Actor Heterogeneity and Explained Variance in Network Models—A Scalable Approach through Variational Approximations

Nadja Klein\textsuperscript{1,*} and Göran Kauermann\textsuperscript{2}

\textsuperscript{1}Technische Universität Dortmund, \textsuperscript{2}Ludwig-Maximilians-Universität München

Abstract

The analysis of network data has gained considerable interest in recent years. This also includes the analysis of large, high-dimensional networks with hundreds and thousands of nodes. While exponential random graph models serve as workhorse for network data analyses, their applicability to very large networks is problematic via classical inference such as maximum likelihood or exact Bayesian estimation owing to scaling and instability issues. The latter trace from the fact that classical network statistics consider nodes as exchangeable, i.e., actors in the network are assumed to be homogeneous. This is often questionable. One way to circumvent the restrictive assumption is to include actor-specific random effects, which account for unobservable heterogeneity. However, this increases the number of unknowns considerably, thus making the model highly-parameterized. As a solution even for very large networks, we propose a scalable approach based on variational approximations, which not only leads to numerically stable estimation but is also applicable to high-dimensional directed as well as undirected networks. We furthermore demonstrate that including node-specific covariates can reduce node heterogeneity, which we facilitate through versatile prior formulations and a new measure that we call \textit{posterior explained variance}. We illustrate our approach in three diverse examples, covering network data from the Italian Parliament, international arms trading, and Facebook; and conduct detailed simulation studies.

Keywords: Exponential random graph model; node heterogeneity; random effects; reparameterization trick; social network analysis; stochastic variational inference

* Correspondence should be directed to Nadja Klein at nadja.klein@tu-dortmund.de.
1 Introduction

Until about two decades ago, the analysis of network data was relatively rare in the literature. However, it has since become a continuously emerging field in statistics, allowing the investigation of links and relationships between nodes representing, for instance, social entities, genes, diseases, and many others (see Goldenberg et al.; 2009; Kolaczyk; 2009; Fienberg; 2012; Kolaczyk and Csardi; 2014; Biagini et al.; 2019, for examples of overviews on this topic).

A key statistical model for network data analyses is the exponential random graph model (ERGM), originally proposed by Frank and Strauss (1986). ERGMs may certainly be considered as the workhorses in statistical network data analyses, as they allow for interpretable models as well as extensions in various ways. Nowadays, ERGMs are widely used in economics, sociology, and political science, amongst others, to analyse (social) networks. The key idea is to consider a network with $N$ nodes as a binary adjacency matrix $Y \in \{0, 1\}^{N \times N}$, where $Y_{ij} = 1$ if an edge from node $i$ to node $j$ exists, and $Y_{ij} = 0$ otherwise. The diagonal is left undefined, i.e., edges connecting a node to itself are not allowed, and we set $Y_{ii} = 0$. The network may be directed or undirected, depending on the relationships between the actors in the network. Compared to directed networks, undirected networks fulfil the symmetry property that $Y_{ij} = Y_{ji}$ for all $1 \leq i < j \leq N$. The adjacency matrix $Y$ can be considered as a random variable with a probability distribution that is based on a set of sufficient network statistics $s_k(y)$, for $k = 0, \ldots, p$. This leads to the probability model

$$P(Y = y \mid \beta) = \frac{\exp(s(y)^T \beta)}{\kappa(\beta)},$$

(1)

where $s(\cdot) = (s_0(\cdot), s_1(\cdot), \ldots, s_p(\cdot))^T$ is a vector of sufficient network statistics, such as the number of edges or two-stars in a network (see e.g. Snijders et al.; 2006, and Supplement A for relevant network statistics) and $\beta = (\beta_0, \beta_1, \ldots, \beta_p)^T \in \mathbb{R}^{p+1}$ is the parameter vector of model coefficients. Since $s(y)$ depends on the network only, its components are endogenous. The model in (1) represents an exponential family distribution, and the interpretation of an ERGM and its coefficients $\beta$ is similar to that of a binary logistic regression model. That is, a tie in a network is the outcome, and the characteristics of network members and network structures aid in explaining or predicting the probability of a tie (Hunter et al.; 2008). However, unlike in logistic regression, the normalization constant $\kappa(\beta) = \sum_{y^* \in \mathcal{Y}} \exp(s(y^*)^T \beta)$ involves a sum over all possible networks represented by $\mathcal{Y}$ being the set of all (symmetric for undirected and non-symmetric for directed networks) $\{0, 1\}^{N \times N}$ matrices. This is intractable except for very small networks. Estimation of $\kappa(\beta)$ in model (1) therefore needs to be carried out approximately or based on simulations (see also Hunter et al.; 2012, for a general survey on computational methods used in network analysis).

An early reference for estimating ERGMs is Snijders (2002), who adapted so-called Markov Chain Monte Carlo (MCMC) maximum likelihood estimation (MLE) (MCMC-MLE Geyer and Thompson; 1992). A numerically stable routine thereof has been proposed in Hummel et al. (2012) using a so-called stepping algorithm. However, MCMC-MLE may have exponentially slow convergence, making estimation impractical for a large class of ERGMs (Chatterjee and Diaconis; 2013). Bayesian estimation of ERGMs is challenging as well and known as a doubly intractable problem, since not only $\kappa(\beta)$ but also the normalizing
constant of the posterior is intractable. Caimo and Friel (2011) therefore proposed an MCMC algorithm that samples from the likelihood using a “tie no tie” sampler (Hunter et al.; 2008) coupled with the exchange algorithm of Murray et al. (2006) to sample from the posterior. Reducing the numerical burden of Bayesian estimation in model (1) is also pursued by Yin and Butts (2020) or by Bouranis et al. (2018), who propose adjusted pseudolikelihood estimation in the context of Bayesian model selection.

Besides the challenges in estimation, a critical shortcoming of the ERGM in its classical formulation (1) is that it assumes node homogeneity, given the network statistics. In other words, the actors in the network can be permuted without changing the model. In practice, this can be a crucial caveat, in particular when modelling large networks, and the inclusion of latent node heterogeneity in the model is advisable. Accounting for such heterogeneity traces back to the so-called $p_1$ and $p_2$ models, which explain the existence of an edge purely with external nodal covariates or random effects, respectively (Holland and Leinhardt; 1981; Duijn et al.; 2004). In this model setup, Wang et al. (2023) recently proposed variable selection in the presence of node heterogeneity. The ideas of node heterogeneity were extended in Koskinen (2009) and further on in Thiemichen et al. (2016a), who combined the node-specific random effects of the $p_2$ model with ERGMs and proposed Bayesian estimation via MCMC. While conceptually straight-forward, the MCMC approach becomes numerically infeasible in larger networks. As an illustration, take the large undirected social network depicted in Figure 1 with about 4,000 nodes and nearly 90,000 edges, a set of Facebook profiles with edges representing friendships. Heterogeneity in the nodes and their connectedness is directly visible. We will account for this by including latent node-specific heterogeneity. Box-Steffensmeier et al. (2018) propose approximating estimation

Figure 1: Facebook egos.

Illustration of the network. The left plot depicts the complete network with 4039 nodes including the egos. The right plot depicts the network with 3953 nodes after exclusion of the egos and all nodes only having connections to egos.

through a pseudolikelihood approach, which does work in large networks, but has its own problems such as bad behaviour or void inference (see e.g., Duijn et al.; 2009). Kevork
and Kauermann (2021) propose pseudolikelihood estimation in networks with nodal heterogeneity and extend it to bipartite networks in Kevork and Kauermann (2022). However, this suffers from biased inference.

If node- or edge-specific covariates, denoted as $x$, are also available, including these in the model can reduce nodal heterogeneity. In this case, (1) extends to

$$P(Y = y | \beta) = \frac{\exp(s(y, x)^\top \beta)}{\kappa(\beta)},$$

(2)

where $s(y, x)$ is a vector of statistics built from both the endogenous $y$ and the exogenous components $x$. The main assumption of model (2) is that all nodal heterogeneity is captured through the exogenous covariates $x$. As such, $x$ can be seen as a set of confounding variables that capture node-specific heterogeneity. However, in real applications, one might not have included all covariates to explain heterogeneity; that is to say, some nodal heterogeneity may remain, which cannot be explained through the included confounders. We will therefore also extend model (2) towards including additional nodal heterogeneity to account for such effects not explained by $x$.

If random nodal heterogeneity is required, covariates $x$ do not fully explain differences between the nodes. Vice versa, if the nodal heterogeneity is low or not required in the model with covariates, nodal heterogeneity is fully explained by the external covariates as generally desired for interpretability. Taking this view, we may state that reducing nodal heterogeneity through the inclusion of covariates $x$ allows quantification of the amount of posterior explained variance, comparable to the coefficient of determination $R^2$ in classical regression models. We facilitate this idea through Bayesian reasoning using versatile penalized complexity priors (Klein and Kneib; 2016; Simpson et al.; 2017) on variance parameters of the priors for model coefficients associated with the nodal random effects.

We illustrate this extended approach in two further examples. Figure 2 visualizes the considered collaboration network of the members of the Italian Parliament in an undirected network with edge-specific covariates. Next, we consider a directed network of international arms trading in 2016. Figure 3 illustrates the respective network with directed edges indicating the export directions. We showcase that controlling for important confounders through the inclusion of node-specific covariates (such as gross domestic product) can reduce nodal random effects, thus providing a way of reducing unobserved heterogeneity. This observation is confirmed in a simulation study with nodal covariates and is not necessarily the case for edge-specific covariates, as we will see in the parliament data.

To make estimation feasible, even for large networks with nodal heterogeneity, we propose the use of variational inference (VI) as a scalable and stable alternative to existing estimation procedures for ERGMs. We propose a computationally efficient variational Bayes (VB) estimator (Jordan et al.; 1999; Ormerod and Wand; 2010) to compute approximate posterior inference quickly, even when the network and parameter dimension are large. VI is an optimization-based technique for approximate Bayesian inference that has gained in popularity over the last few years, as it provides a computationally efficient alternative to sampling methods that scales well to high-dimensional problems and highly parameterized models (Blei et al.; 2017). Variational methods typically seek to minimize the Kullback–Leibler (KL) divergence between the possibly complex true posterior and a more tractable so-called variational density, which can be shown to be equivalent to maximizing a lower bound $\mathcal{L}$ on the log-marginal likelihood. We consider stochastic VI (SVI;
Figure 2: Political collaboration network.

Illustration of the network. It represents the Italian Parliament using a binary network with an edge representing at least one co-sponsorship.

cf. e.g., Nott et al.; 2012; Paisley et al.; 2012; Salimans and Knowles; 2013), which does not require expectations to be evaluated analytically, but enables the use of an unbiased Monte Carlo estimate of the gradient of $\mathcal{L}$ to make inference tractable. The VB estimator is based on a Gaussian approximation with a sparse factor representation of its covariance matrix (Ong et al.; 2018) and applicable to ERGMs with node heterogeneity even for large networks. It has proven to be highly accurate in a number of simulations conducted. These simulations also allow us to define suitable default values for involved tuning and optimization options. To further facilitate the use of our approach, we also propose feasible options to answer model-fit and model-selection questions. Variational approximations in ERGMS have been used before in Mele and Zhu (2021), who propose a mean-field-type variational approximation, and Tan and Friel (2020), who develop a variety of variational methods for ERGMs, but their respective models do not account for heterogeneity. For other network models with block or mixture components, variational methods have been used in e.g., Latouche et al. (2012); McDaid et al. (2013), or more recently in Babkin et al. (2020) and Yin et al. (2022).

Overall, we view the contributions of this paper as follows. First, our VI approach scales up to high dimensions and highly-parameterized models, in which available estimation techniques for network data analysis meet their limits. We are thus able to estimate networks with thousands of nodes and accordingly thousands of nodal random heterogeneity effects. Secondly, if node-specific covariates are available, we liaise posteriors of nodal random effects for model validation and model selection, which indeed allows us to quantify the amount of (posterior) explained uncertainty, similar to classical linear regression models. Finally, we also propose heuristic amendments for inference based on standard error corrections of our variational approximation, leading to more reliable quantification.
Figure 3: International arms trading.

Illustration of the network. Each node represents a country, with all country abbreviations explained in Table E.1 in the supplement. The size of the nodes relates to the outdegree of each node (the more outgoing edges, the larger the node). The arrows indicate the export directions.
of uncertainty.

We begin with a review on directed and undirected Bayesian ERGMs with nodal random effects and make our choices for prior distributions in Section 2. Section 3 details our estimation approach in these models through VB, while Section 4 discusses practical options for model selection. Three up-to-date illustrations on network data from the Italian Parliament, international arms trading, and Facebook egos in Section 5 underpin the benefits of VB for ERGMs including heterogeneity. Section 6 concludes. A detailed supplement contains the employed network statistics (A), further derivations and calculations relevant to our VI approach (B–D), additional material on the real-data examples (E), and extensive simulations (F). To explore the performance of our VI approach, we specifically investigate its accuracy and robustness, validity of (corrected) uncertainty estimates, model selection through approximate Bayes factors and posterior explained variance, as well as benchmarking with exact Bayesian inference in small networks. Overall, the simulation results are satisfying.

2 Bayesian ERGMs with Nodal Random Effects

This section describes our Bayesian ERGM with nodal random effects. We review ERGMs with latent nodal heterogeneity in Section 2.1 for undirected and directed graphs. Our prior choices used for Bayesian inference are discussed in Section 2.2. For notational simplicity we omit possible covariates $x$ in the notation and write the statistics as $s(y)$ even though all results directly apply to statistics of the form $s(y, x)$ as in (2).

2.1 Mixed ERGMs

To compensate for heterogeneity in the nodes of a network in ERGMs of the form (1), Thiemichen et al. (2016a) consider combining the $p_2$ model of Duijn et al. (2004) with (1) to a so-called mixed ERGM of the form

$$p(y \mid \beta, \gamma) : = \mathbb{P}(Y = y \mid \beta, \gamma) = \frac{\exp(s(y)^\top \beta + t(y)^\top \gamma)}{\kappa(\beta, \gamma)},$$

(3)

where $t(y)$ contains the degree statistics of the $N$ vertices. For an undirected graph, $t(y) = (t_1(y), \ldots, t_N(y))^\top$ counts the ties for each node $i = 1, \ldots, n$, i.e. $t_i(y) = \sum_{j=1}^N Y_{ij}$. The associated coefficient vector $\gamma = (\gamma_1, \ldots, \gamma_N)^\top$ is assumed to be normally distributed, $\gamma_i \overset{i.i.d.}{\sim} N(\mu_\gamma, \sigma_\gamma^2)$, where $N(\mu, \sigma^2)$ denotes a Gaussian distribution with mean $\mu$ and variance $\sigma^2$. The parameter $\mu_\gamma$ thereby captures the average propensity in the network to form a tie. Therefore, $\beta_0$, which is usually the parameter associated with the edge statistic $\beta_{\text{edge}} \equiv \beta_0$, is excluded from $\beta$, i.e. $\beta = (\beta_1, \ldots, \beta_p)^\top$. Alternatively, one can set $\mu_\gamma = 0$. Indeed, there is the relation $\beta_{\text{edge}} = 2\mu_\gamma$ (Thiemichen et al.; 2016a). In the undirected case, the likelihood in (3) arises from the conditional formulation

$$\logit \left[ \mathbb{P}(Y_{ij} = 1 \mid Y_{kl}, (k, l) \neq (i, j); \beta, \gamma_i, \gamma_j) \right] = s_{ij}(y)^\top \beta + \gamma_i + \gamma_j,$$  

(4)
for $1 \leq i \neq j \leq N$ and where $s_{ij}(y)$ denotes the vector of so-called change statistics

$$s_{ij}(y) = s(y_{ij} = 1 \mid Y_{-ij}) - s(Y_{ij} = 0 \mid Y_{-ij}),$$

with $Y_{-ij}$ being the status of the remaining network except for the edge between node $i$ and $j$. When the network is directed, the statistics in model (3) extend to

$$t(y) = (t_{11}(y), \ldots, t_{1N}(y), t_{21}(y), \ldots, t_{2N}(y))^\top,$$

$$\gamma = (\delta_1, \ldots, \delta_N, \phi_1, \ldots, \phi_N)^\top,$$

where $t_{1i}(y) = \sum_{j=1}^N Y_{ij}$, $t_{2i} = \sum_{j=1}^N Y_{ji}$ count the incoming and outgoing edges connected to node $i$, while $\delta_i$ and $\phi_i$ are the corresponding sender and receiver effects, respectively. Similarly to the undirected case, $(\delta_i, \phi_i)^\top$ are random and (4) takes the form

$$\logit [P(Y_{ij} = 1 \mid Y_{kl}, (k, l) \neq (i, j); \beta, \delta_i, \delta_j, \phi_i, \phi_j)] = s_{ij}(y)^\top \beta + \delta_i + \phi_j$$

where additional constraints on the mean values of $\delta_i$ and $\phi_j$ are required, as detailed below.

### 2.2 Prior distributions

We extend the above models now towards a Bayesian treatment by formulating appropriate prior distributions. For the coefficient vector $\beta$ of network statistics and the vector of nodal random effects $\gamma$, we employ Gaussian priors with appropriate covariance structures, depending on whether the network is directed or undirected. We then make further prior assumptions on the covariances.

**Undirected Bayesian mixed ERGM** In the undirected case, we have $\beta = (\beta_1, \ldots, \beta_p)^\top$ and $\gamma = (\gamma_1, \ldots, \gamma_N)^\top$. As mentioned before, it is commonly assumed that $\beta_0 \equiv 0$, such that the intercept (edge statistic) is implicitly modelled through the mean $\mu$ of the Gaussian prior for $\gamma$. Overall, we make the following prior assumptions:

$$\beta \sim N(0, \sigma_\beta^2 I_{p \times p}), \quad \sigma_\beta^2 \sim SD(1/2, b_\beta)$$

$$\gamma \sim N(\mu, \sigma_\gamma^2 I_{N \times N}), \quad \mu \sim N(0, b_\mu), \quad \sigma_\gamma^2 \sim SD(1/2, b_\gamma),$$

where $SD(1/2, b)$ denotes the scale-dependent prior of Klein and Kneib (2016) (which corresponds to a Weibull prior with shape parameter 1/2 and scale parameter $b$), respectively. This prior relies on the principles of penalized complexity priors (Simpson et al.; 2017) and has the appealing property of penalizing from a flexible alternative to a properly defined base model. For our case, this corresponds to the situation in which evidence in the data should decide between a nested model without nodal random effects (base model) and a more flexible alternative containing nodal random effects, a topic we further investigate in the presence of nodal covariates in Section 5.2. Empirically, our simulations are rather robust against the specific choices of hyperparameters $b_\mu$, $b_\beta$, and $b_\gamma$, such that we set $b_\mu = 100$, $b_\beta = 100$, and $b_\gamma = 100$, see also Supplement F.1 for empirical evidence on robustness against these choices. We denote the vector of all model parameters in the undirected Bayesian mixed ERGM with dimension $\dim(\vartheta) = p_\vartheta = p + N + 3$ as

$$\vartheta = (\beta^\top, \gamma^\top, \sigma_\beta^2, \mu, \sigma_\gamma^2)^\top.$$  

Figure 4 presents a graphical illustration of the undirected Bayesian mixed ERGM.
Undirected Bayesian ERGM with Nodal Random Effects

Undirected Bayesian ERGM

\[ p(\beta, \gamma, \sigma_\beta^2, \mu, \sigma_\gamma^2 | y) \propto p(y | \beta, \gamma) p(\beta | \sigma_\beta^2) p(\gamma | \mu, \sigma_\gamma^2) p(\sigma_\beta^2 | b_\beta) p(\mu) p(\sigma_\gamma^2) \]

\[ \beta | \sigma_\beta^2 \sim N(0, \sigma_\beta^2) \]

\[ \gamma | \sigma_\gamma^2 \sim N(\mu, \sigma_\gamma^2) \]

\[ \sigma_\beta^2 | b_\beta \sim SD(\frac{1}{b_\beta}) \]

\[ \sigma_\gamma^2 | b_\gamma \sim SD(\frac{1}{b_\gamma}) \]

\[ s(y) \]

\[ \exp[s(y)^T \beta + t(y)^T \gamma] \]

\[ \kappa(\beta, \gamma) \]

\[ \text{if } \beta_{\text{edge}} = 0: m_\gamma = \mu_{\gamma} \sim N(0, b_\mu) \]

\[ \text{else: } m_\gamma = 0 \]

\[ b_\mu \]

Figure 4: Graphical representation of the undirected Bayesian ERGM with nodal effects. Ellipses are stochastic nodes and rectangles are deterministic/logical nodes. Single arrows are stochastic edges and double arrows are logical/deterministic edges. In simulations in Section F, the cases \( \beta_{\text{edge}} = 0 \) and \( \mu_{\gamma} = 0 \) are compared and denoted with the suffix “-het(\( \beta_{\text{edge}} = 0 \))” and “-het(\( \mu_{\gamma} = 0 \))”, respectively.

**Directed Bayesian mixed ERGM**

In the directed case, we have \( \beta = (\beta_0, \beta_1, \ldots, \beta_p)^T \) and \( \gamma = (\delta_1, \ldots, \delta_N, \phi_1, \ldots, \phi_N)^T \). In this setting, it is notationally more convenient to include \( \beta_0 \) as edge effect. While the priors for \( \beta \) and \( \sigma_\beta^2 \) are the same as in the undirected case, the hierarchical prior for \( \gamma \) is

\[ \gamma \sim N(0, \Sigma), \]

\[ \Sigma = \begin{bmatrix} \sigma_\delta^2 & \sigma_\phi^2 \\ \sigma_\delta^2 & \sigma_\phi^2 \end{bmatrix} \otimes I_N = \begin{bmatrix} \sigma_\delta^2 & \sigma_\delta \sigma_\phi \rho \\ \sigma_\delta \sigma_\phi \rho & \sigma_\phi^2 \end{bmatrix} \otimes I_N, \]

\[ \sigma_\delta^2 \sim SD(1/2, b_\delta), \sigma_\phi^2 \sim SD(1/2, b_\phi), \rho \sim Beta(a_\rho, b_\rho), \]

where Beta(\( a, b \)) denotes a beta distribution with parameters \( a, b \). In all our simulations and applications, we set \( b_\delta = b_\phi = 100, a_\rho = b_\rho = 1 \), resulting in weakly informative priors for the marginal variances and uniform priors for \( \rho \). In similarity to the undirected case, posterior results are rather robust against exact choices for these hyperparameters (cf. Supplement F.1). Finally, the vector of all model parameters in the directed Bayesian mixed ERGM with dimension \( p_\theta = p + 2N + 5 \) is

\[ \theta = (\beta^T, \gamma^T, \sigma_\beta^2, \sigma_\delta^2, \sigma_\phi^2, \rho)^T. \]

For posterior estimation, some parameters are re-parameterized to the real line \( \mathbb{R} \). Specifically, \( \sigma_\beta^2 \) is log-transformed, similar to \( \sigma_\gamma^2 \) (undirected case) and \( \sigma_\delta^2, \sigma_\phi^2 \) (directed case). For the directed model, a Fisher-z transformation is used for \( \rho \), see Supplement B for resulting priors on the transformed parameters.
3 Variational Inference for Bayesian Mixed ERGMs

In this section, we review basic ideas of VI and introduce a scalable VI method for the Bayesian mixed ERGM.

3.1 Variational inference in a nutshell

VI methods are a promising approach to scaling approximate Bayesian inference to work in large datasets and highly parameterized models. The general idea of VI is to approximate a posterior density $p(\vartheta|y) \propto p(y|\vartheta)p(\vartheta)$ by a more tractable density $q_\lambda(\vartheta)$, the so-called variational density. Here, $p(y|\vartheta)$ is the conditional likelihood at (3), and $\lambda$ is a vector of variational parameters that are calibrated by minimizing some measure of closeness between $q_\lambda(\vartheta)$ and $p(\vartheta|y)$. Commonly, the measure of closeness adopted is the Kullback-Leibler divergence (KL) from $q_\lambda(\vartheta)$ to $p(\vartheta|y)$ given by

$$
\text{KL}(q_\lambda(\vartheta)||p(\vartheta|y)) = \int \log\left(\frac{q_\lambda(\vartheta)}{p(\vartheta|y)}\right) q_\lambda(\vartheta) d\vartheta.
$$

(7)

Since the KL is non-negative,

$$
\mathcal{L}(\lambda) = \int q_\lambda(\vartheta) \log \left\{ \frac{p(y, \vartheta)}{q_\lambda(\vartheta)} \right\} d\vartheta
= \int q_\lambda(\vartheta) \log \left\{ \frac{p(y|\vartheta)p(\vartheta)}{q_\lambda(\vartheta)} \right\} d\vartheta,
$$

(8)

is a lower bound on $\log(p(y))$ known as the variational lower bound or evidence lower bound (ELBO). Because the left-hand side of (7) does not depend on $\lambda$, minimizing the KL with respect to $\lambda$ is equivalent to maximizing $\mathcal{L}$ with respect to $\lambda$, which is a more convenient objective not involving the intractable marginal likelihood. Introductory overviews on variational inference can be found in Ormerod and Wand (2010); Blei et al. (2017).

3.2 Stochastic variational inference

Maximizing $\mathcal{L}(\lambda)$ directly to obtain an optimal variational approximation (VA) is often difficult, since $\mathcal{L}(\lambda)$ is defined as an integral that is generally intractable, as it is in our case. However, (8) is an expectation with respect to $q_\lambda(\vartheta)$

$$
\mathcal{L}(\lambda) = E_{q_\lambda} \{ \log(h(\vartheta)) - \log(q_\lambda(\vartheta)) \}.
$$

(9)

The expectation (9) enables unbiased Monte Carlo (MC) estimation, which extends to the estimation of the gradient of $\mathcal{L}(\lambda)$ after differentiating under the integral sign. Doing so, the gradient $\nabla_\lambda \mathcal{L}(\lambda)$ results in an expectation with respect to $q_\lambda$,

$$
\nabla_\lambda \mathcal{L}(\lambda) = E_{q_\lambda} \{ \nabla_\lambda \log(q_\lambda(\vartheta))[\log(h(\vartheta)) - \log(q_\lambda(\vartheta))] \},
$$

(10)
where the so-called log-derivative trick $E_{q_\lambda}(\nabla_\lambda \log(q_\lambda(\vartheta))) = 0$ was employed. This is often used with stochastic gradient ascent (SGA) methods and there is now a large literature surrounding the application of this idea, also called stochastic variational inference (SVI; see Nott et al.; 2012; Paisley et al.; 2012; Hoffman et al.; 2013; Salimans and Knowles; 2013; Kingma and Welling; 2014; Rezende et al.; 2014; Ranganath et al.; 2014; Titsias and Lázaro-Gredilla; 2015; Kucukelbir et al.; 2017, among others). Denoting with $\nabla_\lambda L(\lambda)$ an unbiased MC estimate of the gradient $\nabla_\lambda L(\lambda)$, SGA methods proceed as follows. Choose an initial value $\lambda^{(0)}$ and for $t = 0, 1, \ldots$ perform the update

$$\lambda^{(t+1)} = \lambda^{(t)} + \nu^{(t)} \circ \overline{\nabla_\lambda L(\lambda^{(t)})}$$

recursively, where $\circ$ denotes the Hadamard (element-by-element) product of two random vectors and $\{\nu^{(t)}\}_{t \geq 0}$ is a sequence of vector-valued learning rates with dimension $\dim(\lambda)$. The update is continued until a stopping condition is satisfied. The learning rate sequence is chosen to satisfy the Robbins–Monro conditions $\sum_t \nu_j^{(t)} = \infty$ and $\sum_t (\nu_j^{(t)})^2 < \infty$ (Robbins and Monro; 1951), $j = 1, \ldots, \dim(\lambda)$, which ensures that the iterates $\lambda^{(t)}$ converge to a (possibly local) optimum as $t \to \infty$ under suitable regularity conditions (Bottou; 2010). In practice, it is important to consider adaptive learning rates, and these are set here using the ADADELTA method of Zeiler (2012), as in Ong et al. (2018).

For the SGA algorithm to be efficient, the estimate $\overline{\nabla_\lambda L(\lambda)}$ should exhibit low variance, and the references above on SVI differ in the way an unbiased estimate $\overline{\nabla_\lambda L(\lambda)}$ is constructed and how its variance is reduced. Here we consider the so-called re-parameterization trick (Kingma and Welling; 2014; Rezende et al.; 2014). Xu et al. (2019) recently provided evidence that employing this method is often much more efficient than existing alternatives. We give details on how to employ the re-parameterization trick in our case in Supplement C.2.

### 3.3 Choice of the variational approximation

Successful application of the variational methods described above requires a suitable and numerically tractable approximation density $q_\lambda(\vartheta)$. We follow Ong et al. (2018) and employ a Gaussian variational approximation $q_\lambda(\vartheta) = \phi(\vartheta; \mu, \Upsilon)$, where the covariance matrix is a parsimoniously structured factor covariance matrix with $K$ factors. This choice allows for a flexible full covariance structure, while keeping the number of unknowns feasible. Furthermore, the Gaussian approximation enables the use of the aforementioned re-parameterization trick. We refer to Supplement C.1–C.3 for details on the variational density, variance reduction through the re-parameterization trick, as well as implementation of the SGA and involved gradients. From Supplement F.1, we choose $K = 20$ as our default, Yielding a good balance between accuracy and computational efficiency.
3.4 Estimation of $E_{\beta,\gamma}(s(y))$ and $E_{\beta,\gamma}(t(y))$

Computation of the gradients with respect to $\beta$ and $\gamma$ involves the derivatives $\frac{\partial \log(\kappa(\beta,\gamma))}{\partial \beta}$ and $\frac{\partial \log(\kappa(\beta,\gamma))}{\partial \gamma}$, which are — similar to $\kappa(\beta,\gamma)$ — themselves analytically intractable, since

$$\frac{\partial \log(\kappa(\beta,\gamma))}{\partial \beta} = \sum_{y \in Y} \exp(\beta^\top s(y) + \gamma^\top t(y)) \frac{s(y)}{p(y|\beta,\gamma)} = \sum_{y \in Y} p(y|\beta,\gamma)s(y) = \mathbb{E}_{y|\beta,\gamma}[s(y)]$$

$$\frac{\partial \log(\kappa(\beta,\gamma))}{\partial \gamma} = \sum_{y \in Y} \exp(\beta^\top s(y) + \gamma^\top t(y)) \frac{t(y)}{p(y|\beta,\gamma)} = \sum_{y \in Y} p(y|\beta,\gamma)t(y) = \mathbb{E}_{y|\beta,\gamma}[t(y)].$$

Tan and Friel (2020) consider three options for approximating $\mathbb{E}_{y|\beta,\gamma}[s(y)]$ and $\mathbb{E}_{y|\beta,\gamma}[t(y)]$ numerically, namely MC sampling and (adaptive) importance sampling ((A)IS). In our simulations (F.1), we find that (A)IS is the slightly faster method for very small parameter spaces. However, the larger the parameter space, the worse the approximation quality of (A)IS becomes. Even for a network of only 40 nodes with random effects, MC sampling is more efficient. These findings are in line with the statements made in Tan and Friel (2020); we therefore employ MC sampling as default. At each iteration, $L$ networks are simulated using the “tie-no-tie” sampler in the `ergm` package (Hunter et al.; 2008), which is a Metropolis-Hastings sampler. As the estimation only needs to be unbiased, it is sufficient to sample $L = 5$ networks (with burn-in phase of 5000), as demonstrated empirically in Supplement F.1.

3.5 Uncertainty quantification

In principle, standard errors for $\hat{\vartheta}$ can be directly computed using the VA $q_{\hat{\lambda}} = N(\hat{\mu}, \hat{\Sigma})$. Even though it has been demonstrated in some situations that VI does not suffer from accuracy in terms of posterior predictive densities (e.g., Braun and McAuliffe; 2010; Kucukelbir et al.; 2017), it is known that VI generally underestimates the variance of the posterior density (Blei et al.; 2017), which is a consequence of its objective function. A few papers try to match more closely the inferences made by MCMC (e.g., Giordano et al.; 2018). However, these are often computationally expensive or preliminary designed for mean field VB, which is different from our stochastic fixed-form VI (compare Miller; 2021, for a general discussion).

To improve the coverage of credible intervals of $\theta = (\beta^\top, \gamma^\top)^\top \in \mathbb{R}^{p_\theta}$ derived from our $q_{\hat{\lambda}}$, we employ the following simple covariance correction for $\hat{\Sigma}$. We define with $V := F_\theta^{-1} = \left[\text{Var}(s(y), t(y))^\top\right]^{-1}$ the inverse Fisher information, which is estimated through

$$\hat{\Sigma} = \left(\frac{1}{B} \sum_{b=1}^{B} (s(y^b), t(y^b))^\top(s(y^b), t(y^b))\right)^{-1}$$

Tan and Friel (2020) consider three options for approximating $\mathbb{E}_{y|\beta,\gamma}[s(y)]$ and $\mathbb{E}_{y|\beta,\gamma}[t(y)]$ numerically, namely MC sampling and (adaptive) importance sampling ((A)IS). In our simulations (F.1), we find that (A)IS is the slightly faster method for very small parameter spaces. However, the larger the parameter space, the worse the approximation quality of (A)IS becomes. Even for a network of only 40 nodes with random effects, MC sampling is more efficient. These findings are in line with the statements made in Tan and Friel (2020); we therefore employ MC sampling as default. At each iteration, $L$ networks are simulated using the “tie-no-tie” sampler in the `ergm` package (Hunter et al.; 2008), which is a Metropolis-Hastings sampler. As the estimation only needs to be unbiased, it is sufficient to sample $L = 5$ networks (with burn-in phase of 5000), as demonstrated empirically in Supplement F.1.

3.5 Uncertainty quantification

In principle, standard errors for $\hat{\vartheta}$ can be directly computed using the VA $q_{\hat{\lambda}} = N(\hat{\mu}, \hat{\Sigma})$. Even though it has been demonstrated in some situations that VI does not suffer from accuracy in terms of posterior predictive densities (e.g., Braun and McAuliffe; 2010; Kucukelbir et al.; 2017), it is known that VI generally underestimates the variance of the posterior density (Blei et al.; 2017), which is a consequence of its objective function. A few papers try to match more closely the inferences made by MCMC (e.g., Giordano et al.; 2018). However, these are often computationally expensive or preliminary designed for mean field VB, which is different from our stochastic fixed-form VI (compare Miller; 2021, for a general discussion).

To improve the coverage of credible intervals of $\theta = (\beta^\top, \gamma^\top)^\top \in \mathbb{R}^{p_\theta}$ derived from our $q_{\hat{\lambda}}$, we employ the following simple covariance correction for $\hat{\Sigma}$. We define with $V := F_\theta^{-1} = \left[\text{Var}(s(y), t(y))^\top\right]^{-1}$ the inverse Fisher information, which is estimated through

$$\hat{\Sigma} = \left(\frac{1}{B} \sum_{b=1}^{B} (s(y^b), t(y^b))^\top(s(y^b), t(y^b))\right)^{-1}$$

Tan and Friel (2020) consider three options for approximating $\mathbb{E}_{y|\beta,\gamma}[s(y)]$ and $\mathbb{E}_{y|\beta,\gamma}[t(y)]$ numerically, namely MC sampling and (adaptive) importance sampling ((A)IS). In our simulations (F.1), we find that (A)IS is the slightly faster method for very small parameter spaces. However, the larger the parameter space, the worse the approximation quality of (A)IS becomes. Even for a network of only 40 nodes with random effects, MC sampling is more efficient. These findings are in line with the statements made in Tan and Friel (2020); we therefore employ MC sampling as default. At each iteration, $L$ networks are simulated using the “tie-no-tie” sampler in the `ergm` package (Hunter et al.; 2008), which is a Metropolis-Hastings sampler. As the estimation only needs to be unbiased, it is sufficient to sample $L = 5$ networks (with burn-in phase of 5000), as demonstrated empirically in Supplement F.1.

3.5 Uncertainty quantification

In principle, standard errors for $\hat{\vartheta}$ can be directly computed using the VA $q_{\hat{\lambda}} = N(\hat{\mu}, \hat{\Sigma})$. Even though it has been demonstrated in some situations that VI does not suffer from accuracy in terms of posterior predictive densities (e.g., Braun and McAuliffe; 2010; Kucukelbir et al.; 2017), it is known that VI generally underestimates the variance of the posterior density (Blei et al.; 2017), which is a consequence of its objective function. A few papers try to match more closely the inferences made by MCMC (e.g., Giordano et al.; 2018). However, these are often computationally expensive or preliminary designed for mean field VB, which is different from our stochastic fixed-form VI (compare Miller; 2021, for a general discussion).

To improve the coverage of credible intervals of $\theta = (\beta^\top, \gamma^\top)^\top \in \mathbb{R}^{p_\theta}$ derived from our $q_{\hat{\lambda}}$, we employ the following simple covariance correction for $\hat{\Sigma}$. We define with $V := F_\theta^{-1} = \left[\text{Var}(s(y), t(y))^\top\right]^{-1}$ the inverse Fisher information, which is estimated through

$$\hat{\Sigma} = \left(\frac{1}{B} \sum_{b=1}^{B} (s(y^b), t(y^b))^\top(s(y^b), t(y^b))\right)^{-1}$$

Tan and Friel (2020) consider three options for approximating $\mathbb{E}_{y|\beta,\gamma}[s(y)]$ and $\mathbb{E}_{y|\beta,\gamma}[t(y)]$ numerically, namely MC sampling and (adaptive) importance sampling ((A)IS). In our simulations (F.1), we find that (A)IS is the slightly faster method for very small parameter spaces. However, the larger the parameter space, the worse the approximation quality of (A)IS becomes. Even for a network of only 40 nodes with random effects, MC sampling is more efficient. These findings are in line with the statements made in Tan and Friel (2020); we therefore employ MC sampling as default. At each iteration, $L$ networks are simulated using the “tie-no-tie” sampler in the `ergm` package (Hunter et al.; 2008), which is a Metropolis-Hastings sampler. As the estimation only needs to be unbiased, it is sufficient to sample $L = 5$ networks (with burn-in phase of 5000), as demonstrated empirically in Supplement F.1.
based on $B$ simulated networks $y^1, \ldots, y^B$ from $p(y|\hat{\beta}, \hat{\gamma})$. We further define $S = \text{diag}(s_1, \ldots, s_p)$ as the diagonal matrix, such that $s_i = \hat{V}_{ii} / \hat{\Upsilon}_{ii}$ holds for $i = 1, \ldots, p$. We now construct a corrected version of the full covariance matrix $\hat{\Upsilon}$ as $\hat{\Upsilon}_{\text{corrected}} = S^{1/2} \hat{\Upsilon} S^{1/2}$. We investigate the coverage derived from $\hat{\Upsilon}$ and $\hat{\Upsilon}_{\text{corrected}}$ in Supplement F.3. The main conclusion is that applying the suggested correction generally leads to coverages closer to the nominal levels, with the tendency that $\hat{\Upsilon}$ underestimates the standard errors, while $\hat{\Upsilon}_{\text{corrected}}$ yields slightly too conservative credible intervals.

An alternative way to construct credible intervals for $\theta$ would be to re-estimate the networks $y^1, \ldots, y^B$ to obtain a sample $\{\hat{\theta}^1, \ldots, \hat{\theta}^B\}$ from which credible intervals could be constructed. However, if the networks are large, this can also be computationally demanding, since it requires the training of $B$ additional networks.

### 3.6 VI algorithm for Bayesian mixed ERGMs

Algorithm C.2 in Supplement C.6 calibrates our proposed VA to the augmented posterior using SGA with the re-parameterization trick and the ADADELTA learning rate. The choice of starting values for $\vartheta$, stopping criterion, and computation of point estimates is detailed in Supplement C.4 and C.5. In Supplement F.2, we evaluate our VI approach to mixed ERGMs and compare it to exact inference via MCMC as proposed in (Thiemichen et al.; 2016b) using mixbergm (Thiemichen and Caimo; 2018) and which is computationally feasible for small networks only. We find that here VI performs en par with MCMC, while being considerably faster and feasible when MCMC is not.

### 4 Bayesian Inference, Model Selection & Goodness-of-Fit

Important yet challenging aspects in network analyses are to find the best specification of the model and to evaluate the overall model fit. For mixed ERGMs, it is not only of interest to decide which network statistics to include but also to decide whether nodal random effects should be present in the model or not. In other words, we question whether the statistics included fully describe the network structure or whether unobserved nodal heterogeneity remains. To tackle these questions, we propose three approaches. Firstly, we use the marginal posteriors of variances of the random nodal effects as a graphical device to measure the node heterogeneity across competing models. Secondly, we rely on (approximate) Bayes factors (BFs; Kass and Wasserman; 1995). Thirdly, we propose Bayesian goodness-of-fit (BGOF; Hunter et al.; 2008) measures.

#### 4.1 Explained variance through exogenous covariates

The marginal posteriors of variances associated with the nodal random effects (i.e. $\sigma_\gamma^2$ in the undirected cases and $\sigma_\delta^2, \sigma_\phi^2$ in the directed cases, respectively) allow us to quantify the unexplained variability, i.e., the heterogeneity that cannot be explained by the network statistics $s(y)$. This becomes particularly interesting in the presence of node and/or edge-specific covariates $x$, as in model (2). We may then investigate the influence of including the covariates on the heterogeneity of the nodes. We propose to do this by regarding
the differences in the respective posteriors in models fitted with and without covariates (i.e., \( s(y, x) \) vs \( s(y) \)). This exhibits how much variability can be explained (or vice versa is induced) by including \( x \) and defines a novel (graphical) measure to quantify the extent of nodal heterogeneity in competing network models in the presence of covariates that has not been used before. To be specific, we define the posterior explained variance as follows. 

**Definition 4.1** (Posterior explained variance). Let \( \bullet \in \{ \gamma, \delta, \phi \} \) and \( \mathcal{M}_1^*, \mathcal{M}_2^* \) be two models with nodal random effects and the same network statistics but without and with exogenous covariates \( x \), respectively. Let \( p_{\bullet^*, \mathcal{M}_1^*} \| y, p_{\bullet^*, \mathcal{M}_2^*} \| y \) be the respective marginal posteriors. Then, we define the posterior explained variance as

\[
R_\bullet = \mathbb{P}(\sigma_{\bullet^*, \mathcal{M}_2^*}^2 < \sigma_{\bullet^*, \mathcal{M}_1^*}^2 \mid y) \\
= \int_0^\infty \left\{ \int_0^s p_{\sigma_{\bullet^*, \mathcal{M}_2^*}^2 \mid y}(t) dt \right\} p_{\sigma_{\bullet^*, \mathcal{M}_1^*}^2 \mid y}(s) ds \\
\approx \int_0^\infty \left\{ \int_0^s q_{\sigma_{\bullet^*, \mathcal{M}_2^*}^2}(t) dt \right\} q_{\sigma_{\bullet^*, \mathcal{M}_1^*}^2}(s) ds,
\]

where \( q_{\sigma_{\bullet^*, \mathcal{M}_1^*}^2} \), \( q_{\sigma_{\bullet^*, \mathcal{M}_2^*}^2} \) are the respective marginal variational densities.

The applicability of the posterior explained variance is investigated empirically in Supplement F.4, where we demonstrate the ability to reduce heterogeneity when the model contains nodal covariates. We also exemplify this in Section 5.2. However, when covariates are edge-specific, a reduction of the heterogeneity is not guaranteed, as we will see in Section 5.1.

### 4.2 Approximate Bayes factors

The BF for comparing any two models \( \mathcal{M}_1 \) and \( \mathcal{M}_2 \), is defined as

\[
\text{BF}_{12} = \frac{p(y \mid \mathcal{M}_1)}{p(y \mid \mathcal{M}_2)},
\]

where \( p(y \mid \mathcal{M}_j) = \int p(y \mid \vartheta, \mathcal{M}_j)p(\vartheta \mid \mathcal{M}_j) d\vartheta, \ j = 1, 2 \) is the marginal likelihood under \( \mathcal{M}_j \) and \( p(\vartheta \mid \mathcal{M}_j), p(\vartheta \mid \mathcal{M}_j) \) are the respective likelihood and prior distributions. Generally, when \( \text{BF}_{12} > 1 \), the data favours \( \mathcal{M}_1 \) over \( \mathcal{M}_2 \). If \( 0 < \text{BF}_{12} < 1 \), \( \mathcal{M}_2 \) is favoured instead.

According to Bayes’ theorem, the integration can be avoided and the marginal likelihood \( p(y) \) (suppressing the dependence on the model \( \mathcal{M} \)) can be obtained via

\[
p(y) = \frac{p(y, \vartheta)}{p(\vartheta \mid y)} = \frac{p(y \mid \vartheta)p(\vartheta)}{p(\vartheta \mid y)}
\]

which involves the posterior \( p(\vartheta \mid y) \) in the denominator. Let now \( \vartheta_1, \vartheta_2 \) be the set of all model parameters under \( \mathcal{M}_1 \) and \( \mathcal{M}_2 \) with corresponding network statistics \( s_1(\cdot) \) and \( s_2(\cdot) \), respectively. Then, the BF can also be written as

\[
\text{BF}_{12} = \frac{\kappa(\beta_2, \gamma_2) \exp(\beta_1^T s_1(y) + \gamma_1^T t(y)) p(\vartheta_1) p(\vartheta_2 \mid y)}{\kappa(\beta_1, \gamma_1) \exp(\beta_2^T s_2(y) + \gamma_2^T t(y)) p(\vartheta_2) p(\vartheta_1 \mid y)}
\]

The posteriors \( p(\vartheta_1 \mid y), p(\vartheta_2 \mid y) \) under \( \mathcal{M}_1, \mathcal{M}_2 \) are approximated by \( q_{\lambda_1} \) and \( q_{\lambda_2} \) evaluated at their point estimates \( \hat{\vartheta}_1 \) and \( \hat{\vartheta}_2 \), respectively, which we obtain from the variational
approximations \( q_{\lambda_j} \) (see Supplement C.5 for details). Plugging these also into the remaining terms, we obtain our approximate BF denoted by \( \hat{BF}_{12} \) as

\[
\hat{BF}_{12} = \frac{\kappa(\hat{\beta}_2, \hat{\gamma}_2) \exp(\hat{\beta}_1^T s_1(y) + \hat{\gamma}_1^T t(y)) p(\hat{\theta}_1) q_{\lambda_2}(\hat{\theta}_2)}{\kappa(\hat{\beta}_1, \hat{\gamma}_1) \exp(\hat{\beta}_2^T s_2(y) + \hat{\gamma}_2^T t(y)) p(\hat{\theta}_2) q_{\lambda_1}(\hat{\theta}_1)}.
\]

(14)

In (14), all but the first factor \( \kappa(\hat{\beta}_2, \hat{\gamma}_2)/\kappa(\hat{\beta}_1, \hat{\gamma}_1) \) can be directly evaluated analytically. However, as the ratio of the normalizing constants is intractable, it needs to be approximated. To do so, we use thermodynamic integration (path sampling ; Caimo and Friel; 2013; Thiemichen et al.; 2016b), and distinguish two situations:

(I) Nested models  If the models \( \mathcal{M}_1 \) and \( \mathcal{M}_2 \) are nested, two situations are possible, where w.l.o.g. we assume that \( \mathcal{M}_1 \) is nested in \( \mathcal{M}_2 \).

(I).1 \( \mathcal{M}_1 \) and \( \mathcal{M}_2 \) contain the same network statistics but \( \mathcal{M}_2 \) also accounts for nodal heterogeneity. Assuming \( s_1(\cdot) \) and \( s_2(\cdot) \) contain an intercept, we have \( \gamma_1 \equiv 0 \).

(I).2 Both models \( \mathcal{M}_1 \) and \( \mathcal{M}_2 \) contain the sociality effects, but \( \mathcal{M}_2 \) includes not only the network statistics of \( \mathcal{M}_1 \) but also further ones, i.e. \( s_1(\cdot) \subset s_2(\cdot) \) and \( \dim(\beta_1) < \dim(\beta_2) \).

The path sampling approach of Gelman and Meng (1998) can be applied to approximate numerically the expectation involved in computing \( \log \left\{ \kappa(\hat{\beta}_2, \hat{\gamma}_2)/\kappa(\hat{\beta}_1, \hat{\gamma}_1) \right\} \) using the trapezoid rule and repeated sampling from model (1) on a grid in (0,1) (see Section 3.2 of Thiemichen et al.; 2016b, for details).

(II) Non-nested models  If models \( \mathcal{M}_1 \) and \( \mathcal{M}_2 \) are non-nested, augmenting \( \beta_1, \gamma_1 \) into \( \beta_2, \gamma_2 \) is no longer possible, such that the usual path sampling approach cannot be applied. Instead, path sampling has to be performed twice, for \( \log \left\{ \kappa(\phi_2)/\kappa(0) \right\} \) and \( \log \left\{ \kappa(0)/\kappa(\phi_1) \right\} \) separately, with \( \kappa(0) \) being the normalizing constant of a null model, in which all parameters are set to 0 (see Section 3.3 of Thiemichen et al.; 2016b, for further details). As computing time is almost doubled, (I) should be used whenever two models are nested.

A generic representation of the computation of our BFs is provided in Algorithm D.1 in Supplement D, while Section F.5 in the Supplement demonstrates that, overall, the BFs are able to decide correctly whether or not node heterogeneity is present and which network statistics should be retained in a model.

4.3 Bayesian goodness-of-fit diagnostics

Hunter et al. (2008) consider the conditional distribution of “out-of-model” statistics at the MLE, and compare it to the observed graph. Subsequent Bayesian work has done the same with posterior predictive distributions as adequacy checking. The latter is also referred to as Bayesian goodness-of-fit diagnostics (BGOFs) for ERGMs by comparing high-level statistics of observed networks with those of corresponding networks simulated from the estimated network, in order to evaluate the model fit in terms of posterior predictive assessment. The estimated posterior distribution of the model parameters is approximated by \( q_{\lambda} \) in our VI approach. The set of statistics used for the comparison is the

- degree distribution, which counts the nodes with degree \( k \) (i.e. \( k \) connected nodes);
• geodesic distance distribution, which is defined as the shortest path length between two nodes (or infinity if there is no such path); and
• edge-wise shared partners distribution, which expresses the tendency for tied nodes to have multiple shared partners. Specifically, the edge-wise shared partner statistic counts all nodes $i$ and $j$ that are connected and also have an edge to a third node $k$.

The measures can be visualised via boxplots using the `bgof()` function in the `bergm` package (Caimo and Friel; 2014). The function requires a number of simulated networks; we set this equal to 100 later in Section 5. For formal definitions of the statistics, see Supplement A.

5 Empirical Analyses

We now consider three applications of our approach for networks requiring actor-specific information. In Section 5.1, we first consider an undirected political network with 663 nodes, 20,049 edges, and edge-specific covariates representing the Italian Parliament, in which one node represents a member of parliament. In Section 5.2, we consider a directed network of international arms trading in 2016 involving 163 countries, each represented by a node, and their export and import information. Previous methods typically cannot deal with all present challenges, i.e. the need of nodal effects, nodal covariates, and the fact that the network is directed. Finally, in Section 5.3, we illustrate the scalability of our VI method along a large undirected network with 4,039 nodes from Facebook. Owing to its size, previous work has mostly analysed subsets of this database. Further material can be found in Supplement E.

5.1 Political collaboration network

We consider data from 2008–2013, which determines the last legislative period with Silvio Berlusconi as Prime Minister, though he resigned in 2011 before the end of the election period. The 663 nodes in the network are the members of parliament during the time window and edges define the number of co-sponsorships of a law proposal.

Model specification  We look at the binary network with an edge representing at least one co-sponsorship. As network statistics we include the following:

• $s_{\text{edge}}(y)$, the number of edges in the network;
• $s_{2\text{-star}}(y)$, the number of 2-stars, which measures whether co-sponsorship is driven by the number of co-authorships one of the members of parliament has;
• $s_{\text{gwesp}}(y)$, the number of co-sponsorship-wise shared members of parliament in a geometrically weighted form. This statistic stabilizes the estimation.

Moreover, as exogenous quantities we include

• $s_{\text{male}}(y) = \sum_{i=1}^{N} \sum_{j>i} y_{ij} I\{\text{male}_i = \text{male}_j\}$, which questions whether males are more likely to co-sponsor a proposal, i.e. male homophily;
• $s_{\text{female}}(y)$ being the same for females
• $s_{\text{party}}(y) = \sum_{i=1}^{N} \sum_{j>i} y_{ij} I\{\text{party}_i = \text{party}_j\}$ as indicator whether co-sponsors belong to the same party, and finally
• $s_{\text{age}}(y) = \sum_{i=1}^{N} \sum_{j>i} y_{ij} |\text{age}_i - \text{age}_j|$, which quantifies age homophily.
We start with a model containing the network statistics only, denoted by $M_1$. Next, we augment this model by the respective edge-specific covariates, denoted by $M_2$. Finally, both models are further augmented by nodal random effects, which we label $M_1^*$ and $M_2^*$. Computing times for 1,000 VI iterations were 3.7, 5, 4, and 5.3 minutes for models $M_1$, $M_1^*$, $M_2$, and $M_2^*$, respectively.

**Results** As Table 1 depicts, models containing nodal effects outperform the respective models without. In addition, the model with covariates outperforms the one without covariates. BGOFs presented in the Supplement, Figure E.2 confirm this observation. However, looking at posterior explained variances comparing models $M_2^*$ and $M_1^*$, we obtain $R_\gamma = 2.6e^{-09}$. Hence, the covariates cannot explain heterogeneity as can be seen in Figure 5. Table 2 lists posterior mean estimates (together with 95% corrected credible intervals) of network statistics for all four models. We find strong homophily for the party, which indeed is not surprising. Additionally, we obtain a strong and significant gender homophily.

### 5.2 International arms trading

With our second example, we aim to understand why (and when) countries trade arms. We use ERGMs to shed light on this question by considering international arms trading in 2016 as a directed network consisting of 163 countries (nodes) and 407 edges, where a directed edge refers to recorded arms trading in that year. The data were taken from the Stockholm International Peace Research Institute (www.sipri.org). Economically as well as politically, it is of interest to understand the driving forces behind arms trading. Particular
Table 2: Political collaboration network.

| Statistics/covariate | $M_1$          | $M^*_1$       | $M_2$          | $M^*_2$        |
|----------------------|----------------|---------------|----------------|----------------|
| $s_{\text{edge}}(y)$ | -6.253         | -6.754        | -6.754         | 0.003          |
|                      | (-6.284, -6.221) | (-6.758, -6.750) |                |                |
| $s_{\text{2-star}}(y)$ | 1.3e-04        | 0.003         | 0.003          | 0.003          |
|                      | (7.2e-06, 2.6e-04) | (0.0027, 0.032) | (0.0025, 0.0033) |                |
| $s_{\text{gwesp}}(y)$ | 0.242          | 0.214         | 0.211          | 0.211          |
|                      | (0.239, 0.245) | (0.214, 0.215) | (0.211, 0.211) |                |
| $s_{\text{male}}(y)$ | 0.193          | 0.161         |                |                |
|                      | (0.184, 0.203) | (0.154, 0.168) |                |                |
| $s_{\text{female}}(y)$ | 0.277          | 0.223         |                |                |
|                      | (0.276, 0.277) | (0.219, 0.227) |                |                |
| $s_{\text{party}}(y)$ | 0.799          | 0.771         |                |                |
|                      | (0.798, 0.801) | (0.765, 0.778) |                |                |
| $s_{\text{age}}(y)$ | 0.001          | -0.001        |                |                |
|                      | (0.000, 0.002) | (-0.002, 0.001) |                |                |

Posterior mean estimates together with 95% corrected credible intervals of coefficients of network statistics and covariates for models $M_1$, $M^*_1$, $M_2$, $M^*_2$. Effects not containing the zero within the respective credible interval are highlighted in bold.

Interest lies in identifying which covariates have a direct influence on the probability that one country exports arms to another. Hence, in addition to network statistics, it is of interest to include nodal as well as bi-nodal information. Perkins and Neumayer (2010) argue that there is a time delay between the date arms are ordered and their delivery date. Therefore, all exogenous covariates are based on a two-year lag.

Model specification  With respect to including relevant covariates, we follow previous work (see e.g. Thurner et al.; 2019; Lebacher et al.; 2021a); using the (log) gross domestic product for the receiver as well as for the sender ($\text{lgdp}_{\text{in}}/\text{lgdp}_{\text{out}}$), and the logarithmic military expenditure ($\text{lmilex}$) for the receiving country. Furthermore, we account for information on alliances between countries (alliance) and the regime dissimilarity between two partners by measuring the absolute difference between the country’s so-called polity score ($\text{polity} \in (-10, 10)$). In addition to these exogenous quantities, we include, besides the number of edges, the following endogenous network statistics:

- $s_{\text{mutual}}(y)$, which counts how many reciprocal relations exist in a network, i.e. countries which mutually trade with each other.
- $s_{\text{2-star-out}}(y)$, which counts 2-star out constellations, i.e. one country exporting to two different countries;
- $s_{\text{2-star-in}}(y)$, which counts 2-star in constellations, i.e. one country importing from two different countries;
- $s_{\text{transitivity}}(y)$, which counts constellations according to “the trade partner of my trade partner is my trade partner”, i.e., triangles of the form that country $i$ sells weapons to countries $j$ and $k$ which themselves trade in that $j$ sells weapons to $k$. 
We start with a model containing the network statistics only, i.e.
\[ M_{1} : \exp \left( \beta_{\text{mutual}} \cdot s_{\text{mutual}}(y) + \beta_{\text{2-star-out}} \cdot s_{\text{2-star-out}}(y) + \beta_{\text{2-star-in}} \cdot s_{\text{2-star-in}}(y) + \beta_{\text{transitivity}} \cdot s_{\text{transitivity}}(y) \right) \]
and contrast it against a model with node-specific heterogeneity, i.e.
\[ M_{1}^{*} : \exp \left( \beta_{\text{mutual}} \cdot s_{\text{mutual}}(y) + \beta_{\text{2-star-out}} \cdot s_{\text{2-star-out}}(y) + \beta_{\text{2-star-in}} \cdot s_{\text{2-star-in}}(y) + \beta_{\text{transitivity}} \cdot s_{\text{transitivity}}(y) + t(y)^{\top} \gamma \right). \]
The models are identical, despite the \( 2N = 322 \) random effects for receiver and sender that are not included in \( M_{1} \). To demonstrate that exogenous variables can explain some of the unobserved heterogeneity, we contrast \( M_{1} \) and \( M_{1}^{*} \) to the corresponding models including covariates, i.e.
\[ M_{2} : \exp \left( \beta_{\text{lgdp out}} \cdot s_{\text{lgdp out}}(y) + \beta_{\text{gdp in}} \cdot s_{\text{gdp in}}(y) + \beta_{\text{lmilex in}} \cdot s_{\text{lmilex in}}(y) + \beta_{\text{alliance}} \cdot s_{\text{alliance}}(y) + \beta_{\text{mutual}} \cdot s_{\text{mutual}}(y) + \beta_{\text{2-star-out}} \cdot s_{\text{2-star-out}}(y) + \beta_{\text{2-star-in}} \cdot s_{\text{2-star-in}}(y) + \beta_{\text{transitivity}} \cdot s_{\text{transitivity}}(y) \right) \]
\[ M_{2}^{*} : \exp \left( \beta_{\text{lgdp out}} \cdot s_{\text{lgdp out}}(y) + \beta_{\text{gdp in}} \cdot s_{\text{gdp in}}(y) + \beta_{\text{lmilex in}} \cdot s_{\text{lmilex in}}(y) + \beta_{\text{alliance}} \cdot s_{\text{alliance}}(y) + \beta_{\text{mutual}} \cdot s_{\text{mutual}}(y) + \beta_{\text{2-star-out}} \cdot s_{\text{2-star-out}}(y) + \beta_{\text{2-star-in}} \cdot s_{\text{2-star-in}}(y) + \beta_{\text{transitivity}} \cdot s_{\text{transitivity}}(y) + t(y)^{\top} \gamma \right). \]

Computing times for 1,000 VI iterations were 0.9, 1.5, 1.3, and 1.6 minutes for models \( M_{1} \), \( M_{1}^{*} \), \( M_{2} \), and \( M_{2}^{*} \), respectively.

**Results**

The posterior explained variances comparing models \( M_{2}^{*} \) and \( M_{1}^{*} \) are \( R_{\delta} = 0.55 \) and \( R_{\phi} = 0.52 \) for the sender and receiver, respectively. Quantile functions of marginal posteriors of the variance parameters are shown in Figure 6. In addition, the respective posterior expectations of models \( M_{1}^{*} \) vs \( M_{2}^{*} \) are 61.8 vs 45.2 and 84.8 vs 63.8 for the sender and receiver, respectively. These measures demonstrate in general that the included covariates can contribute to the reduction of unobserved heterogeneity for both exports and imports. Moreover, the BGOFs in Figure E.3 in the Supplement illustrate that retaining the nodal random effects in addition to the covariates improves the model fit, such that \( M_{2}^{*} \) is preferred over model \( M_{2} \) without nodal effects and also over \( M_{1}^{*} \) without covariates.

Table 3 lists the posterior mean estimates (together with 95% corrected credible intervals) of network statistics for all four models. We see a strong negative effect for mutual trade. In other words, it is not likely that countries sell weapons to a country they buy weapons from. Transitivity is positive so that arms trading between two importing countries of the same importer is likely. Moreover, 2-in-star is negative, which implies that countries prefer to import from only a few countries. In contrast, 2-out-star is positive, which demonstrates that countries exporting arms tend to do so to multiple countries. As would be expected, military expenditure, GDP, as well as the indicator as to whether the countries share an alliance have a positive effect, i.e., promote the trading of weapons. The difference in polity score is not significant, and slightly negative when allowing for node heterogeneity.
Figure 6: International arms trading.

Marginal posterior quantile functions of variance parameters in $M_1^*$ (excluding nodal covariates) and $M_2^*$ (including nodal covariates).

Table 3: International arms trading.

| Statistics/covariate | $M_1$          | $M_1^*$         | $M_2$          | $M_2^*$         |
|----------------------|----------------|-----------------|----------------|-----------------|
| $s_{\text{edge}}(y)$ | -5.836 (-5.847, -5.824) | -4.655 (-4.673, -4.637) | -5.958 (-5.958, -5.957) | -5.888 (-5.889, -5.886) |
| $s_{\text{mutual}}(y)$ | -0.762 (-0.762, -0.762) | -0.734 (-0.734, -0.734) | -0.652 (-0.652, -0.652) | -0.600 (-0.601, -0.599) |
| $s_{\text{transitive}}(y)$ | 0.490 (0.490, 0.491) | 0.277 (0.277, 0.278) | 0.409 (0.408, 0.409) | 0.255 (0.254, 0.255) |
| $s_{\text{2-in-star}}(y)$ | 0.098 (0.087, 0.109) | -0.013 (-0.014, -0.013) | -0.029 (-0.032, -0.026) | -0.109 (-0.110, -0.108) |
| $s_{\text{2-out-star}}(y)$ | 0.086 (0.075, 0.097) | 0.075 (0.074, 0.076) | 0.054 (0.050, 0.057) | 0.041 (0.040, 0.041) |
| lmilex               | 0.056 (0.050, 0.062) | 0.056 (0.050, 0.062) | 0.056 (0.050, 0.062) | 0.056 (0.050, 0.062) |
| gdp$_{\text{out}}$   | 0.358 (0.348, 0.367) | 0.138 (0.118, 0.159) | 0.138 (0.118, 0.159) | 0.138 (0.118, 0.159) |
| gdp$_{\text{in}}$    | 0.054 (0.049, 0.058) | -0.131 (-0.145, -0.118) | 0.054 (0.049, 0.058) | -0.131 (-0.145, -0.118) |
| polity               | -0.023 (-0.058, 0.011) | -0.041 (-0.060, -0.022) | -0.023 (-0.058, 0.011) | -0.041 (-0.060, -0.022) |
| alli                 | 0.526 (0.525, 0.527) | 0.372 (0.371, 0.374) | 0.526 (0.525, 0.527) | 0.372 (0.371, 0.374) |

Posterior mean estimates together with 95% corrected credible intervals of coefficients of network statistics and covariates for models $M_1$, $M_1^*$, $M_2$, $M_2^*$. Effects not containing the zero within the respective credible interval are highlighted in bold.
5.3 Facebook ego network

The third example is a benchmark dataset taken from the Stanford Large Network Dataset Collection (SNAP datasets; Leskovec and Krevl; 2014). The dataset provides information on friend lists from ten anonymized Facebook users called egos. Given the fact that the egos are connected to all their friends, the egos (and all nodes only having connections to egos) are excluded before analysing the network, as too much importance would otherwise be attributed to those nodes; see Figure 1. However, most papers so far have only considered a subsample of the network due to its size (e.g., Thiemichen and Kauermann; 2017). The focus here is to demonstrate that the variational approach allows us to fit and select complex models for large networks, even in the presence of heterogeneity.

Model specification  We select the model with two major aims, i) to identify relevant network statistics and ii) decide whether or not nodal effects improve the model fit. For i) we specifically compare the three models $M_1$ to $M_3$ with the following model specifications:

$$
M_1 : \exp(\beta_{\text{edge}}s_{\text{edge}}(y) + \beta_{\text{2-star}}s_{\text{2-star}}(y) + \beta_{\text{triangle}}s_{\text{triangle}}(y))
$$

$$
M_2 : \exp(\beta_{\text{edge}}s_{\text{edge}}(y) + \beta_{\text{2-star}}s_{\text{2-star}}(y) + \beta_{\text{gwesp}}s_{\text{gwesp}}(y))
$$

$$
M_3 : \exp(\beta_{\text{edge}}s_{\text{edge}}(y) + \beta_{\text{2-star}}s_{\text{2-star}}(y) + \beta_{\text{triangle}}s_{\text{triangle}}(y) + \beta_{\text{gwesp}}s_{\text{gwesp}}(y)).
$$

For ii) we include nodal random effects in each model and denote these as $M_1^*$ to $M_3^*$.

Results  The computing times for 1,000 VI iterations were 14, 19.1, and 37.7 minutes for $M_1$ to $M_3$ and 142.5, 156.3, and 162.2 minutes for $M_1^*$ to $M_3^*$, respectively. As can be seen in Table 4, models containing nodal effects outperform the respective ones without. $M_2^*$ and $M_3^*$ outperform $M_1^*$ whereas $M_3^*$ is preferred over $M_3^*$ in terms of BFs. This observation is confirmed by the BGOFs in the Supplement, Figure E.5.

Table 5 lists the posterior mean estimates (together with 95% corrected credible intervals) of network statistics for all six models. A deeper discussion on interpreting effects of network statistics in general is provided in Snijders et al. (2006). Here, we briefly highlight some findings in the best model $M_2^*$ (4th row in Table 5). The effect $\beta_{\text{2-star}}$ is (statistically significantly) negative, which indicates that the likelihood of a tie decreases if an additional 2-star exists in the network, meaning one node has two friends in common. This is a partial effect, given the effect $\beta_{\text{gwesp}}$, which is (statistically significantly) positive meaning that, overall, there is a tendency to increase the number of joint partners. However, as nodal heterogeneity is required following the BF-based model selection, the actors in the network are too heterogeneous to describe Facebook friendships just by the selected statistics.
Table 5: Facebook egos.

| Model | Statistic | \( s_{\text{edge}}(y) \) | \( s_{\text{triangles}}(y) \) | \( s_{\text{2-star}}(y) \) | \( s_{\text{gwesp}}(y) \) | \( \gamma \) |
|-------|-----------|-----------------|-----------------|-----------------|-----------------|---------|
| \( \mathcal{M}_1 \) | -6.157    | 0.581            | -0.016          | No              |
|        | (-6.159, -6.156) | (0.580,0.581) | (-0.017, -0.015) |                  |
| \( \mathcal{M}^*_1 \) | 0.594    | -0.0246          | Yes             |
|        | (0.559,0.629) | (-0.02464,-0.0245) |                  |
| \( \mathcal{M}_2 \) | -7.217    | -0.012           | 0.554           | No              |
|        | (-7.240, -7.193) | (-0.021, -0.003) | (0.384,0.724) |                  |
| \( \mathcal{M}^*_2 \) | -0.018   | 0.586            | Yes             |
|        | (-0.0188,-0.0174) | (0.503,0.668) |                  |
| \( \mathcal{M}_3 \) | -6.955    | 0.026            | -0.0165         | No              |
|        | (-6.978,-6.932) | (-0.011,0.063) | (-0.023, -0.010) | (0.412, 0.636) |
| \( \mathcal{M}^*_3 \) | 0.067    | -0.035           | Yes             |
|        | (0.059,0.075) | (-0.036,-0.035) | (0.527,0.573) |                  |

Posterior mean estimates together with 95\% corrected credible intervals of coefficients of network statistics for all models. Effects not containing the zero within the credible interval are highlighted in bold.

### 6 Conclusion

In this paper, we have developed variational inference for the analysis of large scale networks with nodal heterogeneity. Our approach comes with a number of merits and solutions in comparison to existing methods. Firstly, it allows the incorporation of nodal heterogeneity in the network, both in undirected as well as in directed networks. Secondly, while previous Bayesian network models are unsuitable for large networks owing to their numerical complexity, the variational approach pushes this limit, allowing us to analyse networks with thousands of nodes even when node heterogeneity is included. Thirdly, we contribute to model selection and model validation, utilizing the information obtained through the (approximate) posterior distributions. In particular, comparing models with and without nodal heterogeneity effects provides a novel framework for assessing how much external node or edge-specific covariates contribute to explaining the existence of edges. This is demonstrated in a directed network on arms trading. Lastly, we propose a simple correction step, so that the posterior standard errors are closer to the true ones.

Overall, we demonstrate the great potential of variational methods in the context of network analyses with a large number of edges and nodal heterogeneity. In the future, it would be of interest to leverage this potential further to networks that are beyond the scope of this paper, e.g. for dynamic (Lebacher et al.; 2021b) or multi-edge (Brandenberger et al.; 2019) networks. In the context of such networks, other choices of variational approximation may also be investigated, such as methods based on implicit copulas (Smith and Loaiza-Mayta; 2022) or mixture models (Gunawan et al.; 2021).

### Acknowledgments

The authors would like to thank Jana Kleinemeier and Tim Bündert for assistance in coding and evaluation of simulation results and Prof. Michael Smith for...
an initial discussion on this project. Andrew Entwistle kindly provided his English proofreading expertise. We thank Cornelius Fritz and Michael Lebacher for data sharing and useful discussions on the empirical illustrations.

**Funding** The first author Nadja Klein was supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) through the Emmy Noether grant KL 3037/1-1.

**Supplementary Material** This supplement contains the employed network statistics (A), further derivations and calculations relevant to our VI approach (B–D), additional material on the two real data examples (E), and extensive simulations evaluating the accuracy and robustness of our estimator, as well as benchmarking with exact Bayesian inference in small networks (F).

**References**

Babkin, S., Stewart, J. R., Long, X. and Schweinberger, M. (2020). Large-scale estimation of random graph models with local dependence, *Computational Statistics & Data Analysis* **152**: 107029.

Biagini, F., Kauermann, G. and Meyer-Brandis, T. (eds) (2019). *Network Science - An Aerial View*, 1 edn, Springer.

Blei, D. M., Kucukelbir, A. and McAuliffe, J. D. (2017). Variational inference: A review for statisticians, *Journal of the American Statistical Association* **112**(518): 859–877.

Bottou, L. (2010). Large-scale machine learning with stochastic gradient descent, *in Y. Lechevallier and G. Saporta (eds), Proceedings of the 19th International Conference on Computational Statistics (COMPSTAT2010)*, pp. 177–187.

Bouranis, L., Friel, N. and Maire, F. (2018). Bayesian model selection for exponential random graph models via adjusted pseudolikelihoods, *Journal of Computational and Graphical Statistics* **27**(3): 516–528.

Box-Steffensmeier, J. M., Christenson, D. P. and Morgan, J. W. (2018). Modeling unobserved heterogeneity in social networks with the frailty exponential random graph model., *Political Analysis* **26**(1): 3–19.

Brandenberger, L., Casiraghi, G., Nanumyan, V. and Schweitzer, F. (2019). Quantifying triadic closure in multi-edge social networks, *Proceedings of the 2019 IEEE/ACM International Conference on Advances in Social Networks Analysis and Mining*, Association for Computing Machinery, New York, USA, pp. 307—310. **URL:** https://doi.org/10.1145/3341161.3342926

Braun, M. and McAuliffe, J. (2010). Variational inference for large-scale models of discrete choice, *Journal of the American Statistical Association* **105**(489): 324–335.

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

Caimo, A. and Friel, N. (2013). Bayesian model selection for exponential random graph models, *Social Networks* **35**(1): 11–24.

Caimo, A. and Friel, N. (2014). Bergm: Bayesian exponential random graphs in R, *Journal
Chatterjee, S. and Diaconis, P. (2013). Estimating and understanding exponential random graph models, *The Annals of Statistics* 41(5): 2428–2461.

Duijn, M. A. J., Snijders, T. A. and Zijlstra, B. J. H. (2004). p2: A random effects model with covariates for directed graphs, *Statistica Neerlandica* 58(2): 234–254.

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

Fienberg, S. E. (2012). A brief history of statistical models for network analysis and open challenges, *Journal of Computational and Graphical Statistics* 21(4): 825–839.

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

Gelman, A. and Meng, X.-L. (1998). Simulating normalizing constants: from importance sampling to bridge sampling to path sampling, *Statistical Science* 13(2): 163–185.

Geweke, J. and Zhou, G. (1996). Measuring the Pricing Error of the Arbitrage Pricing Theory, *The Review of Financial Studies* 9(2): 557–587.

Geyer, C. J. and Thompson, E. A. (1992). Constrained Monte Carlo maximum likelihood for dependent data, *Journal of the Royal Statistical Society: Series B* 54(3): 657–683.

Giordano, R., Broderick, T. and Jordan, M. I. (2018). Covariances, robustness, and variational Bayes, *Journal of Machine Learning Research* 19(51): 1–49.

Goodreau, S., Kitts, J. and Morris, M. (2009). Birds of a feather, or friend of a friend? using exponential random graph models to investigate adolescent social networks, *Demography* 46: 103—125.

Gunawan, D., Kohn, R. and Nott, D. (2021). Flexible variational bayes based on a copula of a mixture of normals, *arXiv:2106.14392*.

Handcock, M. S., Hunter, D. R., Butts, C. T., Goodreau, S. M., Krivitsky, P. N. and Morris, M. (2021). *ergm: Fit, Simulate and Diagnose Exponential-Family Models for Networks*. R package version 3.11.0.

Hoffman, M. D., Blei, D. M., Wang, C. and Paisley, J. (2013). Stochastic variational inference, *Journal of Machine Learning Research* 14(4): 1303–1347.

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

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

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

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

Jordan, M. I., Ghahramani, Z., Jaakkola, T. S. and Saul, L. K. (1999). An introduction to variational methods for graphical models, *Machine Learning* 37(2): 183–233.

Kass, R. E. and Wasserman, L. (1995). A reference Bayesian test for nested hypotheses and its relationship to the Schwarz criterion, *Journal of the American Statistical Association*
Kevork, S. and Kauermann, G. (2021). Iterative estimation of mixed exponential random graph models with nodal random effects, *Network Science* 9(4): 478–498.

Kevork, S. and Kauermann, G. (2022). Bipartite exponential random graph models with nodal random effects, *Social Networks* 70: 90–99.

Kingma, D. P. and Welling, M. (2014). Auto-encoding variational Bayes, in Y. Bengio and Y. LeCun (eds), *2nd International Conference on Learning Representations*.

Klein, N. and Kneib, T. (2016). Scale-dependent priors for variance parameters in structured additive distributional regression, *Bayesian Analysis* 11(4): 1071–1106.

Kolaczyk, E. D. (2009). *Statistical Analysis of Network Data*, 1 edn, Springer.

Kolaczyk, E. D. and Csardi, G. (2014). *Statistical Analysis of Network Data with R*.

Koskinen, J. (2009). Using latent variables to account for heterogeneity in exponential family random graph models, in S. Ermakov, V. Melas and A. Pepelyshev (eds), *Proceedings of the 6th St. Petersburg Workshop on Simulation*, Vol. 2, pp. 845–849.

Kucukelbir, A., Tran, D., Ranganath, R., Gelman, A. and Blei, D. M. (2017). Automatic differentiation variational inference, *J. of Machine Learning Research* 18(1): 430–474.

Latouche, P., Birmelé, E. and Ambroise, C. (2012). Variational Bayesian inference and complexity control for stochastic block models, *Statistical Modelling* 12: 93–115.

Lebacher, M., Thurner, P. and Kauermann, G. (2021a). Censored regression for modelling small arms trade volumes and its “forensic” use of exploring unreported trades, *Journal of the Royal Statistical Society: Series C*. https://doi.org/10.1111/rssc.12491.

Lebacher, M., Thurner, P. W. and Kauermann, G. (2021b). A dynamic separable network model with actor heterogeneity: An application to global weapons transfers, *Journal of the Royal Statistical Society: Series A (Statistics in Society)* 184(1): 201–226.

Leskovec, J. and Krevl, A. (2014). SNAP Datasets: Stanford large network dataset collection, [http://snap.stanford.edu/data](http://snap.stanford.edu/data).

Lusher, D., Koskinen, J. and Robins, G. (eds) (2012). *Exponential Random Graph Models for Social Networks: Theory, Methods, and Applications*, Structural Analysis in the Social Sciences, Cambridge University Press.

McDaid, A. F., Murphy, T., Friel, N. and Hurley, N. (2013). Improved Bayesian inference for the stochastic block model with application to large networks, *Computational Statistics & Data Analysis* 60: 12–31.

Mele, A. and Zhu, L. (2021). Approximate Variational Estimation for a Model of Network Formation, *The Review of Economics and Statistics* pp. 1–30.

Miller, J. W. (2021). Asymptotic normality, concentration, and coverage of generalized posteriors., *J. Mach. Learn. Res.* 22: 168–1.

Morris, M., Handcock, M. S. and Hunter, D. R. (2008). Specification of exponential-family random graph models: Terms and computational aspects, *Journal of Statistical Software* 24(4): 1—24.

URL: [https://www.jstatsoft.org/index.php/jss/article/view/v024i04](https://www.jstatsoft.org/index.php/jss/article/view/v024i04)

Murray, I., Ghahramani, Z. and MacKay, D. J. C. (2006). MCMC for doubly-intractable distributions, *Proceedings of the Twenty-Second Conference on Uncertainty in Artificial Intelligence*, pp. 359—366.

Nott, D. J., Tan, S. L., Villani, M. and Kohn, R. (2012). Regression density estimation with variational methods and stochastic approximation, *Journal of Computational and Graphical Statistics* 21(3): 797–820.
Ong, V. M., Nott, D. and Smith, M. (2018). Gaussian variational approximation with a factor covariance structure, *Journal of Comp. and Graph. Statistics* 27(2): 465–478.

Ormerod, J. T. and Wand, M. P. (2010). Explaining variational approximations, *The American Statistician* 64(2): 140–153.

Paisley, J., Blei, D. M. and Jordan, M. I. (2012). Variational bayesian inference with stochastic search, in J. Langford and J. Pineau (eds), *Proceedings of the 29th International Conference on Machine Learning*, pp. 1363–1370.

Perkins, R. and Neumayer, E. (2010). The organized hypocrisy of ethical foreign policy: Human rights, democracy and Western arms sales, *Geoforum* 41(2): 247–256.

Ranganath, R., Gerrish, S. and Blei, D. (2014). Black Box Variational Inference, in S. Kaski and J. Corander (eds), *Proceedings of the Seventeenth International Conference on Artificial Intelligence and Statistics*, Vol. 33, pp. 814–822.

Rezende, D. J., Mohamed, S. and Wierstra, D. (2014). Stochastic backpropagation and approximate inference in deep generative models, in E. P. Xing and T. Jebara (eds), *Proc. 31st International Conference on Machine Learning*, Vol. 32, pp. 1278–1286.

Robbins, H. and Monro, S. (1951). A Stochastic Approximation Method, *The Annals of Mathematical Statistics* 22(3): 400–407.

Salimans, T. and Knowles, D. A. (2013). Fixed-form variational posterior approximation through stochastic linear regression, *Bayesian Analysis* 8(4): 837–882.

Simpson, D., Rue, H. Martins, T. G., Riebler, A. and Sørbye, S. H. (2017). Penalising model component complexity: A principled, practical approach to constructing prior, *Statistical Science* 32(1): 1–28.

Smith, M. S. and Loaiza-Maya, R. (2022). Implicit copula variational inference, *Journal of Computational and Graphical Statistics* 0(0): 1–13.

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

Snijders, T. A. B., Pattison, P. E., Robins, G. L. and Handcock, M. S. (2006). New specifications for exponential random graph models, *Sociological Methodology* 36(1): 99–153.

Tan, L. S. L. and Friel, N. (2020). Bayesian variational inference for exponential random graph models, *Journal of Computational and Graphical Statistics* 29(4): 910–928.

Thiemichen, S. and Caimo, A. (2018). mixbergm. Code available at https://github.com/acaimo/Bergm-nodal-effects.

Thiemichen, S., Friel, N., Caimo, A. and Kauermann, G. (2016a). Bayesian exponential random graph models with nodal random effects, *Social Networks* 46: 11–28.

Thiemichen, S., Friel, N., Caimo, A. and Kauermann, G. (2016b). Bayesian exponential random graph models with nodal random effects, *Social Networks* 46: 11–28.

Thiemichen, S. and Kauermann, G. (2017). Stable exponential random graph models with non-parametric components for large dense networks, *Social Networks* 49: 67–80.

Thurner, P. W., Schmid, C. S., Cranmer, S. J. and Kauermann, G. (2019). Network interdependencies and the evolution of the international arms trade, *Journal of Conflict Resolution* 63(7): 1736–1764.

Titsias, M. and Lázaro-Gredilla, M. (2015). Local expectation gradients for black box variational inference, in C. Cortes, N. Lawrence, D. Lee, M. Sugiyama and R. Garnett (eds), *Advances in Neural Information Processing Systems*, Vol. 28.

Wang, J., Cai, X., Niu, X. and Li, R. (2023). Variable selection for high-dimensional
nodal attributes in social networks with degree heterogeneity, *Journal of the American Statistical Association* 0(0): 1–14.

**URL:** [https://doi.org/10.1080/01621459.2023.2187815](https://doi.org/10.1080/01621459.2023.2187815)

Williams, R. J. (1992). Simple statistical gradient-following algorithms for connectionist reinforcement learning, *Machine Learning* 8(4): 229—256.

Xu, M., Quiroz, M., Kohn, R. and Sisson, S. A. (2019). Variance reduction properties of the reparameterization trick, in K. Chaudhuri and M. Sugiyama (eds), *Proceedings of the Twenty-Second International Conference on Artificial Intelligence and Statistics*, Vol. 89, pp. 2711–2720.

Yin, F. and Butts, C. (2020). Kernel-based approximate Bayesian inference for exponential family random graph models, *arXiv:2004.08064v2*.

Yin, F., Shen, W. and Butts, C. T. (2022). Finite mixtures of ergms for modeling ensembles of networks, *Bayesian Analysis* 1(1): 1–39.

Zeiler, M. D. (2012). ADADELTA: An adaptive learning rate method, *arXiv:1212.5701v1*.