Finite Mixtures of ERGMs for Ensembles of Networks *

Fan Yin
Department of Statistics, University of California, Irvine
Weining Shen
Department of Statistics, University of California, Irvine
Carter T. Butts
Department of Statistics, Sociology, Computer Science, and EECS, and Institute for Mathematical Behavioral Sciences, University of California, Irvine

October 28, 2019

Abstract

Ensembles of networks arise in many scientific fields, but currently there are few statistical models aimed at understanding their generative processes. To fill in this gap, we propose characterizing network ensembles via finite mixtures of exponential family random graph models, employing a Metropolis-within-Gibbs algorithm to conduct Bayesian inference. Simulation studies show that the proposed procedure can recover the true cluster assignments and cluster-specific parameters. We demonstrate the utility of the proposed approach using an ensemble of political co-voting networks among U.S. Senators.

Keywords: Mixture model; Exponential-family random graph models (ERGMs); MCMC; Deviance information criterion (DIC); Political co-voting networks

1 Introduction

Data involving ensembles of networks - that is, multiple independent networks - arise in various scientific fields, including sociology (Slaughter and Koehly, 2016; Stewart et al., 2019), neuroscience (Simpson et al., 2011; Obando and De Vico Fallani, 2017), molecular biology (Unhelkar et al., 2017).

*This work was supported in part by NSF award DMS-1361425; corresponding author Carter T. Butts (buttsc@uci.edu)
Grazioli et al. 2019), and political science (Moody and Mucha 2013) among others. Typically, ensembles of networks represent the action of multiple generative processes, with different processes being prominent in different settings. A reasonable starting point for analysis of such data is to posit that this variation can be represented in terms of discrete set of subpopulations, such that the networks drawn from any given subpopulation tend to be produced by similar generative processes.

Given a set of potential generative models, one would then like to identify the subsets of networks drawn from a particular subpopulation, or a probabilistic mixture of multiple subpopulations. It is natural to view this as a hierarchical finite mixture problem, with the base distributions being parametric distributions on graphs.

As a plausible approximation to the underlying data generating process, the hierarchical finite mixture framework also provides a flexible approach for predictive modeling of ensemble of networks. If one seeks to predict graph structures drawn from a heterogeneous (super)population learned from observed data, one needs to average over the possible generative processes that might end up producing the observation that one wants to predict. Such a view is similar in spirit to model averaging techniques (Hoeting et al. 1999; Hjort and Claeskens 2003), especially if interpreted in terms of a hierarchical problem in which we seek to predict an outcome of interest (e.g., co-voting prevalence among U.S. senators) by first predicting network structure and then predicting the behavior of a process on that network. In that setting, if it turned out that there were $k$ types of possible network formation processes and we did not know which one ours happened to be, we would certainly want to average across the types.

There is a growing body of literature on the analysis of ensembles of networks. This includes work on discriminative analysis of networks via distance or similarity measures (e.g. Banks and Carley 1994; Butts and Carley 2005; Fitzhugh et al. 2015), which can be broadly viewed as mapping the ensemble of interest into some high-dimensional space (e.g., the Hamming space of graphs), and then employing standard multivariate analysis techniques (e.g., hierarchical clustering, multidimensional scaling) to seek an informative low-dimensional approximation. Other approaches work with user-selected graph statistics, either directly (e.g., Prulj 2007; Sweet et al. 2019) or by e.g., modeling quantiles of the observed statistics relative to a reference distribution to control for size and density effects (Butts 2011). As such, these approaches do not attempt to provide generative models for the networks within the ensemble, though they may in some cases
provide generative models for summary statistics (e.g., predicting the conditional uniform graph quantile for the transitivity of a new graph drawn from the same ensemble).

In the category of generative models for complex networks, a common approach is to employ multilevel models with exponential random graph models (ERGMs, a general family of parametric models for networks (see, e.g. Robins et al., 2007 for a review)), as base distributions. Faust and Skvoretz (2002) introduced both multivariate meta-analysis of ERGM parameters from a common model family (fit to an ensemble of graphs) and predicted conditional edge probabilities from the generative base models as tools for leveraging ERGMs to compare networks. More elaborate meta-analytic procedures and hierarchical models for single populations of networks were subsequently developed by, among others, Zijlstra et al. (2006); Slaughter and Koehly (2016); McFarland et al. (2014); Butts (2017), and Stewart et al. (2019). Nonparametric models (e.g., latent space or block models) have also been employed for studying sets of networks, e.g. hierarchical mixed membership stochastic blockmodels for multiple networks (Sweet et al., 2014). In general, this prior work has either not posited a generative model for the parameters of the base distribution (as in descriptive meta-analytic approaches), has not attempted to jointly estimate population-level and network-level parameters (as in conventional meta-analysis), or has assumed a simple hierarchical form in which coefficients are taken to be drawn from a simple population distribution (often Gaussian) with common mean and variance. The latter work well for homogeneous (super)populations, but where the network ensemble reflects higher levels of heterogeneity, more structure is required. By contrast, work such as that of Durante and Dunson (2018) or Lehmann (2019) explicitly considers heterogeneity within graph subpopulations, but assumes that the subpopulation labels are observed. Joint modeling of population-level and network-level parameters where subpopulation memberships are unknown - or where the true generative process otherwise involves a mixture of graph distributions - has remained to date an open problem in the ERGM context.

In this paper, we propose using a mixture of ERGMs to model the generative process of ensembles of networks in which the group labels are not available, under the general framework of finite mixture models (McLachlan and Basford, 1988; Fraley and Raftery, 2002; Bouveyron et al., 2019). Such a formulation provides a useful probabilistic interpretation of the results and allows for convenient statistical inference; we also note that related approaches have proven to be efficacious for modeling structure within networks (e.g. Salter-Townshend and Murphy, 2015).
We develop a Metropolis-within-Gibbs algorithm to perform Bayesian inference for the proposed model, with both the cluster assignments and the ERGM parameters in the clusters being estimated simultaneously. Given that our primary focus is developing a practical procedure that can obtain meaningful clusters, we employ a pseudo-likelihood approximation to the ERGM likelihood for efficient computation; while we show here that this approach can work well, more advanced MCMC techniques can also be deployed to obtain more accurate estimates when the interest lies mainly in the inference of cluster-specific parameters. (It is also possible to use the pseudo-likelihood when updating cluster assignment parameters and then use high-accuracy MCMC-based likelihood calculations to update cluster-specific parameters, offering additional options for speed/accuracy tradeoffs.)

We approach the problem of choosing number of clusters from a model selection perspective, and in particular we use a version of deviance information criterion to choose the number of clusters to employ.

The remainder of this paper is structured as follows. In section 2 we briefly introduce the exponential-family random graph models (ERGMs) and common estimation techniques. Section 3 describes the idea of mixtures of ERGMs, along with our estimation algorithms and our proposed method for selecting the number of clusters. Section 4 presents a simulation study showing that the proposed method can recover the true cluster assignment and model parameters. Section 5 shows the results of our method applied to a political co-voting data. Section 6 concludes with a discussion.

2 Exponential-family Random Graph Models (ERGMs)

In recent years, ERGMs have found applications in empirical research in a wide range of scientific fields. Recent examples include the study of large friendship networks (Goodreau 2007), genetic and metabolic networks (Saul and Filkov 2007), disease transmission networks (Groendyke et al. 2012), conflict networks in the international system (Cranmer and Desmarais 2011), the structure of ancient networks in various of archaeological settings (Amati et al. 2019), the structural comparison of protein structure networks (Grazioli et al. 2019), the effects of functional integration and functional segregation in brain functional connectivity networks (Simpson et al. 2011; Sinke et al. 2016; Obando and De Vico Fallani 2017), and the impact of endogenous network effects.
on the formation of interhospital patient referral networks (Caimo et al., 2017). While addressing very different problems in different empirical settings, what these studies have in common is a clear methodological commitment to modeling network mechanisms directly via parametric effects, rather than just attempting to “control for” unspecified dependence among the observations (e.g., via latent structure). The ability to provide generative and interpretable models of complex network structure is an important asset of this approach, which we leverage here in the context of graph ensembles.

2.1 Definition

Exponential-family random graph models (ERGMs) (Holland and Leinhardt, 1981; Frank and Strauss, 1986; Snijders et al., 2006; Hunter and Handcock, 2006), also known as $p$-star models (Wasserman and Pattison, 1996), are a family of parametric statistical models developed for explicitly modeling the complex stochastic processes that govern the formation of edges within pairs of nodes in a network. We introduce them first in the single-network case. Consider the set of nodes in the network of interest, $V$, and let $n \equiv |V|$ be its cardinality, i.e. the number of nodes in the network. We represent the network’s structure via an order-$n$ random adjacency matrix $Y$, in which each element takes 1 or 0 representing the presence or absence of a tie between incident nodes. Letting $Y_n$ be the set of all possible network configurations on $n$ nodes, we write the probability mass function (pmf) of $Y$ taking a particular configuration $y$ in the form of a discrete exponential family as

$$P_{\eta}(Y = y | X; \theta) = \exp \left( \eta(\theta)^T g(y; X) - \psi_{g,\eta,X,Y_n}(\theta) \right) h(y), \quad y \in Y_n, \quad (1)$$

where $\theta = (\theta_1, \ldots, \theta_q) \in \mathbb{R}^q$ is a vector of (curved) model parameters, mapped to the natural parameters by $\eta(\theta) = (\eta_1(\theta), \ldots, \eta_p(\theta)) \in \mathbb{R}^p$. The natural parameters $\eta$ may depend on the sizes of the networks and may be non-linear functions of a parameter vector $\theta$. The user-defined sufficient statistics $g : Y_n \rightarrow \mathbb{R}^p$ may incorporate fixed and known covariates $X$ that are measured on the nodes or dyads. The sufficient statistics typically incorporate features of the network of interest that are believed to be crucial to the social process which had produced it (see, e.g., Morris et al., 2008). Here $h$ defines the reference measure for the model family; often chosen to be the counting measure on $Y_n$ for unvalued graphs with fixed $n$, other reference measures can
make more sense in different settings. As discussed below, we employ a sparse graph reference that leads to a mean degree that is asymptotically constant in $n$. Finally, the normalizing factor $\psi_{g,n,X,Y_n}(\theta) = \log \sum_{y' \in Y_n} \exp \{ \eta(\theta)^\top g(y'; X) \} h(y')$ ensures that (1) sums up to 1 over the support $Y_n$.

Exact evaluation of the normalizing factor involves integrating an extremely rough function over all possible network configurations ($2^\binom{n}{2}$ non-negative terms for an undirected network of size $n$). This cannot be done by brute force except for trivially small graphs, and the roughness of the underlying function precludes simple Monte Carlo strategies; thus, alternative approaches that approximate or avoid this calculation are of substantial interest (see Hunter et al., 2012, for a review). To date, the most frequently used approaches include: maximum pseudo-likelihood estimation (MPLE; Besag (1974)) adapted by Strauss and Ikeda (1990); Markov Chain Monte Carlo MLE (MCMC MLE; Geyer and Thompson (1992)) by Handcock (2003); Hunter and Handcock (2006); Stochastic approximation (SA; Robbins and Monro (1951); Pflug (1996)) by Snijders (2002); and Bayesian inference based on approximate exchange algorithm (Caimo and Friel, 2011).

Recent developments on ERGM estimation have concentrated on: (1) finding better initial values for simulation-based MLE, including the partial stepping technique (Hummel et al., 2012) and contrastive divergence (CD; Hinton (2002))-based techniques adapted to ERGMs by Krivitsky (2017); and (2) more accurate tractable approximations to ERGM likelihood than pseudo-likelihood, such as the adjusted pseudo-likelihood (Bouranis et al., 2017, 2018) for faster Bayesian inference. Despite the computational challenges, these and related strategies have made ERGM inference practical for well-posed model families.

### 2.2 Size-adjusted parameterizations

It is worth noting that the behavior of Eq. (1) across $n$ is highly dependent on the choice of reference measure, $h$. In particular, the counting measure - while a mathematically convenient choice - implicitly sets the base distribution of the network to be the uniform distribution on $Y_n$, and has the side effect of generating graphs whose densities are ceteris paribus constant in $n$. When network size varies, this is not always realistic: in many networks, mean degree is approximately constant in $n$, implying that density must scale as $n^{-1}$. To correct for this, Krivitsky et al. (2011) propose the reference measure $h(y) = n^{-M(y)}$, where $M$ is the edge count. This is equivalent to
adding a size-dependent offset of $-\log n$ to the natural parameter associated with the edge count, i.e.
\[ \eta_1(\theta) = \theta_1 - \log n, \] (2)
where $\theta_1 \in \mathbb{R}$ is a parameter that does not depend on the network size. In the present work, we employ the Krivitsky reference measure as above, although other size-adjusted parameterizations are also possible (e.g., Butts and Almquist, 2015; Kolaczyk and Krivitsky, 2015).

3 Finite mixtures of ERGMs

We assume a population of networks $(Y^{(1)}, V^{(1)}, X^{(1)}), \ldots, (Y^{(m)}, V^{(m)}, X^{(m)})$, where $Y^{(i)}$ is a graph structure on vertex set $V^{(i)}$ with covariate set $X^{(i)}$. Our interest is in modeling $Y^{(1)}, \ldots, Y^{(m)}$ given $(V^{(1)}, X^{(1)}), \ldots, (V^{(m)}, X^{(m)})$, where it will be assumed that the respective graph structures are conditionally independent given the generative process, vertex sets, and covariates.

3.1 Model

We model the generative process for the network ensemble as a finite mixture, with each mixture component (equivalently, “cluster”) being an ERGM distribution with cluster-specific parameters. (See Figure 1.) Given $K$ clusters, the a priori probability for a network to belong to cluster $k$ is $\tau_k$ for $k = 1, 2, \ldots, K$, and the probability law governing the formation of the network in group $k$ is parameterized by Eq. (1) with cluster-specific parameter vector $\theta_k \in \mathbb{R}^{q_k}$ and cluster-specific mapping to the natural parameters $\eta_k(\theta_k) = (\eta_{k,1}(\theta_k), \ldots, \eta_{k,p_k}(\theta_k)) \in \mathbb{R}^{p_k}$. For notational simplicity, we omit the subscripts $\eta_k$’s for the remainder of the paper.

More specifically, the marginal likelihood for network $Y^{(i)}$, with $|V^{(i)}| = n_i$, takes the following form
\[ P(Y^{(i)} = y^{(i)}|X^{(i)}; \tau, \theta) = \sum_{k=1}^{K} \tau_k \exp \left( \eta_k(\theta_k)^\top g_k(y^{(i)}; X^{(i)}) - \psi_{g_k,\eta_k,Y_{n_i}}(\theta_k) \right) h_i(y^{(i)}), y^{(i)} \in \mathcal{Y}_{n_i} \] (3)

where $\tau = (\tau_1, \ldots, \tau_K)$ and $\theta = (\theta_1, \ldots, \theta_K)$ are the model parameters, and the former satisfies the constraint $\sum_{k=1}^{K} \tau_k = 1, \tau_k \geq 0$ for $k = 1, \ldots, K$.

The ensemble of networks consists of $m$ independent observations $Y = (y^{(1)}, \ldots, y^{(m)})$ with fixed covariate set $X = (X^{(1)}, \ldots, X^{(m)})$ and fixed vertex set $V = (V^{(1)}, \ldots, V^{(m)})$, and hence
the joint likelihood is
\[ P(Y = y | X; \tau, \theta) = \prod_{i=1}^{m} \left[ \sum_{k=1}^{K} \tau_k \exp \left( \eta_k(\theta_k)^\top g_k(y^{(i)}; X^{(i)}) - \psi_{g_k, \eta_k, X^{(i)}, Y_i}^{(i)}(\theta_k) \right) h_i(y^{(i)}) \right], \quad (4) \]
where we have absorbed the support constraint into the reference measure.

To facilitate statistical inference, we consider the representation of (4) from a latent variable perspective. Let \( Z_i, i = 1, \cdots, m \) be latent variables following a categorical distribution with \( K \) values and probability parameter \( \tau \), such that \( Z_i = k \) if \( Y^{(i)} \) belongs to cluster \( k \). We may then treat \( Y^{(i)} \) as arising from a process in which \( Z_i \) is first drawn from \( \text{Categorical}(\tau) \), and \( Y^{(i)} \) is then drawn from the ERGM distribution corresponding to cluster \( Z_i \). While one could allow the reference measure to also vary by cluster, we focus on the case of ERGMs specified relative to the Krivitsky reference measure if the sizes of the networks vary.

### 3.2 Bayesian estimation

Bayesian estimation is a natural choice for parameter inference here, since (1) it is more robust to initialization and less prone to converge to local minima than maximum likelihood; (2) interval estimation is straightforward and does not rely on the assumption of approximate normality; and
(3) it provides principled answers in fixed-$n$, $m$ settings. Our strategy is to employ Metropolis-within-Gibbs sampling to obtain MCMC samples from the joint posterior distribution of $\theta$ and $\tau$.

We specify prior distributions for the parameters as follows,

$$\tau \sim \text{Dirichlet}(\alpha),$$

$$\theta_k \overset{i.i.d.}{\sim} \text{MVN}(\mu, \Psi), \quad k = 1, \cdots, K,$$

where $\alpha = (\alpha_1, \ldots, \alpha_K)$, $\mu$ and $\Psi$ are hyper-parameters to be specified by the user. For typical use cases, a reasonable choice of hyperparameters are $\alpha_1 = \cdots = \alpha_K = 3$, which puts low probability on any group being extremely small, and $\Psi = 25I_p$, which is fairly flat over the typical range of variation for common parameterizations. A convenient choice of $\mu$ is $0$, but this can be problematic because it will rarely be true that we want to shrink the edge parameter (which governs density) towards 0. It can hence be important to incorporate empirical knowledge into the specification of $\mu$; in particular, set the hyperparameter associated with edge term to be negative (e.g., $-\log n$) when modeling social networks under the counting measure, as most social networks are sparse. Under the Krivitsky reference measure, using the log of the a priori expected degree (based either on theory or analysis of similar data sets) is an appropriate choice.

As noted, we perform posterior inference via MCMC. Our algorithm iterates over the model parameters $(\theta, \tau)$ with the priors given above, and the latent variables $Z = (Z_1, \cdots, Z_m)$. Where possible we sample from the full conditional posterior distributions; otherwise we use Metropolis-Hastings steps.

The proposal distribution $q(\cdot|\theta)$ in the Metropolis step is set by the user to achieve good performance of the algorithm. On the basis of some experimentation, we use the symmetric proposal $\mathcal{N}(\theta, \sigma^2 I_q)$, where $\sigma = 0.05$. At each MCMC iteration, we permute the labels to impose ordering constraints on the first common element of the parameter vectors (e.g., total number of edges), $\theta_{11} < \theta_{21} < \cdots < \theta_{K1}$ for model identifiability purposes.

To deal with the intractability of $P(\mathbf{y}^{(i)}|\mathbf{X}^{(i)}; \theta)$, there are at least three possible solutions in ERGM literature:

- Work with a tractable approximation in the place of ERGM likelihood, e.g. pseudo-likelihood
Algorithm 1 Metropolis-within-Gibbs sampler for the ERGM mixture model

1: **Initialization**: Set $\tau^0$, $\theta^0$ and $Z^0$ to initial values (e.g., prior means).

2: for $t = 1, 2, \cdots, T$ do

3: Generate $Z_t^i$ ($i = 1, \cdots, m$, $k = 1, \cdots, K$) from $P(Z_t^i = k | \eta_{t-1}^i, \theta_{t-1}^i, y^{(i)}) \propto \eta_{t-1}^i P(y^{(i)} | X^{(i)}; \theta_{t-1}^i)$

4: Compute $\nu_t^k = \sum_{i=1}^m 1_{Z_t^i = k}$, $k = 1, \cdots, K$

5: Generate $\tau^t$ from Dirichlet($\alpha_1 + \nu_t^1, \cdots, \alpha_K + \nu_t^K$)

6: for $k = 1, \cdots, K$ do

7: Propose $\theta_t^k \sim q(\cdot | \theta_{t-1}^k)$

8: Accept $\theta_t^k$ with probability equal to $\frac{\pi(\theta_t^k) \prod_{Z_t^i = k} P(y^{(i)} | X^{(i)}; \theta_t^k) q(\theta_{t-1}^k | \theta_t^k)}{\pi(\theta_{t-1}^k) \prod_{Z_t^i = k} P(y^{(i)} | X^{(i)}; \theta_{t-1}^k) q(\theta_t^k | \theta_{t-1}^k)}$

9: end for

10: end for

(Strauss and Ikeda, 1990), fully adjusted pseudo-likelihood (Bouranis et al., 2018), or other composite likelihoods (Austad and Friel, 2010; Asuncion et al., 2010).

- Use importance sampling to approximate the ERGM likelihood (Koskinen, 2004, 2008).

- Use auxiliary-variable based MCMC algorithms to eliminate the intractable normalizing factor in ERGM likelihood (Caimo and Friel, 2011).

In fact, updating $\theta_k$’s using the Metropolis-Hastings ratio in (8) is a doubly-intractable problem, which can be approached using various advanced MCMC techniques (see Park and Haran, 2018 for a review). However, these advanced techniques all require simulating networks from ERGMs at each MCMC iteration to approximate the true likelihood Eq. (1), which can be expensive for large networks. When the major goal is clustering instead of estimation on cluster-specific parameters, we propose to work with the most common form of tractable approximation, the pseudo-likelihood, in which the full likelihood of each network is approximated by a product of full conditional distributions of edge variables $y_{ij}$ in $y$,

$$f_{PL}(y | X; \theta) = \prod_{(i,j) \in D} P(y_{ij} | y_{-ij}; X; \theta) = \prod_{(i,j) \in D} \frac{1}{1 + \exp \left\{ -\eta(\theta)^t \Delta_{i,j}g(y; X) \right\}},$$

(5)
where $\Delta_{i,j}g(y; X) = g(y_{ij}^+; X) - g(y_{ij}^-; X)$ are the so-called change statistics associated with the dyad $(i, j)$, representing the change in sufficient statistics when $y_{ij}$ is toggled from 0 ($y_{ij}^-$) to 1 ($y_{ij}^+$) with the rest of the network remaining unchanged; $\mathcal{D}$ denotes the set of all pairs of dyads. For directed networks, $\mathcal{D} = \{(i, j) | i, j \in \mathcal{N}, i \neq j\}$, while for undirected networks, $\mathcal{D} = \{(i, j) | i, j \in \mathcal{N}, i < j\}$. In the frequentist paradigm, maximizing (5) gives the so-called MPLE, which is relatively fast, algorithmically convenient, and able to provide approximate parameter estimates for even badly-specified models. While empirical observations show that MPLE can cause bias and underestimate standard errors (Van Duijn et al., 2009) (especially for models with strong dyadic dependence), it has been the default choice for initialization of MCMC-MLE algorithms. There is also promising work on using bootstrapped MPLE to construct confidence intervals (Schmid and Desmarais, 2017) for large and sparse networks, as the MPLE is usually close to MLE in such cases (Desmarais and Cranmer, 2010). Similar logic has motivated the use of Bayesian bootstrap estimation based on “pseudo-MAP” estimates using the PL approximation to the likelihood (Grazioli et al., 2019).

3.3 Choosing the number of clusters

We recast the problem of choosing the number of clusters as a model selection problem. Each number of clusters corresponds to a different statistical model, and we use a version of the observed deviance information criteria (DIC) introduced by Celeux et al. (2006), which is an extension of the original DIC (Spiegelhalter et al., 2002) for generalized linear models, to compare the models with latent variables. Given posterior draws $\tau^l, \theta^l = (\theta^l_1, \ldots, \theta^l_K)$ and observed ensemble of networks $\mathbf{y} = (y^{(1)}, \ldots, y^{(m)})$, the observed DIC is defined by

$$DIC_K = -4E[\log P(\mathbf{y}; \mathbf{X}; \theta)] + 2\log \hat{P}(\mathbf{y}; \mathbf{X}; \theta),$$

where

$$\hat{P}(\mathbf{y}; \mathbf{X}; \theta) = \prod_{i=1}^m \hat{P}(y^{(i)}; \mathbf{X}^{(i)}; \theta) = \prod_{i=1}^m \left( \frac{1}{m} \sum_{l=1}^L \sum_{k=1}^K \tau^l_k P(y^{(i)}; \mathbf{X}^{(i)}; \theta^l_k) \right),$$

and

11
\[ E[\log \mathbb{P}(y|X, \theta)|y] = \frac{1}{m} \sum_{i=1}^{L} \sum_{l=1}^{m} \log \left\{ \sum_{k=1}^{K} \tau_k \mathbb{P}(y^{(i)}|X^{(i)}; \theta_k^{(i)}) \right\}. \]

As practitioners often seek for parsimonious models to represent the clusters, we present a rule-of-thumb to identify the point where there is diminishing return by further increasing the number of clusters, and hence to avoid potential over-fitting. Define the relative difference (RD) in DIC as

\[ RD(k) = \frac{DIC_k - DIC_{k-1}}{DIC_{k-1}}, k = 2, 3, \ldots. \]

Then we define the optimal number of clusters by \( k_{opt} = \min_k \{ k | RD(k) \geq -0.5\% \} \) as a rule-of-thumb in practice, in the sense that if the improvement of DIC is below 0.5% by including an additional cluster in the model then we will stop there.

We note that having an ensemble of networks makes it possible to assess the out-of-sample performance of mixture of ERGMs using the traditional statistical principle of cross-validation (CV). In particular, to reduce the possibility of accidentally dropping all graphs in a single cluster completely by holding out too many graphs simultaneously, leave-one-out CV should be favored. The loss function for the cross-validation procedure can be negative log-likelihood evaluated on the held-out data as well as prediction error with respect to any structural properties of interest (obtained by simulating from estimated model using training data). Though the CV is not Bayesian and violates the likelihood principle, it is easy to implement and obviates the need to choose a threshold for when to stop adding clusters based on the predictive power of the model.

### 3.4 Posterior probability of cluster membership

An appealing aspect of performing cluster analysis via a mixture model is that the posterior probability of individuals belonging to each cluster (alternately: graphs having been generated by a particular process) can be conveniently obtained as

\[ \mathbb{P}(Z_i = k|y^{(i)}) = \int \frac{\tau_k \mathbb{P}(y^{(i)}|X^{(i)}; \theta_k)}{\sum_{k=1}^{K} \tau_k \mathbb{P}(y^{(i)}|X^{(i)}; \theta_k)} \pi(\theta, \tau|y) d\theta d\tau, \quad (7) \]

where \( \pi(\theta, \tau|y) \) is the posterior distribution of \( \theta, \tau \). The integral (7) is computationally intractable. Hence we use posterior samples \( \theta^1, \ldots, \theta^L \) and \( \tau^1, \ldots, \tau^L \) to obtain its Monte-Carlo
approximation,
\[ \hat{P}(Z_i = k|y^{(i)}) = \frac{1}{L} \sum_{l=1}^{L} \frac{\tau_k^l P(y^{(i)}|X^{(i)}; \theta_k^l)}{\sum_{k=1}^{K} \tau_k^l P(y^{(i)}|X^{(i)}; \theta_k^l)}. \]  

Given the goal of obtaining a deterministic cluster for each observed network \( y^{(i)} \), then the posterior mode, i.e., the \( k \) that yields the largest \( \hat{P}(Z_i = k|y^{(i)}) \) will be used.

4 Simulation studies

We conduct simulation studies to show that the proposed approach is capable of identifying the true cluster memberships and recovering the true model parameters. The ground truth is available for the synthetic dataset, as we simulate 30, 15 and 15 undirected networks of size 100 from each of 3 ERGM distributions defined on 3 commonly used network sufficient statistics but with distinct parameters,

- \( g_1(y) = \sum_{i<j} y_{ij} \), total number of edges.
- \( g_2(y) = e^\phi \sum_{k=1}^{n-2} \left\{ 1 - (1 - e^{-\phi})^k \right\} EP_k(y) \), geometrically weighted edgewise shared partner (GWESP). Here \( EP_k(y) \) is the number of connected pairs that have exactly \( k \) common neighbors, which measures local clustering in a network. The decay parameter \( \phi \) controls the relative contribution of \( EP_k(y) \) to the GWESP statistic, and it is fixed at 0.25 in this case.
- \( g_3(y; X) = \sum_{i<j} y_{ij} 1_{(X_i = X_j)} \), total number of edges with endpoints sharing same value on nodal covariate \( X \), often known as nodematch term.

We set nodal covariate \( X \) to be fixed, binary feature, and let one half of the nodes take value 0, while the other half take value 1 on \( X \). We select the true model parameters as

\[ \tau_{true} = \begin{pmatrix} 0.5 \\ 0.25 \\ 0.25 \end{pmatrix}, \quad \theta_{true} = \begin{pmatrix} -5.5 & 2.25 & 0.25 \\ -4.0 & 0.25 & 2.00 \\ -2.2 & 0.00 & 0.00 \end{pmatrix}. \]

to generate the data. Clustering ensembles of networks produced by this model is by no means a trivial task, especially as the cluster-level parameter values have been chosen to produce networks
Despite the apparent similarity of the networks produced by the three generative processes, we are able to infer the latter from the observed ensemble.

of similar densities ($\approx 0.10$) as shown in Figure 2. While these networks appear superficially similar, we can recover the distinct processes that generated them.

We then apply our algorithm for fitting a mixture of ERGMs and selecting the number of clusters as described in Section 3. In particular, we initialize the cluster membership indicator randomly according to the prior,

$$Z^0_i \sim \text{Cat}\left(\frac{\alpha_1}{\sum_{j=1}^K \alpha_j}, \cdots, \frac{\alpha_K}{\sum_{j=1}^K \alpha_j}\right), i = 1, \cdots, m,$$

then $\tau^0 = \left(\frac{\alpha_1}{\sum_{j=1}^K \alpha_j}, \cdots, \frac{\alpha_K}{\sum_{j=1}^K \alpha_j}\right)$. For $\theta$, we set the initial values for coefficients associated with edge parameters as $-2$, that is, $\theta_{11} = \cdots = \theta_{K1} = -2$; and initialize all other elements as 0.

We replicate this experiment for 20 times and allow the candidate number of clusters to range from 1 to 5. Each chain consists a total of 80,000 MCMC iterations with burn-in as 30,000, and the thinning interval was chosen as 50 to obtain high-quality, weakly correlated draws from the posterior. All computations in this paper are implemented in R (R Core Team, 2018), and we use software suite statnet (Handcock et al., 2008) to simulate networks from ERGMs.

In Figure 3, the DICs unanimously flatten out after $K = 3$ for all 20 replicates. In some runs, the DIC values are observed to decrease after $K = 3$, indicating that the smallest DIC might not always correspond to the true number of clusters, but the diminishing return yielded by further partitioning observed networks into smaller clusters is very informative for the identification of
the correct number of clusters. Figure 3 displays the traceplots of the posterior draws for a representative experiment run, and we can see that the chains mix well.

As for the parameter estimation, we compute the means of posterior means over 20 runs,

$$\hat{\tau} = \begin{pmatrix} 0.48 \\ 0.26 \\ 0.26 \end{pmatrix}, \quad \hat{\theta} = \begin{pmatrix} -5.51 & 2.26 & 0.25 \\ -4.02 & 0.25 & 2.02 \\ -2.20 & 0.00 & -0.01 \end{pmatrix}. $$

and the standard deviations of posterior means across the 20 runs are

$$SD(\hat{\tau}) = \begin{pmatrix} 0.002 \\ 0.001 \\ 0.002 \end{pmatrix}, \quad SD(\hat{\theta}) = \begin{pmatrix} 0.08 & 0.06 & 0.02 \\ 0.03 & 0.02 & 0.01 \\ 0.03 & 0.01 & 0.03 \end{pmatrix}. $$

This shows that the proposed method can yield fairly accurate estimation of cluster-specific parameters, and mixture weight parameters $\tau$. 

Figure 3: DIC vs number of clusters, 20 replicates
Figure 4: Posterior samples for a representative replicate (samples drawn during burn-in period were discarded). Rows 1, 2, 3 correspond to clusters 1, 2, 3, respectively. Columns 1, 2, 3 correspond to edges, gwesp(0.25) and nodematch(X), respectively.

5 Case study

In this section, we apply the proposed method to cluster the co-voting patterns among U.S. Senators from 1867 (start year of Congress 40) to 2014 (end year of Congress 113), which was a subset of the data first analyzed by Moody and Mucha (2013) using modularity and role-based blockmodels. The co-voting tendencies are represented by networks based on the roll call voting data from http://voteview.com, which contains the voting decision of each Senator (yay, nay, or abstain) for every bill brought to Congress.\(^1\) The nodes in the co-voting network represent Senators and an edge is placed between two nodes if the corresponding Senators vote concurrently (both yay of both nay) on at least 75% of the bills to which they were both present. Here we aim at identifying subgroups of networks that appear to have similar generating characteristics within the group but different characteristics across groups.

---

\(^1\)The data is available online in the R package VCERRGM, https://github.com/jihuilee/VCERGM
Figure 5: Co-voting networks of 61st, 89th and 111th Congress, which were formed in the year of 1909, 1965 and 2009, respectively. Colors indicate Senators’ party affiliations, blue = Democrats(D), red = Republican(R).

5.1 Model specification and estimation

Figure 5 shows that the co-voting networks vary in structure on different years, and the party-affiliation appears to be a key factor affecting the co-voting patterns among Senators. Therefore we consider an ERGM model with following sufficient statistics $g(y) = (g_1(y), g_2(y), g_3(y), g_4(y))$, where

$$g_1(y) = \sum_{i<j} y_{ij}, \text{ total number of edges;}$$

$$g_2(y; X) = \sum_{i<j} y_{ij} I\{X_i = X_j = D\}, \text{ total number of edges between Democrats;}$$

$$g_3(y; X) = \sum_{i<j} y_{ij} I\{X_i = R, X_j = D\}, \text{ total number of edges between Democrats and Republicans;}$$

$$g_4(y) = e^\phi \sum_{k=1}^{n-2} \left\{1 - (1 - e^{-\phi})^k\right\} E P_k(y), \text{ GWESP statistic}$$

The decay parameter of GWESP term is fixed as $\phi = 0.25$ as often used in ERGM literature. We note that these networks vary in size (range: 69 – 112) and thus include an offset term (2) to adjust for network size. (This is equivalent to using the Krivitsky reference measure, which provides a parameterization with constant baseline expected degree.)

Figure 5 indicates that the DIC reaches its minimum at $K = 3$, and hence $K = 3$ appears to be a plausible choice for the number of clusters. Under $K = 3$, the posterior mean estimates of cluster-specific parameters are
Figure 6: DIC vs Number of Clusters, Congress co-voting networks

\[
\hat{\tau} = \begin{pmatrix}
0.36 \\
0.47 \\
0.17 \\
\end{pmatrix}
\quad \hat{\theta} = \begin{pmatrix}
1.69 & 0.01 & -2.49 & 1.42 \\
2.04 & -0.12 & -3.09 & 2.14 \\
2.47 & 0.92 & -4.47 & 2.63 \\
\end{pmatrix}
\]

We note that the size-invariant parameters for edge term (first column) can be interpreted as the log of the baseline mean degree (rather than the logit of the baseline density, as in the case of the counting measure), suggesting expected degrees varying from approximately 5.5 to 12 across clusters prior to consideration of other effects.

Based on these estimates, we have the following observations regarding the co-voting patterns. Across all clusters, we see both inhibition of cross-party ties (third column) and strong triadic closure (fourth column). Clusters do differ, however. Cluster 1 shows essentially symmetric behavior by party (column two), with lower levels of cross-group inhibition and triadic closure bias than in the other clusters; overall, cluster 1 suggests a relatively low level of polarization by party, with voting only loosely restricted by party lines. By contrast, cluster 2 reflects a much more polarized regime, with more activity overall and co-voting being more concentrated.
within party. Like cluster 1, however, cluster 2 shows little party asymmetry (apart from a fairly weak tendency towards lower levels of co-voting among Democrats). Such asymmetry is much more strongly pronounced within cluster 3, with intraparty Democratic ties being approximately 2.5 times as likely (ceteris paribus) as ties within the GOP. This cluster also reflects extremely high levels of polarization, with cross-party co-voting being strongly inhibited and high levels of triadic closure. Over the period studied here, the most common pattern (probability 0.47) is the symmetric polarization of cluster 2, with the loose, low polarization pattern of cluster 1 also being fairly common (probability 0.36). The asymmetric, highly polarized regime of cluster 3 is less common, but is still estimated to account for approximately 17% of the observed cases. Interestingly, we do not see a corresponding asymmetric pattern in which the GOP shows high intraparty vote density, as might be anticipated; thus, there appear to be latent differences in how the two parties behave during the period that, while not manifest in every congress, always have the potential to arise.

One advantage of working with a fully generative model is the ability to perform “what-if” analyses that separate effects due to observed covariates from differences in structure arising from differences in generative processes. To probe the impact of the three behavioral regimes inferred from the co-voting data, we consider how the entire ensemble Congressional networks would be expected to have been different, if each respective regime had governed the U.S. Congress for the entire study period. To perform such an analysis, we first simulate a set of posterior predictive networks for each Congress during the study period, with parameters drawn from the posterior distribution of each respective cluster. Each collection of networks can be thought of as a simulated “alternate history,” in which the size and composition of each Congress were held to their real-world values but the behavioral tendencies that shaped the co-voting networks throughout the period were reflective of only one of the three clusters. Systematic differences in network structure across sets thus provide insight into the potential impact of behavioral regime, controlling for size and composition.

One important property that can be probed in this way is the expected incidence of voting coalitions, which play an important role in party politics. Here, we focus on minimal coalitions, defined as sets of three legislators who consistently vote together (i.e., triangles). Within-party coalitions can be sources of party cohesion, although they also act as blocks that can sometimes
resist (and must be negotiated with by) party leaders; cross-party coalitions, by contrast, pose significant challenges to party cohesion, but can also serve as foci for sponsorship and promotion of bipartisan legislation. Both are hence significant, with distinct implications for the political landscape. To examine the coalition structures that would have been expected to occur under our three behavioral regimes, we simulate 10 “alternate histories” from the posterior distributions of each cluster, calculating the realized proportions of intra-Democratic, intra-Republican, and inter-Party triangles. (That is, the counts of fully connected triads with all three members as Democrats, all three members as Republicans, or members from both parties, scaled by their maximum possible values.) Using proportions rather than raw counts ensures these metrics are normalized for network size and the distribution of party affiliations in each Congress; substantively, this choice of scaling tells us how close each party (or the cross-party cut) is to forming a perfect coalition, in which all members vote in concert. Figure 7 shows the realized proportion of intra-party triangles in simulated networks, and Figure 8 shows the realized proportion of intra-party triangles in the simulated networks. Both figures show substantial differences in coalition structure, implying that the behavioral regimes associated with the three inferred clusters would be expected to have a meaningful impact on the political process. Specifically, we note the following:

- The regime of cluster 1 is marked by the formation of very few voting coalitions, either within party or between party). As suggested by the parameter values, we see little difference in coalition formation between the two parties, both having little cohesion.

- By contrast, the regime of cluster 2 shows a much higher incidence of intra-party coalition formation, with roughly 10-20% of the potential intra-party coalitions being present. Coalition incidence differs little by party, with at best a small average increment in the rate of coalition incidence for Republicans versus Democrats. Interestingly, this regime also shows the highest rate of cross-party coalition formation; while the rate is very low overall, it is considerably higher than that observed under cluster 1.

- Finally, the regime of cluster 3 favors extremely high levels of intra-party cohesion, with rates approaching 50% of the maximum possible for Republicans and 75% for Democrats. As this implies, the resulting networks are also highly asymmetric, with the Democratic party expected to generate a much more cohesive coalition structure than the GOP. Interestingly,
this strong intra-party coalition formation does not exist entirely at the expense of cross-
party coalitions: we find an expected rate of cross-party coalition formation that is only
slightly less than that expected for networks arising under cluster 2. That said, the much
higher incidence of intra-party coalition formation under cluster 3 leads inter-party coalitions
to be a smaller fraction of the total coalition set than under cluster 2, potentially making
them less critical to the legislative process.

Taken together, these observations suggest that the cluster 1 regime tends to generate uniformly
loose voting networks with very few coalitions of any kind. These networks may resist polarization,
but their high level of fragmentation may make it more difficult to assemble the sorts of alliances
needed to push through controversial legislation. By contrast, the regime of cluster 2 tends to
produce uniformly clustered networks with moderately high levels of coalition formation in both
parties coupled with relatively high numbers of cross-party coalitions. These networks may pose
particular challenges for party leaders, as they contain a mix of multiple local coalitions that must
be courted for votes, “lone wolves” outside of coalitions who must be approached individually, and
likely defectors whose cross-party coalitions provide a bullwark against within-party influence.
Finally, the regime of cluster 3 tends to produce party-cohesive networks dominated by dense
intra-party coalitions on both sides of the aisle (but with substantially higher levels of cohesion
among Democratic legislators). This regime offers party leaders the greatest chance of being able
to mobilize members in support of legislation, at the cost of potential legislative deadlock during
periods of high inter-party conflict.

In addition to examining the potential impact of different behavioral regimes on voting net-
works, our model also provides insight into the incidence of these regimes over time. For instance,
Figure 9 shows maximum probability cluster assignments over the study period. We see that the
relatively symmetric cultures represented by cluster 1 and cluster 2 alternate in the nineteenth
and twentieth centuries, while the culture of asymmetric polarization represented by cluster 3 be-
comes dominant after late 1990’s. Such finding is in line with the current trend of political party
polarization \cite{Moody and Mucha 2013}. Table 1 shows the breakdown of congresses into \(3 \times 2\)
sub-categories according to the estimated co-voting pattern and the observed majority party. We
examine the independence of co-voting pattern assignment and the majority party using Pearson’s
\(\chi^2\) test, and we fail to reject the null hypothesis that the majority party is independent of the
Figure 7: Proportion of realized intra-party triangles in simulated networks. Colors indicate the party affiliation (blue = Democratic (D), red = Republican (R)).

Figure 8: Proportion of realized inter-party triangles in simulated networks.
Figure 9: Maximum probability cluster assignments over study period. Colors indicate the majority party in the corresponding Congress (blue = Democratic (D), red = Republican (R)). Regimes of voting behavior are visibly correlated over time.

co-voting patterns \(\chi^2 = 1.07, \text{ p-value } = 0.58\). Thus, while the regimes of party behavior are quite visibly autocorrelated, this pattern does not seem to be related to which party has control of congress at any given time.

Table 1: Tabulation of co-voting pattern by majority party (from Congress 40 to Congress 113).

| Co-voting Pattern | Democratic | Republican |
|-------------------|------------|------------|
| 1                 | 16         | 11         |
| 2                 | 17         | 19         |
| 3                 | 5          | 6          |

5.2 Model assessment

To assess the adequacy of the above ERGM mixture model, we consider a simulation-based method \cite{Hunter2008}, with the basic insight that a fitted ERGM model should be able to reproduce in simulation structural properties similar to those of the observed networks. Instead of simulating from a single point estimate, we propose to simulate networks from estimated posterior distribution, following practices of posterior predictive assessment in the Bayesian literature \cite{Gelman2013}.
The structural property of interest here is the modularity score (assessed by party), which can be interpreted as a measure of the polarization of networks with respect to party structure. By definition, the modularity score ranges from $-1$ to $1$, with larger values indicating higher levels of polarization. The evaluation procedure proceeds as follows:

1. Simulate 20 networks from the ERGM mixture distribution using the posterior samples, for each vertex set in the observed co-voting networks.

2. Compute and compare the modularity score of the observed ensemble of networks and the simulated networks.

Figure 10 shows that the resulting mixture model can capture the variation of the modularity scores of the observed ensemble of co-voting networks to a large extent. The remaining discrepancy between observed modularity scores and those of simulated networks may be mitigated by more accurate estimation algorithms for cluster-specific parameters (e.g., using importance sampling techniques).
to approximate ERGM likelihood rather than the pseudo-likelihood), at higher computational expense.

6 Conclusion

In this paper, we proposed a mixture of ERGMs approach for modeling the generative process leading to heterogeneous network ensembles. We developed a Metropolis-within-Gibbs algorithm to fit ERGM mixtures and obtained Bayesian estimates of clustering assignment probabilities and the cluster-specific ERGM parameters. To account for the difference in the size of the observed networks, we used a size-adjusted parameterization for ERGMs. We also tailored a version of the observed DIC and then defined a rule-of-thumb to select the number of clusters. The simulation studies showed that the proposed approach can accurately recover the cluster membership and cluster-specific parameters, without requiring much effort on initialization.

We applied the proposed approach to study the political co-voting networks among U.S. Senators, and identified three clusters that represent vastly different co-voting patterns. After matching the clusters with temporal information, we observed that one symmetric co-voting pattern and another mildly asymmetric co-voting patterns alternate in nineteenth and twentieth century, and there appeared to be an abrupt shift in the co-voting pattern towards the direction of political party polarization in last two decades.

Compared to other methods in the literature, our proposed method allows straightforward statistical inference of heterogeneous generative process of ensemble of networks, and is conveniently interpretable. We believe that the proposed method can prove to be a highly effective tool for both exploratory and inferential analysis of ensembles of networks.

In closing, we comment on two important directions of future research that could prove beneficial to the modeling of ensembles of networks: the development of more sophisticated size-adjusted parameterizations and more accurate tractable approximations of the ERGM likelihood. It is worth remembering that the sizes of the US congresses between 1867 and 2014 range from 69 to 112, non-identical but broadly similar. More importantly, these size changes occur within a social system whose basic structure remains fairly similar throughout the period. In other cases, however, large size differences may be accompanied by increasingly complex internal barriers to interaction or other additional exogenous structure that must be accounted for to obtain realis-
tic predictions. Where this additional structure is not available in the form of covariates, more sophisticated size-adjusted parameterizations may be required; reference measures or other tools facilitating “automatic” correction of such effects would facilitate mixture modeling in such scenarios. With respect to likelihood calculation, it is encouraging that we obtain favorable results in our simulation study using the easily computed pseudo-likelihood approximation. In particular, the main deficiency of the pseudo-likelihood is excessive sharpness near the mode, which could in principle encourage the over-production of mixture components. While we do not see this effect here, more accurate likelihood approximations that are inexpensive enough to perform at each MCMC step for large models would be desirable. As such improved approximations become available, they can be easily integrated into the posterior simulation framework described here.

References

V. Amati, A. Mol, T. Shafie, C. Hofman, and U. Brandes. A framework for reconstructing archaeological networks using exponential random graph models. *Journal of Archaeological Method and Theory*, pages 1–28, 2019.

A. Asuncion, Q. Liu, A. Ihler, and P. Smyth. Learning with blocks: Composite likelihood and contrastive divergence. In *Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics*, pages 33–40, 2010.

H. Austad and N. Friel. Deterministic Bayesian inference for the $p^*$ model. In *13th International conference on Artificial Intelligence and Statistics (AISTATS, 2010), Chia Laguna Resort, Sardinia, Italy, May 13-15 2010*. Journal of Machine Learning Research (JMLR), 2010.

D. Banks and K. M. Carley. Metric inference for social networks. *Journal of Classification*, 11(1): 121–149, 1994.

J. Besag. Spatial interaction and the statistical analysis of lattice systems. *Journal of the Royal Statistical Society. Series B (Methodological)*, pages 192–236, 1974.

L. Bouranis, N. Friel, and F. Maire. Efficient Bayesian inference for exponential random graph models by correcting the pseudo-posterior distribution. *Social Networks*, 50:98–108, 2017.
L. Bouranis, N. Friel, and F. Maire. Bayesian model selection for exponential random graph models via adjusted pseudolikelihoods. *Journal of Computational and Graphical Statistics*, 27(3):516–528, 2018.

C. Bouveyron, G. Celeux, T. B. Murphy, and A. E. Raftery. *Model-Based Clustering and Classification for Data Science: With Applications in R*, volume 50. Cambridge University Press, 2019.

C. T. Butts. Bayesian meta-analysis of social network data via conditional uniform graph quantiles. *Sociological Methodology*, 41(1):257–298, 2011.

C. T. Butts. Baseline mixture models for social networks. *arXiv preprint arXiv:1710.02773*, 2017.

C. T. Butts and Z. W. Almquist. A flexible parameterization for baseline mean degree in multiple-network ERGMs. *The Journal of Mathematical Sociology*, 39(3):163–167, 2015.

C. T. Butts and K. M. Carley. Some simple algorithms for structural comparison. *Computational and Mathematical Organization Theory*, 11(4):291–305, 2005.

A. Caimo and N. Friel. Bayesian inference for exponential random graph models. *Social Networks*, 33(1):41–55, 2011.

A. Caimo, F. Pallotti, and A. Lomi. Bayesian exponential random graph modelling of interhospital patient referral networks. *Statistics in Medicine*, 36(18):2902–2920, 2017.

G. Celeux, F. Forbes, C. P. Robert, and D. M. Titterington. Deviance information criteria for missing data models. *Bayesian Analysis*, 1(4):651–673, 2006.

S. J. Cranmer and B. A. Desmarais. Inferential network analysis with exponential random graph models. *Political Analysis*, 19(1):66–86, 2011.

B. A. Desmarais and S. J. Cranmer. Consistent confidence intervals for maximum pseudolikelihood estimators. In *Proceedings of the Neural Information Processing Systems 2010 Workshop on Computational Social Science and the Wisdom of Crowds*. Citeseer, 2010.

D. Durante and D. B. Dunson. Bayesian inference and testing of group differences in brain networks. *Bayesian Analysis*, 13(1):29–58, 2018.
K. Faust and J. Skvoretz. Comparing networks across space and time, size and species. *Sociological Methodology*, 32(1):267–299, 2002.

S. M. Fitzhugh, J. E. Pixley, and C. T. Butts. A life history graph approach to the analysis and comparison of life histories. *Advances in Life Course Research*, 25:16–34, 2015.

C. Fraley and A. E. Raftery. Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association*, 97(458):611–631, 2002.

O. Frank and D. Strauss. Markov graphs. *Journal of the American Statistical Association*, 81(395):832–842, 1986.

A. Gelman, X.-L. Meng, and H. Stern. Posterior predictive assessment of model fitness via realized discrepancies. *Statistica Sinica*, pages 733–760, 1996.

C. J. Geyer and E. A. Thompson. Constrained Monte Carlo maximum likelihood for dependent data. *Journal of the Royal Statistical Society. Series B (Methodological)*, pages 657–699, 1992.

S. M. Goodreau. Advances in exponential random graph (p*) models applied to a large social network. *Social Networks*, 29(2):231–248, 2007.

G. Grazioli, R. W. Martin, and C. T. Butts. Comparative exploratory analysis of intrinsically disordered protein dynamics using machine learning and network analytic methods. *Frontiers in Molecular Biosciences*, 6:42, 2019.

C. Groendyke, D. Welch, and D. R. Hunter. A network-based analysis of the 1861 Hagelloch measles data. *Biometrics*, 68(3):755–765, 2012.

M. S. Handcock. Assessing degeneracy in statistical models of social networks. Technical report, Center for Statistics and Social Sciences, University of Washington, 2003. [https://www.csss.washington.edu/Papers/wp39.pdf](https://www.csss.washington.edu/Papers/wp39.pdf).

M. S. Handcock, D. R. Hunter, C. T. Butts, S. M. Goodreau, and M. Morris. statnet: Software tools for the representation, visualization, analysis and simulation of network data. *Journal of Statistical Software*, 24(1):1548, 2008.
G. E. Hinton. Training products of experts by minimizing contrastive divergence. *Neural Computation*, 14(8):1771–1800, 2002.

N. L. Hjort and G. Claeskens. Frequentist model average estimators. *Journal of the American Statistical Association*, 98(464):879–899, 2003.

J. A. Hoeting, D. Madigan, A. E. Raftery, and C. T. Volinsky. Bayesian model averaging: a tutorial. *Statistical Science*, pages 382–401, 1999.

P. W. Holland and S. Leinhardt. An exponential family of probability distributions for directed graphs. *Journal of the American Statistical Association*, 76(373):33–50, 1981.

R. M. Hummel, D. R. Hunter, and M. S. Handcock. Improving simulation-based algorithms for fitting ERGMs. *Journal of Computational and Graphical Statistics*, 21(4):920–939, 2012.

D. R. Hunter and M. S. Handcock. Inference in curved exponential family models for networks. *Journal of Computational and Graphical Statistics*, 15(3):565–583, 2006.

D. R. Hunter, S. M. Goodreau, and M. S. Handcock. Goodness of fit of social network models. *Journal of the American Statistical Association*, 103(481):248–258, 2008.

D. R. Hunter, P. N. Krivitsky, and M. Schweinberger. Computational statistical methods for social network models. *Journal of Computational and Graphical Statistics*, 21(4):856–882, 2012.

E. D. Kolaczyk and P. N. Krivitsky. On the question of effective sample size in network modeling: an asymptotic inquiry. *Statistical Science*, 30(2):184, 2015.

J. Koskinen. Bayesian analysis of exponential random graphs-estimation of parameters and model selection. Technical report, Research Report 2004: 2, Department of Statistics, Stockholm University, 2004.

J. H. Koskinen. The linked importance sampler auxiliary variable Metropolis Hastings algorithm for distributions with intractable normalising constants. *MelNet Social Networks Laboratory Technical Report*, pages 08–01, 2008.

P. N. Krivitsky. Using contrastive divergence to seed Monte Carlo MLE for exponential-family random graph models. *Computational Statistics & Data Analysis*, 107:149–161, 2017.
P. N. Krivitsky, M. S. Handcock, and M. Morris. Adjusting for network size and composition effects in exponential-family random graph models. *Statistical Methodology*, 8(4):319–339, 2011.

B. C. L. Lehmann. *Inferring differences between networks using Bayesian exponential random graph models*. PhD thesis, University of Cambridge, 2019.

D. A. McFarland, J. Moody, D. Diehl, J. A. Smith, and R. J. Thomas. Network ecology and adolescent social structure. *American Sociological Review*, 79(6):1088–1121, 2014. doi: 10.1177/0003122414554001.

G. J. McLachlan and K. E. Basford. *Mixture models: Inference and applications to clustering*, volume 84. M. Dekker New York, 1988.

J. Moody and P. J. Mucha. Portrait of political party polarization. *Network Science*, 1(1):119–121, 2013.

M. Morris, M. S. Handcock, and D. R. Hunter. Specification of exponential-family random graph models: terms and computational aspects. *Journal of Statistical Software*, 24(4):1548, 2008.

M. E. Newman. Modularity and community structure in networks. *Proceedings of the National Academy of Sciences*, 103(23):8577–8582, 2006.

C. Obando and F. De Vico Fallani. A statistical model for brain networks inferred from large-scale electrophysiological signals. *Journal of The Royal Society Interface*, 14(128):20160940, 2017.

J. Park and M. Haran. Bayesian inference in the presence of intractable normalizing functions. *Journal of the American Statistical Association*, 113(523):1372–1390, 2018.

G. C. Pflug. *Optimization of Stochastic Models. The Interface Between Simulation and Optimization*. Boston: Kluwer Academic., 1996.

N. Prulj. Biological network comparison using graphlet degree distribution. *Bioinformatics*, 23 (2):e177–e183, 01 2007. ISSN 1367-4803. doi: 10.1093/bioinformatics/btl301. URL https://doi.org/10.1093/bioinformatics/btl301

R Core Team. *R: A Language and Environment for Statistical Computing*. Vienna, Austria: R Foundation for Statistical Computing, 2018.
H. Robbins and S. Monro. A stochastic approximation method. *The annals of mathematical statistics*, pages 400–407, 1951.

G. Robins, T. Snijders, P. Wang, M. Handcock, and P. Pattison. Recent developments in exponential random graph (p*) models for social networks. *Social Networks*, 29(2):192–215, 2007.

M. Salter-Townshend and T. B. Murphy. Role analysis in networks using mixtures of exponential random graph models. *Journal of Computational and Graphical Statistics*, 24(2):520–538, 2015. doi: 10.1080/10618600.2014.923777.

Z. M. Saul and V. Filkov. Exploring biological network structure using exponential random graph models. *Bioinformatics*, 23(19):2604–2611, 2007.

C. S. Schmid and B. A. Desmarais. Exponential random graph models with big networks: Maximum pseudolikelihood estimation and the parametric bootstrap. In *2017 IEEE International Conference on Big Data (Big Data)*, pages 116–121. IEEE, 2017.

M. Schweinberger and M. S. Handcock. Local dependence in random graph models: characterization, properties and statistical inference. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 77(3):647–676, 2015.

S. L. Simpson, S. Hayasaka, and P. J. Laurienti. Exponential random graph modeling for complex brain networks. *PLoS ONE*, 6(5):e20039, 2011.

M. R. Sinke, R. M. Dijkhuizen, A. Caimo, C. J. Stam, and W. M. Otte. Bayesian exponential random graph modeling of whole-brain structural networks across lifespan. *Neuroimage*, 135:79–91, 2016.

A. J. Slaughter and L. M. Koehly. Multilevel models for social networks: hierarchical Bayesian approaches to exponential random graph modeling. *Social Networks*, 44:334–345, 2016.

T. A. Snijders. Markov chain Monte Carlo estimation of exponential random graph models. *Journal of Social Structure*, 3(2):1–40, 2002.

T. A. Snijders and K. Nowicki. Estimation and prediction for stochastic blockmodels for graphs with latent block structure. *Journal of classification*, 14(1):75–100, 1997.
T. A. Snijders, P. E. Pattison, G. L. Robins, and M. S. Handcock. New specifications for exponential random graph models. *Sociological Methodology*, 36(1):99–153, 2006.

D. J. Spiegelhalter, N. G. Best, B. P. Carlin, and A. Van Der Linde. Bayesian measures of model complexity and fit. *Journal of the Royal Statistical Society: Series B (statistical methodology)*, 64(4):583–639, 2002.

J. Stewart, M. Schweinberger, M. Bojanowski, and M. Morris. Multilevel network data facilitate statistical inference for curved ERGMs with geometrically weighted terms. *Social Networks*, to appear, 2019.

D. Strauss and M. Ikeda. Pseudolikelihood estimation for social networks. *Journal of the American Statistical Association*, 85(409):204–212, 1990.

T. M. Sweet, A. C. Thomas, and B. W. Junker. Hierarchical mixed membership stochastic blockmodels for multiple networks and experimental interventions. *Handbook on mixed membership models and their applications*, pages 463–488, 2014.

T. M. Sweet, A. Flynt, and D. Choi. Clustering ensembles of social networks. *Network Science*, pages 1–19, 2019.

M. H. Unhelkar, V. T. Duong, K. N. Enendu, J. E. Kelly, S. Tahir, C. T. Butts, and R. W. Martin. Structure prediction and network analysis of chitinases from the Cape Sundew, Drosera capensis. *Biochimica et Biophysica Acta (BBA)-General Subjects*, 1861(3):636–643, 2017.

M. A. Van Duijn, K. J. Gile, and M. S. Handcock. A framework for the comparison of maximum pseudo-likelihood and maximum likelihood estimation of exponential family random graph models. *Social Networks*, 31(1):52–62, 2009.

S. Wasserman and P. Pattison. Logit models and logistic regressions for social networks: I. an introduction to markov graphs and p*. *Psychometrika*, 61(3):401–425, 1996.

B. J. Zijlstra, M. A. Van Duijn, and T. A. Snijders. The multilevel p2 model. *Methodology: European Journal of Research Methods for the Behavioral and Social Sciences*, 2(1):42–47, 2006.