $g$ with $n^{(1)}(g) = (0, 1, 2, 1)$ and $n^{(2)}(g) = (0, 0, 1, 1, 2, 0)$.](image)

In general, the vector $n^{(d)}(g)$ of length $\binom{n}{d}$ can be defined in the same fashion for connected subgraphs with $d$ nodes (i.e. configurations), and it can be represented in a normalized form, scaled by the number of all $d$-node configurations in the graph. For example, since $\sum_{k=1}^{n-1} n_k(g) = n$, instead of $n^{(1)}(g)$, one can use $n^{(1)}(g)/n$, which is generally called the degree distribution of $g$. In higher orders, $n^{(d)}(g)$ is called the joint degree distribution of $g$, and in particular the normalized $n^{(2)}(g)$ is called the bi-degree distribution of $g$.

Notice also that $n^{(1)}(g)$ is another way of expressing, and hence contains no more information than, the degree partition of the unlabelled graph $g$, that is, $\bar{d}(g) = (d_1(g), \ldots, d_n(g))$, where each $d_i$ represents
the degree of a node in $g$, usually ordered in a way such that $d_1(g) \geq d_2(g) \geq \cdots \geq d_n(g)$. The degree sequence can also be generalized for higher orders to give the joint degree partition of a graph.

**The $dK$-graph models.** The set of graphs constrained by the joint degree distribution is called the $dK$-graphs, where $d$ is the same as above, standing for the number of nodes of the configuration. The joint distribution itself is sometimes called the $dK$-distribution. As a convention, the $0K$-distribution is the average degree, that is, the ratio of the number of edges to the number of nodes in the graph. Thus $n^{(0)}(g)$ can be defined as $e(g)$, the number of edges of $g$. The corresponding model is equivalent to the Erdős-Rényi model after reparameterizing $p$ in the $0K$ model with its odd $p/(1 - p)$.

For the above reason, we refer to the proposed statistical models in exponential family from $\exp\{\sum_{k=0}^{n-1} s_k(g) \alpha_k - \psi(\alpha)\}$, with sufficient statistics $s_k(g) = n^{(d)}(g)$ as the $dK$ models. These models assign the same probability of occurrence to all graphs with the same joint degree distributions of corresponding order.

These models are also hierarchical in the sense that from $n^{(d)}$, all $n^{(d')}$, $0 \leq d' \leq d$, are uniquely determined, whereas the converse is not true. For example, the following observation provides a method for obtaining $n^{(0)}$ from $n^{(1)}$:

$$e(g) = \frac{1}{2} \sum_{k=0}^{n-1} kn_k(g);$$

and the following observations provide a method for obtaining $n^{(1)}$ from $n^{(2)}$:

$$n_k(g) = \frac{1}{k} \sum_{k'=1}^{k} n_{k'k}(g) + \sum_{k'=k}^{n-1} n_{k*k'}(g)), k \in \{1, \ldots, n - 1\};$$

$$n_0(g) = n - \sum_{k=1}^{n-1} n_k(g).$$

Hence by moving from a higher order model to a lower one, one loses some information that can be inferred from the data. This can be seen as the fact that, by moving towards a lower order, there would be a larger sets of graphs with the same sufficient statistics. Lower order models, on the other hand, enable us to infer the structure of a larger set of possible graphs based on the more local characteristics of the observed graphs. Bespeaking, for lower order models, more parameters can be estimated when there are no observations of some joint degree distributions at all.

However, in practice, there are usually very few observations, and in many cases only one observation available; hence it is normally more practical to work with the $1K$ or $2K$ models. This is the direction we take in this paper, and hence we only focus on the $1K$ and $2K$ models.

**Structure of the paper.** In the next section, we study the $1K$ model, discussing the calculation of the normalizing constant, the existence and calculation of maximum likelihood estimation, as well as the asymptotic behavior of the MLE. In Section 3 we apply a parallel theory in order to define the $2K$ model, and we present some ideas and conjectures regarding the maximum likelihood estimation for further work.

### 2 The $1K$ model

**The exponential family form.** As mentioned before, our goal is to model the probability of observing a network $g$ with $n$ nodes. Denote the probability of a node having degree $k$ by $p_k$. Considering the ordered
vector of possible degrees \((0, \ldots, n-1)\) in \(g\), the probability of observing \(g\) can be written as

\[
P(g) = \varphi(p) \prod_{k=0}^{n-1} p_k^{n_k(g)},
\]

where \(n_k(g)\) is the number of nodes with degree \(k\) in \(g\), \(\varphi\) is a normalizing constant, and \(\sum_{k=0}^{n-1} p_k = 1\).

To write (3) in a minimal form, we use the parametrization \(\tilde{p}_k = p_k / \tilde{p}_{n-1}\), which by using the fact that \(\tilde{p}_{n-1} = 1\), implies \(p_{n-1} = 1 / (1 + \sum_{k=0}^{n-2} \tilde{p}_k)\). Therefore, (3) can be rewritten as

\[
P(g) = \varphi(p)p_{n-1}^{\sum_{k=0}^{n-1} n_k(g)} \prod_{k=0}^{n-1} \tilde{p}_k^{n_k(g)} = \frac{\phi(\tilde{p})}{(1 + \sum_{k=0}^{n-2} \tilde{p}_k)^n} \prod_{k=0}^{n-2} \tilde{p}_k^{n_k(g)}.
\]

This in turn can be parametrized in exponential family form as

\[
P(g) = \exp \left\{ \sum_{k=0}^{n-2} n_k(g) \alpha_k - \psi(\alpha) \right\},
\]

where \(\alpha_k = \log \tilde{p}_k\) and \(\psi(\alpha) = n \log (1 + \sum_{k=0}^{n-2} \exp(\alpha_k)) - \log \phi(\tilde{p})\).

We reduced the dimension of the sufficient statistics by arbitrarily removing the element \(n_{n-1}\), to obtain \(n^{(1)}\) as sufficient statistics. We see that this model assigns the same probability to graphs with the same degree distribution, which is the only information the model collects from the data.

**Calculating the normalizing constant.** We know that \(\sum_{g \in G_n} P(g) = 1\), where \(G_n\) is the set of all non-isomorphic graphs with \(n\) nodes. We use this to calculate the normalizing constant \(\psi(\alpha) = \psi_n(\alpha)\) for a fixed \(n\). In this case the normalizing constant can be calculated directly from the set of all graphs with \(n\) nodes. Denote all these graphs by \(G_n = \{g_1, \ldots, g_M\}\), where \(M = 2^{\binom{n}{2}}\).

**Proposition 1.** The normalizing constant for the 1K model can be written as

\[
\psi(\alpha) = \log (1 + \cdots + \prod_{k=0}^{n-2} \tilde{p}_k^{n_k(g_i)} + \cdots + \tilde{p}_0^{n_k(g_M)}) = \log (1 + \cdots + e^{\sum_{k=0}^{n-2} n_k(g) \alpha_k} + \cdots + e^{n \alpha_0}),
\]

where there are \(M\) terms corresponding to each \(g_i \in G_n\), and the first and the last terms correspond to the complete and the null graphs.

**Proof.** Assume that \(g_1\) is the complete graph, \(g_M\) is the null graph, and \(g_i\) is an arbitrary graph with \(n\) nodes. Equation (4) implies that \(P(g_1) = \phi(\tilde{p})/(1 + \sum_{k=0}^{n-2} \tilde{p}_k)^n\), \(P(g_M) = \tilde{p}_0^n \cdot \phi(\tilde{p})/(1 + \sum_{k=0}^{n-2} \tilde{p}_k)^n\), and \(P(g_i) = \prod_{k=0}^{n-2} \tilde{p}_k^{n_k(g_i)} \cdot \phi(\tilde{p})/(1 + \sum_{k=0}^{n-2} \tilde{p}_k)^n\). Now by using \(\sum_{i=1}^{M} P(g_i) = 1\) we obtain \(\phi(\tilde{p}) = (1 + \sum_{k=0}^{n-2} \tilde{p}_k)^n / (1 + \cdots + \sum_{k=0}^{n-2} \tilde{p}_k^{n_k(g_i)} + \cdots + \tilde{p}_0^{n_k(g_M)})\). This, together with \(\alpha_k = \log \tilde{p}_k\) and \(\psi(\alpha) = n \log (1 + \sum_{k=0}^{n-2} \exp(\alpha_k)) - \log \phi(\tilde{p})\), implies (6).

\[\square\]

Notice that in (6) there are repeated terms for different labeling of isomorphic graphs as well as non-isomorphic graphs with the same degree distribution. We illustrate the proposition with an example; see also [14] for asymptotic estimates of the number of graphs in \(G_n\) with a prescribed degree distribution.

**Example 1.** There are 4 non-isomorphic graphs with 3 nodes, where \(g_2\) and \(g_3\) are repeated three times for different labeling:
Proposition \[\text{implies}\]
\[\psi(\alpha) = \log(1 + 3\tilde{p}^2 + 3\tilde{p}^2\tilde{p}_0 + \tilde{p}_0^3) = \log(1 + 3e^{2\alpha_1} + 3e^{2\alpha_1+\alpha_0} + e^{3\alpha_0}).\] (7)
This can be verified by considering \[\text{[4]},\] which implies that \(P(g_1) = \phi(\tilde{p})/(1 + \tilde{p}_0 + \tilde{p}_1)^3,\) \(P(g_2) = \tilde{p}_1^2 \cdot \phi(\tilde{p})/(1 + \tilde{p}_0 + \tilde{p}_1)^3,\) \(P(g_3) = \tilde{p}_1^2 \cdot \tilde{p}_0 \cdot \phi(\tilde{p})/(1 + \tilde{p}_0 + \tilde{p}_1)^3,\) and \(P(g_4) = \tilde{p}_0^3 \cdot \phi(\tilde{p})/(1 + \tilde{p}_0 + \tilde{p}_1)^3,\) and by following the calculations in the proof of Proposition \[\text{[7]}\].

**Degeneracy.** Heuristically, the 1K model should be regarded as relatively unaffected by degeneracy issues, for at least two reasons. First, the change statistic [see \[\text{[19]}\] corresponding to adding an edge between two nodes of degrees \(k\) and \(k'\) is \(\alpha_{k+1} + \alpha_{k'+1} - (\alpha_k + \alpha_{k'}),\) suggesting in general a lack of significant correlation with the number of edges in the graph. Secondly, the growing (in \(n\)) number of parameters and the fact that the degree distributions are negatively correlated prevent the distribution from concentrating on very few configurations as it pushes the probability mass to spread out.

**Existence of the maximum likelihood estimator.** Suppose that \([g_1, \ldots, g_m], m \geq 1\) are \(m\) iid observations of the networks with \(n\) nodes. The log-likelihood function can be written as
\[l(\alpha|g_1, \ldots, g_m) = \left(\sum_{k=0}^{n-2} \alpha_k \sum_{l=1}^{m} n_k(g_l)\right) - m\psi(\alpha).\] (8)
We define the average observed sufficient statistics for the 1K model to be \(\tilde{n}^{(1)}(l) = (\sum_{g=1}^{m} n^{(1)}(g_l))/m\) for \(m\) iid observations \([g_1, \ldots, g_m]\). It is known that, for distributions in exponential families, the MLE exists if and only if the average observed sufficient statistics lie on the interior of the model polytope; see \[\text{[1]}\] and \[\text{[4]}\].

We first explore the corresponding model polytope \(A_{n-1} = \text{convhull}\{n^{(1)}(g), g \in G_n\}\) to derive a necessary and sufficient condition for the existence of the maximum likelihood estimator (MLE) of \(\alpha\), that is, \(\{\hat{\alpha} : l(\hat{\alpha}|g_1, \ldots, g_m) = \max_{\alpha \in \mathbb{R}} l(\alpha|g_1, \ldots, g_m)\}\). We then exploit the well-studied theory of exponential family to calculate the MLE when existing.

In order to study \(A_{n-1}\), we need the two following notations and lemmas: Denote the \(k\)-regular graphs with \(n\) nodes by \(R_k\). In addition, by \(R_{kl}\) denote the graphs with \(n\) nodes such that \(n_k(R_{kl}) = n - 1\) and \(n_l(R_{kl}) = 1\).

**Lemma 1.** For \(0 < k < n\), there exists an \(R_k\) if and only if \(kn\) is even.

**Lemma 2.** Suppose that \(n\) and \(k\) are odd numbers and \(0 \leq l, n\). There exists an \(R_{kl}\) if and only if \(l\) is even.

**Proof.** Suppose that \(l\) is even. We know that there is a \(k\)-regular graph \(H\) with \(n - 1\) nodes. For this graph, consider a matching \(\{(i_0, j_1), \ldots, (i_{(n-1)/2}, j_{(n-1)/2})\}\). Now \(H\) and an isolated node \(h\) provides \(R_{k0}\). By removing the edge between \(i_1\) and \(j_1\) and connecting \(h\) to both \(i_1\) and \(j_1\), we obtain \(R_{k2}\). By this method, we can inductively generate all \(R_{kl}\).

If \(l\) is odd, the sum of degrees of nodes would be an odd number, which is impossible. \(\square\)
Let $B_n = \text{convhull}\{n^{(1)}(g), g \in G_n\}$. In addition, for $0 \leq k < n$, let $e_k = (0, \ldots, 0, n, 0, \ldots, 0)$, where $n$ is the $(k+1)$st element of the vector of length $n$, and for $0 \leq k, l < n$ and $k \neq l$, let $e_{kl} = (0, \ldots, 0, 1, 0, \ldots, 0, n-1, 0, \ldots, 0)$, where $n-1$ is the $(k+1)$st element of the vector and $1$ is the $(l+1)$st element of the vector of length $n$. We observe that $n^{(1)}(R_k) = e_k$ and $n^{(1)}(R_{kl}) = e_{kl}$. The following lemma characterizes $B_n$; see also Lemma 3.

**Lemma 3.** The model polytope $B_n$ is

(if $n$ is even) $n\triangle^{n-1}$, that is, the $(n-1)$-simplex scaled by $n$; and

(if $n$ is odd) the convex hall of the set of extreme points $\{e_l : 0 \leq l < n, l \text{ even}\} \cup \{e_{k,l} : 0 \leq k < n, 0 \leq l < n, k \text{ odd, } l \text{ even}\}$.

**Proof.** $\sum_{k=0}^{n-1} n_k(g) = n$ implies that $A_{n-1} \subseteq n\triangle^{n-1}$. We now need to deal with the two cases separately:

1) $n$ even: By lemma [1] we know that for each $0 \leq k < n$, there exists an $R_k$. The corresponding vectors $e_k$ are all the vertices of $A_{n-1}$; therefore, $A_{n-1} = n\triangle^{n-1}$.

2) $n$ odd: For $0 \leq l < n$ and $l$ even, by lemma [2] there exist $R_l$, and the corresponding $e_l$ are the extreme points. For $0 \leq k, l < n$, odd $k$ and even $l$, by Lemma 2 there exist $R_{kl}$, and it is easy to see that the corresponding $e_{kl}$ cannot be generated by the convex combination of other $n^{(1)}(g)$. Therefore, these are the extreme points too. Now only the vectors with integer entries fewer then $n$ that lie on $n\triangle^{n-1}$ but not on the convex combination of extreme points contain an element $n$ as an entry, which, again by Lemma 1, it is not possible. 

Let $0_i$ be the vector of size $i$ consisting only of zero elements. We can now characterize $A_{n-1}$:

**Proposition 2.** The model polytope $A_{n-1}$ is

(if $n$ is even) the convex hall of the set of extreme points $\{e_k : 0 \leq k < n-1\} \cup \{0_{n-2}\}$; and

(if $n$ is odd) the convex hall of the set of extreme points $\{e_l : 0 \leq l < n-1, l \text{ even}\} \cup \{e_{k,l} : 0 \leq k < n-1, 0 \leq l < n-1, k \text{ odd, } l \text{ even}\} \cup \{0_{n-2}\}$.

**Proof.** By projecting the polytope $B_n$, given in Lemma 3 onto the $(n-1)$-dimensional Euclidean space with coordinates $(n_0, \ldots, n_{n-2})$, we obtain the result. 

In Figure 3, the polytopes $B_3$ and $A_3$, for graphs with three nodes, are depicted.

![Figure 3](image-url)
Therefore, we have the following theorem:

**Theorem 1.** For the 1K model and \( m \) iid observations \( \{g_1, \ldots, g_m\} \), the MLE exists if and only if

- **(if \( n \) is even)** \( \bar{n}_k^{(1)} \neq 0 \) for all \( k \), \( 0 \leq k \leq n - 2 \), and \( \sum_{k=0}^{n-2} \bar{n}_k^{(1)} < n \); and

- **(if \( n \) is odd)** (i) \( \bar{n}_r^{(1)} \neq 0 \) for all \( r \), \( 0 \leq r \leq n - 2 \), and \( \sum_{r=0}^{n-2} \bar{n}_r^{(1)} < n \); and (ii) for every odd \( k \), \( \bar{n}_k^{(1)} < n - 1 \).

**Proof.** The MLE exists if and only if \( \bar{n}_k^{(1)} \in \text{int}(A_{n-1}) \).

In the case that \( n \) is even, a point in \( \text{int}(A_{n-1}) \) is written as \( a_0 e_0 + a_1 e_1 + \cdots + a_{n-2} e_{n-2} + c \Omega_{n-2} \), where \( a_k > 0 \) for \( 0 \leq k < n - 1 \), \( c > 0 \), and \( \sum_{k=0}^{n-2} a_k + c = 1 \). Therefore, \( \bar{n}_k^{(1)} \in \text{int}(A_{n-1}) \) if and only if \( a_k = \bar{n}_k^{(1)} \) and \( c = n - \sum_{k=0}^{n-2} \bar{n}_k^{(1)} \), which implies the result.

In the case that \( n \) is odd, a point in \( \text{int}(A_{n-1}) \) is written as \( \sum_{l=0}^{n-3} a_l e_l + \sum_{k=1}^{n-3} b_{k,l} e_{k,l} + c \Omega_{n-2} \), where \( a_l > 0 \) for even \( l \), \( 0 \leq l < n - 1 \), \( b_{k,l} > 0 \) for odd \( k \) and even \( l \), \( 0 \leq k, l < n - 1 \), \( c > 0 \), and \( \sum_{l=0}^{n-3} a_l + \sum_{k=1}^{n-3} \sum_{l \text{ odd}} b_{k,l} = 1 \).

If \( \bar{n}_k^{(1)} \in \text{int}(A_{n-1}) \), for every odd \( k \), \( \sum_{l=0}^{n-3} b_{k,l} = n_k/(n-1) \), which implies \( n_k > 0 \). In addition, we know that \( \sum_{l=0}^{n-3} b_{k,l} \leq 1 \), which implies that \( n_k < n - 1 \). For every even \( l \), \( a_l = (1/n)(n_l - \sum_{k=1}^{n-2} b_{k,l}) \), which implies \( n_l > 0 \). Now by using \( \sum_{l=0}^{n-3} a_l + \sum_{k=1}^{n-3} \sum_{l \text{ odd}} b_{k,l} < 1 \), we obtain \( \sum_{l=0}^{n-3} n_l < n \).

Conversely, if conditions (i) and (ii) hold, we let \( b_{k,l} = (2n_k)/(n-1)^2 \) and \( a_l = (1/n)(n_l - (2/(n-1)^2 \sum_{k=1}^{n-2} n_k) \). We conclude that \( a_l > 0 \), \( b_{k,l} > 0 \), and \( \sum_{l=0}^{n-3} a_l + \sum_{k=1}^{n-3} \sum_{l \text{ odd}} b_{k,l} < 1 \), which imply the result.

**Corollary 1.** For a single observation in the 1K model, the MLE does not exist.

**Proof.** For an observed \( g \), if \( n_{n-1}(g) \neq 0 \), then \( n_0(g) = 0 \) and vice versa. \( n_{n-1}(g) = 0 \) implies \( \sum_{k=0}^{n-2} \bar{n}_k = n \). Therefore, in either case the MLE does not exist.

**Example 2.** We proceed with Example [7] for networks with 3 nodes, illustrated in Figure 2. Theorem [7] implies that in order for the MLE to exist (i) \( \bar{n}_0 \neq 0 \), \( \bar{n}_1 \neq 0 \), and \( \bar{n}_1 + \bar{n}_0 < 3 \); (ii) one should observe either \( g_1 \) or \( g_4 \) since both \( g_2 \) and \( g_3 \) are of form \( R_{kl} \). If only (i) or (ii) holds, then only one parameter is estimable.

**Estimable parameters.** By partially differentiating the log-likelihood function in (8), we conclude that the MLE \( \hat{\alpha} \) should satisfy the following system of equations:

\[
\frac{\partial \psi(\hat{\alpha})}{\partial \hat{\alpha}_k} = \bar{n}_k, \quad \text{for } k \in \{0, \ldots, n - 2\}.
\]  

(9)

Therefore, from (7), the MLE for 1K model with \( m \) observations must satisfy the following system of equations:

\[
\sum_{i=1}^{M} n_k(g_i)e_{\sum_{i=0}^{n-2} n_i(g_i)\hat{\alpha}_i} = \bar{n}_k, \quad k \in \{0, \ldots, n - 2\}.
\]

(10)

Notice that if for a fixed \( k \), \( \bar{n}_k = 0 \) then \( \sum_{i=1}^{M} n_k(g_i)e_{\sum_{i=0}^{n-2} n_i(g_i)\hat{\alpha}_i} = 0 \). We observe that \( \hat{\alpha}_k \) is the only parameter that appears in all terms and does not appear in all terms of the denominator of the left hand side.
of (10). Therefore, $\hat{\alpha}_k = -\infty$. This corresponds to $\hat{\rho}_k = 0$, or equivalently $\hat{\rho}_k = 0$ since it is that assumed $p_{n-1} \neq 0$.

Thus, based on the MLE, the model implies that the probability of a node having a specific degree is zero when no node with that degree has been observed. Hence, it is plausible to remove such parameters from the model and simply focus on the submodel of exponential family form. The corresponding model polytope would then be simply the same, embedded in the Euclidian space with remaining coordinates. By this method we can still estimate a subset of parameters whose corresponding sufficient statistic is nonzero.

Notice that even with a single observation, there are sometimes a considerable number of parameters that can be estimated. The following proposition deals with the extreme case of such graphs.

**Proposition 3.** There exists a graph $T_n$ of every size $n$ such that $n_0(T_n) = 0$ and $n_k(T_n) \neq 0$ for $k \in \{1, \ldots, n-1\}$.

*Proof.* We prove the result by induction on the number of nodes. For the base, where $n = 2$, the result holds for $K_2$. Suppose that there exists such a graph $T_n$. We prove it for $n + 1$: Since $n_0(T_n) = 0$ there is a $k' \in \{1, \ldots, n-1\}$ such that $n_{k'} = 2$ and $n_k = 1$ if $k \neq k'$. We construct the graph $T_{n+1}$ as follows. We add a node to $T_n$ and start connecting it to the nodes starting from the node with the node with degree $n - 1$ and stop when we reach $k'$. Now regardless of what degree the added node has, there are nodes of all degrees except zero in graph.

Notice, however, that the large sum in (10) entails the common problem with ERG modeling that the computing of the MLE for this model ultimately requires MCMC methods, just like with most other ERGMs.

**Asymptotics.** We have shown that we can estimate a subset of parameters whose corresponding sufficient statistic is nonzero. Here we calculate the probability of a sufficient statistic to be nonzero, and discuss its behaviour asymptotically. In addition, we provide the asymptotical expected value of the number of non-zero sufficient statistics.

Under the 1K-model, for each $k \leq n - 1$, we have the following:

$$
P(n_k(G) > 0) = \frac{\sum_{g \in \mathcal{G}_n, n_k(g) \neq 0} \prod_{k' = 0}^{n-1} p_{k'}^{n_{k'}(g)}}{\sum_{g \in \mathcal{G}_n} \prod_{k' = 0}^{n-1} p_{k'}^{n_{k'}(g)}}. \tag{11}
$$

We will now consider the very special case where all $p_{k'}$ are equal, which implies that they are all equal to $1/n$. In this case we see that the model is the same as the Erdős-Rényi model with $p = 1/2$.

**Proposition 4.** Suppose that $p_i = p$ for all i and let $k = k(n) = (n - 1)/2 + a_n$, where $\{a_n\}$ is a sequence such that $0 \leq a_n \leq (n - 1)/2$ for all $n$. It then holds that

1. $\lim_{n \to \infty} P(n_k(g) > 0) = 1$ if $a_n = O(\sqrt{n})$;
2. $\lim_{n \to \infty} P(n_k(g) > 0) = 0$, if $a_n = \Omega(\sqrt{n \log n})$.

*Proof.* By using (11), we have that $P(n_k(g) > 0) = \frac{\sum_{g \in \mathcal{G}_n, n_k(g) \neq 0} \prod_{k' = 0}^{n-1} p_{k'}^{n_{k'}(g)}}{\sum_{g \in \mathcal{G}_n} \prod_{k' = 0}^{n-1} p_{k'}^{n_{k'}(g)}} = \frac{|\{g \in \mathcal{G}_n : n_k(g) \neq 0\}|}{|\mathcal{G}_n|}$, which is the same as the same probability in the Erdős-Rényi model with $p = 1/2$. Let $\lambda_k(n) = n(n-1)(1/2)^{n-1}$. From the theorem 3.1 in [3], we know that if $\lim_{n \to \infty} \lambda_k(n) = 0$, then $\lim_{n \to \infty} P(n_k(g) > 0) = 0$, and if $\lim_{n \to \infty} \lambda_k(n) = \infty$, then $\lim_{n \to \infty} P(n_k(g) > 0) = 1$. We show that the
latter holds for \(a_n = O(\sqrt{n})\), and the former if \(a_n = \Omega(\sqrt{n \log n})\). By using Stirling’s approximation,

\[
\lambda_k(n) \sim \frac{n(n-1)\cdots(n-k+1)}{n^{n-k/2}2^{k-k/2}k^{k/2}} \approx \frac{(n-1/2)^n}{\sqrt{\pi n}} \propto \frac{n^{n-1/2}}{(1-2\alpha_n(k))(1+2\alpha_n(k))^{2n}} = \frac{2^{n-1}}{\sqrt{n \pi}} \cdot \frac{(1-2\alpha_n(k))(1+2\alpha_n(k))^{2n}}{\sqrt{n}} \frac{1}{\sqrt{n}}
\]

For \(a_n = O(\sqrt{n})\) the previous display is \(\propto \sqrt{n}\) and hence tends to infinity. If \(a_n = \Omega(\sqrt{n \log n})\) the term will vanish instead. The claim is proved.

We now consider the number \(N\) of non-zero entries in the degree distribution and show that it is of order \(O(\sqrt{n \log n})\), which corresponds to the number of estimable parameters in the model.

**Proposition 5.** Suppose that \(p_i = p\) for all \(i\) and let \(N\) denote the number of entries in the degree distribution that are non-zero. Then,

\[
E[N] = O\left(\sqrt{n \log n}\right).
\]

**Proof.** Let \(k_n = \sqrt{cn \log n}\) for some \(c > 0\) which will be set below. Assume that \((n-1)p > k_n\) and let \(A\) denote the event that there exists a node with degree less than \((n-1)p - k_n\) or more than \((n-1)p + k_n\). Let \(D_i\) denote the degree of node \(i\) and notice that \(D_i \sim \text{Bin}(n-1, p)\), for all \(i\). Then \(A = \bigcup \{D_i < 1 - k_n\} \cup \{D_i > 1 + k_n\}\).

By the union bound and Hoeffding inequality we get that, for any \(r > 0\), \(\mathbb{P}(A) \leq n^2 \exp\{-2c \log n\} = \frac{e^c}{n^2}\), provided that \(c = r/2\). It is now easy to see that the expected number of non-zero entries in the degree distribution is of order \(O(\sqrt{n \log n})\). In details, \(E[N] = E[N|A]P(A) + E[N|A^c]P(A^c) \leq \frac{e^c}{n^2} + (1 - \frac{r}{8}) \sqrt{n \log n} = O(\sqrt{n \log n})\).

We have seen that the case \(p_i = p\) for all \(i\) and some \(p \in (0, 1)\) corresponds to the Erdős-Rényi model with \(p = 1/2\). Using (5), this is equivalent to having \(\alpha_k = 0\), for all \(k = 0, 1, \ldots, n - 2\). We now consider the slightly more general case in which the vector \(\alpha = (\alpha_0, \alpha_1, \ldots, \alpha_{n-2})\) belongs to a subset \(A\) of \(\mathbb{R}^{n-1}\) such that \(\log(c_n) \leq \alpha_i \leq \log(C_n)\), where \(c_n \in (0, 1]\) and \(C_n \in [1, \infty)\), for all \(i\). Then it is easy to see that, for any \(\alpha \in A\),

\[
\mathbb{P}_{\alpha}(n_k(G) > 0) \leq \left(\frac{c_a}{c_n}\right)^n \mathbb{P}_0(n_k(G) > 0) \leq \left(\frac{c_a}{c_n}\right)^n \lambda_k(n),
\]

where \(\lambda_k(n)\) is given in the proof or proposition 4 and \(\mathbb{P}_\alpha\) denotes a probability of the random graph \(G\) when sampled from the 1K model with parameter \(\alpha\). Next, for a sequence \(\{a_n\}_{n=1,2,\ldots}\) such that \(0 \leq a_n \leq \frac{C_n}{c_n}\), let \(h_n = (1 - 2a_n)\frac{1}{2} + \frac{a_n}{2} (1 + 2\alpha_n(k))\frac{1}{2} + \frac{a_n}{2}\). Then, by proposition 4, (12) yields that, for \(k = k(n) = (n - 1)/2 + a_n\), \(P_{\alpha}(n_k(G) > 0)\) is bounded by a term that is asymptotically of order \(\left(\frac{c_a}{c_n}\right)^n \sqrt{n} / (h_n)^n\).

Now let \(b = \lim inf_n h_n\). If \(a_n = O(\sqrt{n})\), then \((h_n)^n = O(1)\) from the proof of proposition 4 which yields a trivial bound. Thus assume that \(b \in (1, 2]\) since \(h_n \in [1, n]\) for all \(n\). Then, provided that \(\frac{c_a}{c_n} < b\), the probability \(\mathbb{P}_{\alpha}(n_k(G) > 0)\) vanishes. (Notice that this implies that \(1 < c_n / c_n < 2\).)

**Relation with the Erdős-Rényi model.** Recently and somewhat surprisingly, [5] have shown that some specifications of the ERGM family lead to models which asymptotically behave like Erdős-Rényi (ER) models for appropriate choices of \(p\).
Here we provide some results illustrating the relationships between the ER model and the 1K model. Below we parametrize the 1K model using the natural parameter vector $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{R}^{n-1}$. Notice that we have expunged $n_0$ from the vector of sufficient statistics, a choice that entails no loss of generality.

First off, we make the easy observation that the ER model with probability $p$ can be represented by setting $\alpha_i = i\theta$, $i = 1, \ldots, n-1$, where $\theta = \log \left( \frac{p}{1-p} \right)$. Next, we show that the 1K model is dramatically different from the Erdős–Rényi model in the sense of being almost singular to it whenever the natural parameters have expunged from the vector of sufficient statistics, a choice that entails no loss of generality.

Below, we will denote with $P_p$ the probability distribution of the Erdős-Rényi model with parameter $p \in (0, 1)$ and with $P_\alpha$ the probability distribution of the 1K model with natural parameter vector $\alpha = (\alpha_1, \ldots, \alpha_{n-1}) \in \mathbb{R}^{n-1}$.

**Proposition 6.** Let $p \in (0, 1)$ such that $\min \{|p - 1/2|, 1 - p, p\} > \epsilon$, for a fixed, arbitrarily small $\epsilon > 0$. Then, there exists a sequence of subsets $G_n(p)$ of $G_n$ such that, for any sequence $\{\alpha_n\}$ such that $\alpha_n \in \mathbb{R}^{n-1}$ for all $n$ and $\|\alpha_n\|_\infty = o(n)$,

$$\lim_{n \to \infty} P_p(G_n(p)) = 1 \quad \text{and} \quad \lim_{n \to \infty} P_{\alpha_n}(G_n(p)) = 0.$$

**Proof.** Let $G_n(p)$ be the set of graphs such that $(n-1)p - C\sqrt{n \log n} \leq d_i(g) \leq (n-1)p + C\sqrt{n \log n}$, for all $i = 1, \ldots, n$, where $d_i(g)$ denote the degree of the $i$th node of graph $g$ and $C$ is a positive constant to be specified.

By Heoffding’s inequality, for any $c > 0$, there exists a $C = C(c)$ such that $P_{\alpha_n}(G_n(p)) \geq 1 - \frac{1}{n^c}$, for $n$ large enough that $C\sqrt{\frac{\log n}{n}} < \epsilon$. Next, the probability $P_{\alpha_n}(G_n(p)) = \frac{\sum_{g \in G_n(p)} e^{\sum_{i=1}^{n-1} \alpha_i n_i(g)}}{\sum_{g \in G_n} e^{\sum_{i=1}^{n-1} \alpha_i n_i(g)}}$ can be bounded from above by $\frac{e^{M_n[\hat{G}_n(p)]}}{e^{M_n[G_n(p)]}} = e^{2M_n \mathbb{P}_{1/2}[G_n(p)]}$, a calculation that follows from simple algebra and the fact that, for each $g \in G_n$, $\sum_{i=1}^{n-1} n_i(g) = n - n_0(g) \leq n$.

Then, since $p$ is $\epsilon$-away from $1/2$, Theorem 2.3 in [6] (see also [5]) yields that, for all $n$ large enough, $\mathbb{P}_{1/2}(G_n(p)) \leq e^{-n^2 \epsilon}$, for an appropriate constant $c$, which depends on $p$. Thus, we have shown that, for all $n$ large enough and for each $\alpha$ in an $L_\infty$ ball of $0$ in $\mathbb{R}^{n-1}$ of radius $M$, $P_{\alpha}(G_n(p)) \leq e^{2M-n^{2-\epsilon}}$, which vanishes provided $M = o(n)$.

The case of $p = 1/2$ was not covered by the previous result and one might wonder whether setting all the natural parameters to be equal to a constant vector i.e. $\alpha_i = \theta$ for all $i$, might yield a model close to an ER model with $p = 1/2$. This in fact not the case, as we demonstrate next, unless $\theta = 0$.

Towards this end, notice first that the assumption that $\alpha_i = \theta$, for all $i \geq 1$, is equivalent to $\log \left( \frac{p_i}{p_0} \right) = \theta$. Thus, for any $\theta \in \mathbb{R}$, the probability of observing a graph $g$ is $\frac{e^{-\sum_{j=0}^n |\nu_n(j)|}}{\sum_{\nu=0}^{\nu_n(j)} e^{-\sum_{j=0}^n |\nu_n(j)|}}$, where $\nu_n(j)$ is the number of $n$-graphs with $j$ isolated nodes. It is clear that the above probability is rather different from the ER model with $p = 1/2$. To add more details, it is possible to show that $\nu_n(0) \equiv f(n) = \sum_{k=0}^{n} (-1)^{n-2}(\frac{n}{2})^2(\frac{n}{2})$, and $\nu_n(j) = \binom{n}{j} f(n-j)$. This can be obtained as the solution to the recursion $f(n) = 2f(\frac{n}{2}) - \sum_{i=0}^{n-1} f(i)^{(\frac{n}{2})}$, with the initial conditions $f(0) = 1$ and $f(1) = 0$.

The term $\nu_n(0)$ dominates all the others, in the sense that $\frac{f(n)}{2(\frac{n}{2})} \to 1$, as $n \to \infty$. Thus, when $\theta < 0$ the model will favor networks with many isolated nodes.
3 The 2K model

The exponential family form. Consider the lexicographically ordered vector of possible degrees \(((1, 1), (1, 2), \ldots, (n-1, n-1))\) in \(g\). For \(n_{k_1 k_2}(g)\), the number of edges with endpoint degrees \(k_1\) and \(k_2\) in \(g\), it holds that \(\sum_{k_1=1}^{n-1} \sum_{k_2=k_1}^{n-1} n_{k_1 k_2}(g) = e(g)\), where \(e(g)\) is the number of edges of \(g\), which is still a random quantity. We present an observation with regard to \(n_{k_1 k_2}(g)\) as the following proposition:

**Proposition 7.** The following identity always holds:

\[
\sum_{k_1=1}^{n-1} \sum_{k_2=k_1}^{n-1} \frac{k_1 + k_2}{k_1 k_2} n_{k_1 k_2}(g) = n - n_0(g).
\] (13)

**Proof.** From (2a) and (2b), we obtain \(n - n_0(g) = \sum_{k_1=1}^{n-1} \frac{1}{k_1} (\sum_{k_2=1}^{k_1} n_{k_2 k_2}(g) + \sum_{k_2=k_1}^{n-1} n_{k_1 k_2}(g)) = \sum_{k_1=1}^{n-1} \sum_{k_2=k_1}^{n-1} \frac{1}{k_1 k_2} n_{k_1 k_2}(g)\). In order to write the model in minimal form and since \(\sum_{k_1 < k_2} n_{k_1 k_2}(g) = e(g)\) is still a random quantity, we use the above proposition and let a scaled version of the joint degree distribution, \(\tilde{n}_{k_1 k_2}(g) = ((k_1 + k_2)/(k_1 k_2)) n_{k_1 k_2}(g)\), be the sufficient statistics. Therefore, assuming that the probability of observing graphs with isolated nodes is zero, the probability of observing \(g\) can be written as

\[
P(g) = \varphi(p) \prod_{k_1=1}^{n-1} \prod_{k_2=k_1}^{n-1} \tilde{n}_{k_1 k_2}(g),
\] (14)

where \(\varphi\) is a normalizing constant and \(\sum_{k_1=1}^{n-1} \sum_{k_2=k_1}^{n-1} p_{k_1 k_2} = 1\).

To write (14) in a minimal form, we use the parametrization \(\tilde{p}_{k_1 k_2} = p_{k_1 k_2} / p_{n-1,n-1}\), which by using the fact that \(p_{n-1,n-1} = 1\), implies \(p_{n-1,n-1} = 1/(1 + \sum_{k_1=1}^{n-2} \sum_{k_2=k_1}^{n-1} \tilde{p}_{k_1 k_2})\). Therefore, (14) can be rewritten as

\[
P(g) = \varphi(p) \prod_{k_1=1}^{n-1} \sum_{k_2=k_1}^{n-1} \tilde{n}_{k_1 k_2}(g) \prod_{k_1=1}^{n-1} \prod_{k_2=k_1}^{n-1} \tilde{p}_{k_1 k_2} = \frac{\phi(\tilde{p})}{(1 + \sum_{k_1=1}^{n-2} \sum_{k_2=k_1}^{n-1} \tilde{p}_{k_1 k_2})} \prod_{k_1=1}^{n-2} \prod_{k_2=k_1}^{n-1} \tilde{p}_{k_1 k_2}.
\] (15)

This can be written in exponential family form

\[
P(g) = \exp \left\{ \sum_{k_1=1}^{n-2} \sum_{k_2=k_1}^{n-1} \tilde{n}_{k_1 k_2}(g) \alpha_{k_1 k_2} - \psi(\alpha) \right\},
\] (16)

where \(\alpha_{k_1 k_2} = \log \tilde{p}_{k_1 k_2}\) and \(\psi(\alpha) = n \log (1 + \sum_{k_1=1}^{n-2} \sum_{k_2=k_1}^{n-1} \tilde{p}_{k_1 k_2}) - \log \phi(\tilde{p})\).

The sufficient statistics are in fact \(\tilde{n}_{(2)}(g)\), referring to the vector \(\tilde{n}_{(2)}(g)\) with the arbitrary element \(\tilde{n}_{n-1,n-1}\) removed.

Calculating the normalizing constant. Similar to the 1K case, for a fixed \(n\), \(\psi(\alpha) = \psi_n(\alpha)\) can be explicitly represented. In this case the normalizing constant can be calculated directly from the set of graphs with \(n\) nodes without isolated nodes, which are denoted by \(G_{n-} = \{g_1, \ldots, g_L\}\).

**Proposition 8.** The normalizing constant for the 2K model can be written as

\[
\psi(\alpha) = \log \left( \sum_{l=1}^{L} \prod_{k_1=1}^{n-2} \prod_{k_2=k_1}^{n-1} \tilde{n}_{k_1 k_2}(g_l) \right) = \log \left( \sum_{l=1}^{L} e^{\sum_{k_1=1}^{n-2} \sum_{k_2=k_1}^{n-1} \tilde{n}_{k_1 k_2}(g) \alpha_{k_1 k_2}} \right).
\] (17)
Proof. The proof is similar to the proof of Proposition\textsuperscript{1} by using \textsuperscript{15}.

Example 3. From the graphs in Figure 2, it is apparent that there are 2 non-isomorphic graphs with 3 nodes and without isolated nodes (\(g_1\) and \(g_2\), where \(g_2\) is repeated 3 times). Proposition\textsuperscript{8} implies that 

\[
\psi(\alpha) = \log(1 + 3p_{12}^2) = \log(1 + 3e^{2\alpha_{12}}).
\]

Discussion on the existence of the maximum likelihood estimator and parameter estimation. Suppose that \(\{g_1, \ldots, g_m\}, m \geq 1\) are \(m\) iid observations of the networks with \(n\) nodes and without isolated nodes. The log-likelihood function can be written as 

\[
l(\alpha|g_1, \ldots, g_m) = \left( \sum_{k_1=1}^{n-2} \sum_{k_2=k_1}^{n-1} \alpha_{k_1k_2} \sum_{l=1}^{m} \tilde{n}_{k_1k_2}(g_l) \right) - m\psi(\alpha).
\]

Similar to the 1K model, we study the model polytope 

\[
A_{n-1,n-2} = \text{convhull}(\tilde{n}_{(2)}^*(g), g \in \mathcal{G}_n)
\]

to derive a necessary and sufficient condition for the existence of the MLE. Notice that the \(A_{n-1,n-2}\) lies on an \(n(n-1)/2 - 1\)-dimensional space. Finding this polytope is subject to further work.

In general, however, it is easy to observe that if there are no observations of specific bi-degrees, i.e. \(n_{k_1k_2} = 0\), the corresponding parameter \(\alpha_{k_1k_2}\) is not estimable. For a single observation, we conjecture that asymptotically, there are at most half of the parameters estimable: It is easy to verify that the graph \(T_n\) defined in Proposition\textsuperscript{3} has \((n-1/2)^2\) for \(n\) odd, and \((n-2/2)^2 + n/2\) for \(n\) even, non-zero elements in its bi-degree vector. The ratio of the non-zero elements to the length of the vector \(n(n+1)/2\) tends to 1/2 when \(n\) tends to infinity, which gives a lower bound for the ratio.

On the other hand, we conduct the following numerical experiment: By using Proposition\textsuperscript{7}, we observe that in the vector with maximum non-zeros, ideally every element is 1. Hence we compute all \((k_1 + k_2)/(k_1k_2)\), order them and start adding them until we reach \(n\). The number of elements we have added gives an upper bound for the number of non-zero elements of the bi-degree vector. Figure 4 illustrates the ratio to the vector length, which is decreasing below 0.56.

![Figure 4: An upper bound for the ratio of maximum non-zero elements of the bi-degree vector to its length.](image-url)

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