1 Introduction

Networks are relational data that can be defined as a collection of nodes interacting with each other and connected in a pairwise fashion. From a statistical point of view, networks are relational data represented as mathematical graphs. A graph consists of a set of $n$ nodes and a set of $m$ edges which define some sort of relationships between pair of nodes called dyads. The connectivity pattern of a graph can be described by an $n \times n$ adjacency matrix $y$ encoding the presence or absence of an edge between node $i$ and $j$:

$$y_{ij} = \begin{cases} 1, & \text{if } (i, j) \text{ are connected}, \\ 0, & \text{otherwise}. \end{cases}$$

Two nodes are adjacent or neighbours if there is an edge between them. If $y_{ij} = y_{ji}, \forall i, j$ then the adjacency matrix is symmetric and the graph is undirected, otherwise the graph is directed and it is often called a digraph. Edges connecting a node to itself (self-loops) are generally not allowed in many applications and will not be considered in this context.

2 Exponential random graph models

Introduced by Holland and Leinhardt (1981) to model individual heterogeneity of nodes and reciprocity of their edges, the family of exponential random graph models (ERGMs) was generalised by Frank and Strauss (1986), Wasserman and Pattison (1996) and Snijders et al. (2006). ERGMs constitute a broad class of network models (see (Robins et al., 2007) for an introduction) that assume that the observed network $y$ can be explained in terms of the relative prevalence of a set of network statistics $s(y)$:

$$p(y|\theta) = \frac{\exp\{\theta^t s(y)\}}{z(\theta)} p(\theta) p(y),$$

where the normalising constant $z(\theta)$ is intractable for non trivially-small networks.

Due to the complexity of networks, it is necessary to reduce the information to describe essential properties of the network. Usually this is done via network statistics, a series of counts of sub-graph configurations (e.g., the number of edges, stars, triangles, functions of degree distributions, edgewise shared partners, etc.), catching the relevant information (Snijders et al. 2006).

3 Bayesian inference

In the ERGM context (see (Wasserman and Pattison 1996) and (Robins et al. 2007)), the posterior distribution of model parameters $\theta$ given an observed network $y$ on $n$ nodes may be written as:

$$p(\theta|y) = \frac{p(y|\theta) p(\theta)}{p(y)} = \frac{\exp\{\theta^t s(y)\}}{z(\theta)} \frac{p(\theta)}{p(y)},$$

(2)
where $s(y)$ is a known vector of sufficient network statistics (Morris et al., 2008), $p(\theta)$ is a prior distribution placed on $\theta$, $z(\theta)$ is the intractable likelihood normalising constant, and $p(y)$ is the model evidence. The presence of the intractable ERGM likelihood implies that the usual suite of standard Bayesian inferential methods, especially standard MCMC tools are not possible in this context. However recent work has shown that the ERGM can be given the full Bayesian treatment as we now outline.

### 4 The Bergm package for R

The Bergm package (Caimo and Friel, 2014) for R (R Development Core Team, 2011) implements Bayesian analysis for ERGMs (Caimo and Friel, 2011; 2013; Caimo and Mira, 2015; Thiemichen et al., 2016; Bouranis et al., 2015). The package provides a comprehensive framework for Bayesian inference using Markov chain Monte Carlo (MCMC) algorithms. It can also supply graphical Bayesian goodness-of-fit procedures that address the issue of model adequacy.

The package is simple to use and represents an attractive way of analysing network data as it offers the advantage of a complete probabilistic treatment of uncertainty. Bergm is based on the ergm package (Hunter et al., 2008) which is part of the statnet suite of packages (Handcock et al., 2007) and therefore it makes use of the same model set-up and network simulation algorithms. The ergm and Bergm packages complement each other in the sense that ergm implements maximum likelihood-based inference whereas Bergm implements Bayesian inference. The Bergm package has been continually improved in terms of speed performance over the last years and we feel that this package now offers the end-user a feasible option for carrying out Bayesian inference for networks with several thousands of nodes.

### 5 Approximate exchange algorithm

In order to approximate the posterior distribution $p(\theta|y)$, the Bergm package uses the exchange algorithm described in Section 4.1 of (Caimo and Friel, 2011) to sample from the following distribution:

$$
p(\theta', y', \theta|y) \propto p(y|\theta)p(\theta)e(\theta'|\theta)p(y'|\theta')
$$

where $p(y'|\theta')$ is the likelihood on which the simulated data $y'$ are defined and belongs to the same exponential family of densities as $p(y|\theta)$, $e(\theta'|\theta)$ is any arbitrary proposal distribution for the augmented variable $\theta'$. As we will see in the next section, this proposal distribution is set to be a normal centred at $\theta$.

At each MCMC iteration, the exchange algorithm consists of a Gibbs update of $\theta'$ followed by a Gibbs update of $y'$, which is drawn from $p(\cdot|\theta')$ via an MCMC algorithm (Hunter et al., 2008). Then a deterministic exchange or swap from the current state $\theta$ to the proposed new parameter $\theta'$. This deterministic proposal is accepted with probability:

$$
\min\left(1, \frac{q_0(y')p(\theta')e(\theta|\theta')q_0(\theta)}{q_0(y)p(\theta)e(\theta'|\theta)q_0(y')} \times \frac{z(\theta)z(\theta')}{z(\theta)z(\theta')}\right),
$$

where $q_0$ and $q_0'$ indicate the unnormalised likelihoods with parameter $\theta$ and $\theta'$, respectively. Notice that all the normalising constants cancel above and below in the fraction above, in this way avoiding the need to calculate the intractable normalising constant.

The approximate exchange algorithm is implemented by the bergm function in the following way:

for $i = 1, \ldots, N$

1. generate $\theta'$ from $e(\cdot|\theta)$
2. simulate $y'$ from $p(\cdot|\theta')$
3. update $\theta \to \theta'$ (log) probability:

$$
\min\left(0, [\theta - \theta']^t [s(y') - s(y)] + \log\left(\frac{p(\theta')}{p(\theta)}\right)\right)
$$
where $s(y)$ is the observed vector of network statistics and $s(y')$ is the simulated vector of network statistics. Step 2. above requires a draw from the ERGM likelihood and perfect sampling in principle is a possibility, however practically this is out of reach as no such sampler has yet been developed. Therefore the pragmatic approach we take is to run a Gibbs sampler for $aux.iters$ iterations targeting $p(\cdot|\theta')$. In order to improve mixing a parallel adaptive direction sampler (ADS) approach [Gilks et al. 1994, Roberts and Gilks 1994] is considered as the default procedure.

To illustrate the inferential procedure, we fit a 4-dimensional ERGM to the Faux Mesa High School network data [Resnick et al. 1997] including uniform homophily between students with the same 'grade' (nodematch('Grade')), and statistics capturing the degree distribution (gwdegree) and transitivity effect (gwesp):

```r
> model <- y ~ edges +
  +   nodematch('Grade') +
  +   gwdegree(0.2, fixed = TRUE) +
  +   gwesp(0.2, fixed = TRUE)
```

and we use the `bergm` function with 20,000 auxiliary iterations for network simulation and 6 MCMC chains for the ADS procedure consisting of 2,000 main iterations each:

```r
> bergm.post <- bergm(model,
+   burn.in = 300,
+   main.iters = 2000,
+   aux.iters = 20000,
+   nchains = 6,
+   gamma = 0.6)
```

The estimation took about 200 seconds. A summary of the MCMC results is available via the `bergm.output` command:

```r
> bergm.output(post)
```

| theta1 (edges) | Mean | SD  | Naive SE |
|----------------|------|-----|----------|
|                | -6.4539945 | 0.2269798 | 0.002072032 |
theta2 (nodematch.Grade) 2.0653066 0.1562896 0.001426723
theta3 (gwdegree) 0.1555102 0.2156994 0.001969057
theta4 (gwesp.fixed.0.2) 1.6045295 0.1624254 0.001482734

Time-series SE
theta1 (edges) 0.013682987
theta2 (nodematch.Grade) 0.009303603
theta3 (gwdegree) 0.013919679
theta4 (gwesp.fixed.0.2) 0.009959682

2.5% 25% 50%
theta1 (edges) -6.8988256 -6.6003492 -6.4532048
theta2 (nodematch.Grade) 1.7879473 1.9557575 2.0537140
theta3 (gwdegree) -0.2825274 0.0158655 0.1618899
theta4 (gwesp.fixed.0.2) 1.2841624 1.4983524 1.6031113

75% 97.5%
theta1 (edges) -6.3043630 -6.0255210
theta2 (nodematch.Grade) 2.1665645 2.3952768
theta3 (gwdegree) 0.3118872 0.5568012
theta4 (gwesp.fixed.0.2) 1.7099524 1.9425482

Acceptance rate: 0.1965833

Density and trace plots are produced automatically by the `bergm.output` function:

Posterior predictive goodness-of-fit diagnostics plots are available via the `bgof` command, as shown in the figure below.
> bgof(bergm.post,  
+    aux.iters = 20000,  
+    n.deg = 14,  
+    n.dist = 15,  
+    n.esp = 10)

Bayesian goodness-of-fit diagnostics

The plots in the figure indicate a very good fit of the model in terms of a higher-level network statistics in the data.

6 Pseudo-posterior calibration

An alternative approach to Bayesian inference for ERGMs has been proposed by Bouranis et al. (2015) based on replacing the intractable ERGM likelihood with a tractable pseudo-likelihood approximation. This results in a so-called pseudo-posterior distribution for which it is straightforward to sample from using the usual MCMC toolbox, for example. However it is well understood that Bayesian inference based on the pseudolikelihood can yield poor estimation and this motivated Bouranis et al. (2015) to develop an approach which allows one to correct or calibrate a sample from such a pseudo-posterior distribution so that it is approximately distributed from the target posterior distribution. This is achieved by estimating the maximum a posteriori (MAP) of the posterior distribution and also estimating the Hessian of the posterior distribution at the MAP. Both of these quantities can then be used to define an affine transformation of the pseudo-posterior distribution to one that is approximately distributed as the posterior distribution.

The pseudo-posterior calibration approach can be carried out using the calibrate.bergm function:

> cbergm.post <- calibrate.bergm(model,  
+    iters = 1000,  
+    aux.iters = 20000,  
+    noisy.nsim = 100,  
+    noisy.thin = 1000,  
+    mcmc = 10000)

The estimation took about 80 seconds and the MCMC output can be analysed by using the bergm.output function.

In the plots below, we see that the posterior estimates from the calibrate.bergm function is in good agreement with that corresponding to the bergm function:
7 More information

The Bergm package is available on the CRAN at: https://CRAN.R-project.org/package=Bergm and also on GitHub at: https://github.com/acaimo/Bergm.

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