Bayesian modelling and computation utilising
cycles in multiple network data

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Abstract

Modelling multiple network data is crucial for addressing a wide range of applied research questions. However, there are many challenges, both theoretical and computational, to address. Network cycles are often of particular interest in many applications, e.g. ecological studies, and an unexplored area has been how to incorporate networks’ cycles within the inferential framework in an explicit way. The recently developed Spherical Network Family of models (SNF) offers a flexible formulation for modelling multiple network data that permits any type of metric. This has opened up the possibility to formulate network models that focus on network properties hitherto not possible or practical to consider. In this article we propose a novel network distance metric that measures similarities between networks with respect to their cycles, and incorporate this within the SNF model to allow inferences that explicitly capture information on cycles. These network motifs are of particular interest in ecological studies. We further propose a novel computational framework to allow posterior inferences from the intractable SNF model for moderate sized networks. Lastly, we apply the resulting methodology to a set of ecological network data studying aggressive interactions between species of fish. We show our model is able to make cogent inferences concerning the cycle behaviour amongst the species, and beyond those possible from a model that does not consider this network motif.

Keywords: Doubly intractable distributions, Importance Sampling, Object data analysis, Relational data.
1 Introduction

In many fields, modelling network data is essential to answering the applied research questions of interest. In Ecology, modelling the behaviour of different species within a geographical area can be represented by a network with each species corresponding to a node and the edges representing some form of interaction between species (Delmas et al. (2019); Mittelbach and McGill (2019)). If these interactions are aggressive then this could represent various underlying competitive behaviours within the species’ ecosystem, e.g. certain species vying over a particular food source or type of habitat. In a network these behaviours would be characterised through cycles (Sokhn et al. (2012); Kourtouli et al. (2020)).

Cycles reveal information about network topology (Maugis et al. (2017); Fan et al. (2019)), and is a motif of interest in many applications beyond Ecology. Examples include Neuroscience, where the formation of cycles in a human brain network is crucial for human cognitive functions (Sizemore et al. (2018)), and Biology where RNAs forming covalently closed loop structures, called circular RNAs, have been associated to diseases such as cancer (Han et al. (2017)).

Recent methodological developments permit data to be analysed where each observation is a network. In Ecology, this arises when recording species’ interactions across multiple different areas or sites. In this setting, the goal is to model the underlying mechanism that generates the multiple network data. Recent studies have focused on the problem of modelling multiple network data utilising (a) a latent space framework (Gollini and Murphy (2016); Durante et al. (2017); Wang et al. (2019); Nielsen and Witten (2018); Arroyo et al. (2019)), (b) a measurement error process (Le et al. (2018); Newman (2018); Peixoto (2018); Mantziou et al. (2021)) and (c) distance functions (Lunagómez et al. (2020); Kolaczyk et al. (2017); Ginestet et al. (2017)). However none of these models explicitly consider networks’ cyclical properties in their formulation.

Distance-based models offer a way to encode networks’ cycle information by incorporating this information in a metric measuring similarity between networks. There are a multitude of ways to define a similarity measure between different networks and for a review of these see Donnat and Holmes (2018). However, none of these metrics explicitly consider cycles when measuring network dissimilarity.

In this article we propose a distance-based model for multiple network data that explicitly utilises the cycle information in the distance metric. Specifically, the metric we propose involves counting the number of uncommon cycles between the two networks, denoted as the symmetric difference, and combining this with the Hamming distance (both defined in the next section). The resulting metric is denoted as the Hamming-Symmetric difference (HS) distance metric.

We adopt a Bayesian approach and utilise the Spherical Network Family (SNF) of models (Lunagómez et al. (2020)) to make posterior inferences as this gives us the flexibility to specify the distance metric of our choice, which in our setting is the HS distance. However, the computational challenges associated with fitting the SNF model are significant with the model having an intractable normalising constant which is a sum over the space of graphs. Notably, for an undirected network with \( n \) nodes there are \( 2^{n(n−1)/2} \) possible networks, which means that even for a moderate-sized network with \( n = 20 \) nodes there will be more than \( 1.56 \times 10^{57} \) network configurations which are not practically possible to enumerate. Enumerating cycles within a network is also a computationally intensive task.

The problem of performing inference for intractable distributions has been widely studied
by researchers. Notably, there are two classes of algorithms developed in the literature, (i) the algorithms that use auxiliary variables that allow the cancellation of the normalising constants from the Metropolis-Hastings (MH) ratio (Møller et al. (2006); Murray et al. (2012); Liang (2010)), and (ii) the algorithms that substitute the normalising constant with an approximation in the MH ratio. In the latter case, a common approach for addressing the problem of the intractable normalising constant is using Importance Sampling (IS) (Chen and Shao (1997); Meng and Wong (1996); Gelman and Meng (1994); Everitt, Johansen, Rowing and Evdemon-Hogan (2017); Everitt, Prangle, Maybank and Bell (2017); Atchadé et al. (2013); Beaumont (2003); Andrieu and Roberts (2009); Alquier et al. (2016)). For a detailed review on methods for intractable distributions see Park and Haran (2018).

The methodology proposed in Lunagómez et al. (2020) utilises the auxiliary variable implementation based on Møller et al. (2006) to deal with the double intractability problem, but this does not result in satisfactory performance for making posterior inferences in our setting. We thus develop an alternative computational framework to make posterior inferences through approximating the normalising constant using an Importance Sampler. This was inspired by an approach taken in Vitelli et al. (2017), albeit in a different setting with less computational challenges. The resulting modelling framework performs significantly better in making posterior inferences, and is evaluated on simulated data as well as on data studying species of fish competing over sources of food at various different reefs off the coast of Christmas island in the Indo-Pacific Ocean.

Our key contributions in this paper are thus two-fold. First, we propose and evaluate a novel network distance metric, namely the HS distance, that has not been considered in the network literature. Second, we develop and implement a novel Markov Chain Monte Carlo (MCMC) scheme to make posterior inferences from the Spherical Network Family (SNF) model for multiple network data under the proposed HS distance metric. Specifically, we introduce an Importance Sampling (IS) step within a Metropolis-Hastings (MH) algorithm that allows the approximation of the intractable normalising constant of the SNF model within the MH ratio. The resulting method is computationally intensive and thus motivates us to reduce the burden of computing the cycles through training a non-parametric model within the MCMC that predicts the number of cycles in a network based on other network properties easier (and faster) to obtain. This results in a model that can be implemented in a practical setting to learn about relevant features of interest in an ecological study.

The remainder of this article is organised as follows. Section 2 gives the preliminaries for our study, Section 3 describes our proposed metric as well as an ecological application that motivated its derivation. In Section 4 we give an overview of the SNF model and how Lunagómez et al. (2020) address the problem of the intractable normalising constant. In Section 5 we present how we modify the computations to make posterior inferences for the SNF model. Section 6 illustrates performance of the proposed method in a simulation study. Section 7 applies the method to analyse the ecological application studying aggressive interactions between species of fish. Finally Section 8 ends with some concluding remarks.

2 Relevant network properties and preliminaries

We represent a graph by $\mathcal{G} = (V, E)$, with $V = \{1, \ldots, n\}$ denoting the set of $n$ nodes and $E \in \mathcal{E}_n$ denoting the set of edges in $\mathcal{G}$, with $\mathcal{E}_n = \{(i, j) | i, j \in V\}$. We use an $n \times n$ matrix, namely the adjacency matrix, to represent the presence and absence of edges in graph $\mathcal{G}$. 
Thus, the \((i,j)\)th element of the adjacency matrix for a graph with binary edges is,

\[ A_G(i,j) = \begin{cases} 1, & \text{if an edge occurs between nodes } i \text{ and } j, \\ 0, & \text{otherwise}. \end{cases} \]

By \(G_1, \ldots, G_N\) we represent a population of \(N\) graphs, with corresponding adjacency matrices \(A_{G_1}, \ldots, A_{G_N}\). We further assume that the networks in the population are undirected, with no self-loops, and share the same set of \(n\) nodes. We represent the space of graphs with \(n\) nodes by \(\{G_{[n]}\}\), such that \(\{G_{[n]}\} = \{G = (V,E) : |V| = n\}\). Thus the size of the space of undirected, with no self-loops graphs is \(|\{G_{[n]}\}| = 2^{\binom{n}{2}}\).

A way to quantify similarities among networks is through the use of distance metrics which we denote by \(d_G(\cdot,\cdot)\). Two main types are: (a) structural distances that aim to capture similarities on edge-specific local properties of the graphs, and (b) to spectral distances that aim to capture similarities with respect to global properties of the graphs using a spectral representation (Donnat and Holmes (2018)). A well-known structural distance metric is the Hamming distance, that counts the not in common edges and non-edges between two graphs \(G_k\) and \(G_l\) for \(k,l \in \{1,\ldots,N\}\), defined as:

\[ d_H(A_{G_k},A_{G_l}) = \sum_{i,j} \frac{|A_{G_k}(i,j) - A_{G_l}(i,j)|}{n \cdot (n-1)}. \]

Networks are objects that can exhibit complex structures, thus the derivation of network properties such as the degree distribution is important for evaluating their characteristics. Network cycles are known to be crucial in revealing information about their topology (Maugis et al., 2017). A cycle in an undirected network is a sequence of connected nodes in which the only repeated nodes are the first and the last node in the sequence. An illustrative example of an undirected graph with two cycles is presented in Figure 1. We note here that \(\{1-2-6-1\}\) and \(\{1-3-5-4-1\}\) are considered as the same cycle.

3 Ecological Application and proposed metric

Data have been collected on the aggressive interactions among species of fish in different coral reefs, at Christmas Island in the Indo-Pacific ocean (Keith et al. (2018)). We use a network representation, where nodes represent fish species and edges represent aggressive interactions between them. In Figure 2 we present the resulting undirected networks.

In ecology, it is often of interest to identify competition structures among species that
Figure 2: Networks representing fish species interactions at three Christmas Island reefs.

... to make

1https://www.encyclopedia.com/environment/energy-government-and-defense-magazines/ecological-competition

rily on the same resources \(^1\). The formation of cycles in graphs representing interactions among species can reveal such competitive behaviours (Sokhn et al. (2012); Koutrouli et al. (2020)). Hence, a research question arising here is the following: To what extent are cycles formed from the aggressive interactions between fish in the network data?

An appealing way to answer this research question is with the SNF model (Lunagómez et al. (2020)) that infers a representative network in the population, determined through a user-specified distance metric. In addition, the SNF model involves a dispersion parameter that quantifies the level of dissimilarity between the network data and the network representative, with respect to the specified metric. The flexibility in the choice of the distance metric is a key motivating factor for developing a SNF model to analyse the data.

As our interest lies in cycles formed in the network data, we propose a measure that captures information about dissimilarities between the cycles of two networks. Specifically, we propose a Hamming-Symmetric difference (HS) distance metric consisting of two parts:

1. The Hamming distance counting not in common edges/non-edges between two graphs.

2. The symmetric difference between the cycles formed in two graphs, i.e. counting the number of not in common cycles in two graphs.

Hence, a mathematical representation of the constructed distance metric for two graphs \(G_k, G_l\) for \(k, l \in \{1, \ldots, N\}\) is,

\[
d_{HS}(G_k, G_l) = d_H(A_{G_k}, A_{G_l}) + \lambda \cdot |C_{G_k} \Delta C_{G_l}|,
\]

where \(d_H(\cdot, \cdot)\) denotes the Hamming distance, \(C_{G_i}\) denotes the cycles in graph \(i\), \(\Delta\) indicates the symmetric difference and \(\lambda \in \mathbb{R}\) is a weighting factor. In Supplementary material Section 1.1, we show that HS is a distance metric. Under this construction, we encode information about dissimilarities in the structure of the networks, with respect to both their edges and cycles. The tuning of the \(\lambda\) parameter corresponds to how much influence we allow the symmetric difference to have on the total distance. In Supplementary material Section 1.2, we explore the behaviour of the HS distance for various sizes of \(\lambda\) through synthetic data experiments. In the rest of this article, we assume \(\lambda\) to be equal to 1, suggesting equal importance between the Hamming and the Symmetric difference distance.

The specification of the HS distance metric for the SNF model induces significant challenges when adopting the MCMC framework proposed by Lunagómez et al. (2020) to make
posterior inferences with the SNF model. Notably the mixing of chains is very poor with acceptance rates close to zero. In Supplementary material Section 2, we illustrate this with a simulated data example. This motivated us to develop an alternative computational framework to make posterior inferences with the SNF model and details are given in Section 5.

4 Overview of the SNF model

In this section we provide a brief overview of the SNF model proposed in Lunagómez et al. (2020), and why it is a compelling model to consider for this setting. We also highlight some shortcomings with the current implementation which limits its usefulness in our setting.

4.1 Motivation and Model formulation

Lunagómez et al. (2020) develop a model for network data inspired by the form of a Normal distribution. Specifically, they assume an underlying mean network representing the network population and a dispersion parameter denoting the variation of the networks about this mean. They express the mean network in terms of a Fréchet mean, as seen in the studies of Ginestet et al. (2017) and Kolaczyk et al. (2017), and the dispersion parameter in terms of an entropy. Under this construction, they obtain the probabilistic mechanisms that generate data sets of multiple network data which they denote the SNF model.

Specifically, if we assume we have a population of undirected and unweighted graphs $G_1, \cdots, G_N$ then the joint distribution characterised by the SNF model is given by,

$$P(A_{G_1}, \cdots, A_{G_N} | A_{G^m}, \gamma) \propto \exp \left\{ -\gamma \cdot \sum_{i=1}^{N} \phi(d_G(A_{G_i}, A_{G^m})) \right\},$$

where $G^m$ is the Fréchet mean, $d_G(\cdot, \cdot)$ is a distance metric, $\gamma > 0$ is the dispersion, $\phi(\cdot) > 0$ is a monotone increasing function and the model partition function is the reciprocal of

$$Z(A_{G^m}, \gamma) = \sum_{A_G \in \{G_{[n]}\}} \exp \left\{ -\gamma \cdot \phi(d_G(A_G, A_{G^m})) \right\},$$

where $\{G_{[n]}\}$ is the space of $n$-node networks. The parameters $G^m$, and $\gamma$ can thus be seen to relate to the mean and precision parameters in a Normal distribution.

Lunagómez et al. (2020) show the Centered Erdös-Rényi (CER) model is a special case of a SNF model when the Hamming distance metric is used. Under the CER model a population of networks is generated by perturbing the edges of a centroid network $G^m$ using a Bernoulli distribution with probability $\alpha$, as follows:

$$A_G(i, j) | (A_{G^m}(i, j), \alpha) = |A_{G^m}(i, j) - Z(i, j)|,$$

where $G^m$ is the Frechét mean and $Z(i, j)$’s are iid Ber($\alpha$), with $0 < \alpha < 0.5$. The joint distribution of a population of undirected and unweighted $G_1, \cdots, G_N$ graphs is then

$$P(A_{G_1}, \cdots, A_{G_N} | A_{G^m}, \alpha) = \prod_{i=1}^{N} \alpha^{d_H(A_{G^m}, \alpha)} \cdot (1 - \alpha)^{n\alpha(1-\alpha)/2 - d_H(A_{G^m}, A_{G^m})}$$

where $d_H(\cdot, \cdot)$ denotes the Hamming distance metric and $n$ is the number of nodes.
To make inferences, the authors adopt a Bayesian approach. A prior distribution for $\gamma$ is specified with support on $\mathbb{R}^+$. The prior choice and support is strongly related to the specified distance metric. A prior distribution for the network representative $A_{G^m}$ is specified with the same functional form as that of the SNF model. The priors for the parameters of the CER model are specified in a similar manner, with the prior for the representative having the functional form of the CER model. The prior for $\alpha$ in the CER model requires support on $(0, 0.5)$ with a scaled Beta distribution on $(0, 0.5)$ proposed.

4.2 Addressing the intractable normalising constant

Lunagómez et al. (2020) make posterior inferences using a MCMC scheme to draw samples from the posterior distribution based on a Metropolis-Hastings (MH) algorithm. However, the normalising constant of the SNF model, $Z(A_{G^m}, \gamma)$, depends on the parameters of the model. Thus, the normalising constants do not cancel in the Metropolis-Hastings ratio.

To tackle the intractable normalising constants, Lunagómez et al. (2020) apply the Auxiliary Variable technique presented in Møller et al. (2006). Notably, Møller et al. (2006) consider a likelihood of the form,

$$P(y|\theta) = \frac{q_\theta(y)}{Z(\theta)},$$

where $\theta$ denotes the model parameter, $y$ represents the data, $q_\theta(y)$ the unnormalised density, and $Z(\theta)$ is an intractable normalising constant that depends on $\theta$.

They propose the use of an auxiliary variable $x$ that has the same support as that of $y$, with density $f(x|\theta, y)$ to obtain an unbiased estimator of $Z(\theta)$. In light of Importance Sampling, under Møller et al. (2006) $Z(\theta)$ can be written as,

$$Z(\theta) = \mathbb{E}\left[ \frac{q(x|\theta)}{f(x|\theta, y)} \right],$$

where the expectation is taken with respect to the density of the auxiliary variable $x$, $f(x|\theta, y)$. In this regard, they propose sampling $x$ from $P(\cdot|\theta)$ and use the approximation,

$$Z(\theta) \approx \frac{q(x|\theta)}{f(x|\theta, y)}.$$  

Thus, they can substitute the normalising constant $Z(\cdot)$ by its unbiased estimator $q(x|\cdot)/f(x|\cdot, y)$ in the MH acceptance ratio.

The formulation of the Auxiliary Variable Method in the case of the SNF model involves the simulation of a set of auxiliary variables $G^*$, defined on the same state space as the network data $\{G_i\}_{i=1}^N$. Lunagómez et al. (2020) exploit the probabilistic mechanism of the CER model to specify the conditional density $f(A_{G^m_1}, \ldots, A_{G^m_N} | \{G_i\}_{i=1}^N, A_{G^m}, \tilde{\alpha})$ of the auxiliary network variables $G^*_1, \ldots, G^*_N$. Thence, in each iteration of the MH algorithm a new state of both the model parameters and the auxiliary network variables will be proposed, with the latter sampled from a proposal distribution that has the same functional form as the likelihood. Under this formulation, the normalising constants cancel in the MH ratio. For a more detailed description of this MH algorithm see Lunagómez et al. (2020).

A main challenge in implementing the Auxiliary Variable Method for the SNF model is the slow mixing of the chain for $\gamma$. In Supplementary material Section 2 we illustrate this
in a relevant setting. Notably, we see a very low acceptance rate and thus poor mixing. Depending on the distance metric choice, this issue is apparent even for small network sizes.

The occurrence of this phenomenon can be attributed to the discrepancy between the likelihood, the SNF model, and the choice of auxiliary density, the CER model. Depending on the choice of the distance metric for the SNF model, this discrepancy can increase leading to a bad mixing or, in some cases, the chain not exploring the state space at all.

The poor mixing makes this impractical to consider for our setting and motivates our development of an alternative strategy to approximate the normalising constant. The proposed approach greatly improves performance of the MCMC, allowing it to be applied to similar sizes of networks present in the Ecological data set.

5 Proposed Bayesian inference framework for the SNF model using Importance Sampling

To overcome shortcomings of the Auxiliary Variable approach we develop an alternative method to approximate the intractable normalising constant. Specifically, we formulate an Importance Sampling step within our MCMC equivalent to Ratio Importance Sampling (Chen and Shao, 1997). We were motivated by Vitelli et al. (2017) who also use Importance Sampling to make Bayesian inference from the Mallow’s model (Mallows (1957)), a common model for analysing rank data with the same functional form as the SNF model. Frequentist inference may also be possible, with Mardia and Dryden (1999) developing this for the Watson model that also has the same functional form as the SNF model.

A key difference between the Mallow’s model for rank data and the SNF model is that the normalising constant in the latter involves both the representative network and the dispersion parameter, while for the Mallow’s model the normalising constant depends only on the dispersion parameter, for right-invariant distance metrics considered in Vitelli et al. (2017). This allows an off-line approximation of the normalising constant through IS, using a pseudo-likelihood approximation of the target distribution.

Graphs are more complex objects than rank data, due to diverse structures they exhibit such as the formation of communities and motifs, as well as other topological structures revealed by their spectral decomposition. For networks, the right-invariance property does not hold for the majority of distance functions, with different properties governing rank and network data. Thus, approximating the normalising constant of the SNF model is a more challenging scenario. Unlike Vitelli et al. (2017), we formulate an Importance Sampler within our MCMC to give a good approximation to the normalising constant.

5.1 Formulation of IS step for the SNF model

The normalising constant of the SNF model has the following form,

$$ Z(A_{G^m}, \gamma) = \sum_{A_G \in \{G_n\}} \exp\{-\gamma \cdot \phi(d_G(A_G, A_{G^m}))\}, $$

(4)

this involves computing a sum over the space of $n$-node graphs, $\{G_{[n]}\}$. Clearly when $n$ is modest computing this sum exactly becomes impractical. Instead, using ideas from Impor-
tance Sampling (Robert and Casella (2013)) we can rewrite the sum as

$$
\sum_{A^G \in \{G_n\}} \exp\{-\gamma \cdot \phi(d^G(A^G, A^{G_m}))\} = \sum_{A^G \in \{G_n\}} \frac{\exp\{-\gamma \cdot \phi(d^G(A^G, A^{G_m}))\}}{g(A^G)} g(A^G) = \mathbb{E}_g \left[ \frac{\exp\{-\gamma \cdot \phi(d^G(A^G, A^{G_m}))\}}{g(A^G)} \right],
$$

which can then be approximated by drawing a sample of networks $G_1, \ldots, G_K$ from an Importance Sampling (IS) proposal density $g$ and calculating,

$$
\hat{Z}(A^{G_m}, \gamma) \approx \frac{1}{K} \sum_{k=1}^{K} \frac{\exp\{-\gamma \cdot \phi(d^G(A^G_k, A^{G_m}))\}}{g(A^G_k)}.
$$

One advantage of the IS method is the flexibility with specifying the IS density. In this regard, choices of distributions that are easy to sample from are preferred (Robert and Casella (2013)). In our problem, a natural choice of the IS density is the distance-based CER model.

To sample networks from the CER model, we use MCMC, with the density of the CER model with fixed parameters $\tilde{\alpha}$ and $\tilde{A}^{G_m}$ as the target distribution. This sampling scheme was proposed in Lunagómez et al. (2020) to sample network data from the SNF model. As CER is a member of the SNF, we adopt a similar approach to sample from the CER model.

Thus, the estimator in (6) takes the following form under the CER IS density:

$$
\hat{Z}(A^{G_m}, \gamma) \approx \frac{1}{K} \sum_{k=1}^{K} \frac{\exp\{-\gamma \cdot \phi(d^G(A^G_k, A^{G_m}))\}}{\tilde{\alpha}^{d_H(A^G_k, \tilde{A}^{G_m})} (1 - \tilde{\alpha})^{n(n-1)/2} d_H(A^G_k, \tilde{A}^{G_m})},
$$

where $\{A^G_k\}_{k=1}^{K}$ are networks sampled from the CER model with parameters $\tilde{\alpha}$ and $\tilde{A}^{G_m}$.

We determine $\tilde{\alpha}$ and $\tilde{A}^{G_m}$ by fitting the data to the CER model to obtain the posterior mean of $\tilde{\alpha}$ and posterior mode of $\tilde{A}^{G_m}$. In this way, we encode information about the data that may allow a better approximation of the normalising constant. However, we should be cautious with the size of $\tilde{\alpha}$ as for greater sizes of $\tilde{\alpha}$ there is greater variability between the simulated networks and the centroid, resulting in dense simulated networks for which the task of cycle detection under the HS distance metric can be computationally infeasible.

### 5.2 MCMC scheme with IS step

We now describe our computational framework to obtain posterior draws for the SNF model parameters. As seen in Lunagómez et al. (2020), the joint posterior distribution of the centroid $A^{G_m}$ and the dispersion parameter $\gamma$ can be expressed as

$$
P(A^{G_m}, \gamma | G_{\tilde{G}_1}, \cdots, A^{G_N}) \propto \frac{1}{Z(A^{G_0}, \gamma_0)} \exp\{-\gamma_0 \phi(d^G(A^{G_m}, A^{G_0}))\} P(\gamma | \alpha_0).$$

$$
\frac{1}{Z(A^{G_m}, \gamma)^N} \exp\{-\gamma \sum_{i=1}^{N} \phi(d^G(A^G_i, A^{G_m}))\}.
$$
We follow a largely similar scheme to Lunagómez et al. (2020) to make inferences, using Metropolis-Hastings to sample from the joint posterior of the parameters. However, to overcome the double-intractability problem, we approximate the normalising constant within each iteration of the MCMC using the estimator obtained through Importance Sampling, different to the Auxiliary Variable Method adopted by Lunagómez et al. (2020). Notably, we obtain posterior draws from the target distribution in Equation (8), after substituting the normalising constant in the likelihood with its estimate in Equation (7).

To obtain posterior draws for the parameters $A_G$ and $\gamma$, we follow a similar scheme to Lunagómez et al. (2020). Full details are given in Supplementary material Section 3.2.

5.3 Addressing the challenge of cycle calculation

Cycle detection in networks is computationally intensive, even for moderate-sized networks, resulting in computationally expensive algorithms with respect to the time and memory required to run. In our study we perform cycle detection using the R package igraph (Csardi and Nepusz (2006)). If a network is not sparse, the number of paths connecting two nodes can grow exponentially depending on the number of nodes in the graph. Specifically, in the case of a complete graph with $n$ nodes, the time complexity for performing path detection is $O(n!)$ (Csardi and Nepusz (2006)), making calculations infeasible.

Under the MCMC scheme described in Section 5.2, we draw a new IS sample in each iteration of our algorithm to estimate the normalising constant under equation (7). The estimation involves the calculation of the HS distance between each network in the newly drawn IS sample and the corresponding proposed or current centroid, as seen in the nominator of the sum in equation (7). Thus, the cycles present in each network of the IS sample need to be identified, and this is additionally within each iteration of the MCMC, which leads to a computationally heavy algorithm.

To avoid the exact cycle calculation in every importance sample of every iteration of our MCMC, we consider an approximation of the symmetric difference distance between the cycles of two networks. The formulation exploits the idea that other network distance metrics, less computationally intensive to calculate, can be informative for predicting the symmetric difference distance. In this context, various distance metrics can be thought of as covariates in our problem.

There are a range of different frameworks to perform predictions in Statistics and Machine Learning (Yan and Su (2009); Song and Ying (2015); Biau (2012); Friedman et al. (2001)). In our study, we use supervised learning and specifically the xgboost algorithm (Chen and Guestrin (2016)) to predict the symmetric difference of cycles between networks, using the R package xgboost (Chen et al. (2021)). The basis of supervised learning algorithms, such as xgboost, is the use of a training sample to find the values of the parameters that best fit the data, in order to make predictions for a target variable. The good performance of the xgboost along with its fast execution render it appealing for prediction. However, we note here that other prediction methods could have been equally applied.

In our framework, we train the xgboost in every iteration of the MCMC to make accurate predictions for the newly drawn IS sample. To train the xgboost, we use a single training sample of networks for which we calculate the cycles. Thus the cycle detection task is performed only once in our algorithm. Thence, we calculate distances between the training sample of networks and the current or proposed centroid network, and train the model to identify associations between the distance metrics considered as predictors in our problem,
and the symmetric difference distance which is the target variable. Notably, the distance metrics considered as covariates in our problem are the Hamming distance, the Jaccard distance and the centrality-betweenness distance. For a description of the Jaccard and the centrality-betweenness distances see Supplementary material Section 3.3. Lastly, to estimate the normalising constant from the newly drawn IS sample, we obtain the Hamming, the Jaccard and the centrality-betweenness distance between each network in the new IS sample and the current or proposed centroid, and predict the symmetric difference distance using the current trained xgboost. In this way, we avoid calculating cycles for each newly drawn IS sample in every iteration of the MCMC. Algorithm 1 sketched below illustrates the MH algorithm with IS step and xgboost.

| Algorithm 1: Metropolis-Hastings Algorithm with IS step and xgboost |
|---------------------------------------------------------------|
| **Data:** $G_1, \ldots, G_N$  
| **Hyperparameters:** $G_0, \gamma_0, \alpha, \hat{\gamma}^m$ |
| **Initialisation:** Randomly generate $G^{m(0)}, \gamma^{(0)}$. Draw training sample of networks $G^0_1, \ldots, G^0_K \sim \text{CER}(\hat{\gamma}, \hat{\gamma}^m)$ for xgboost and calculate cycles in networks of training sample $G^0_1, \ldots, G^0_K$.  
| **Train xgboost:** Calculate $d_{\text{symm}}(G^*_k, G^{m(0)}), d_{\text{Hamm}}(G^*_k, G^{m(0)}), d_{\text{Jacc}}(G^*_k, G^{m(0)}), d_{\text{centr}}(G^*_k, G^{m(0)})$ and train xgboost using as labels the $d_{\text{symm}}(G^*_k, G^{m(0)}), \gamma^{(0)}$ for $k \in \{1, \ldots, K\}$ (1) |
| **for** $i \leftarrow 1$ to $M$ **do**  
| **MH step with a mixture of kernels:** Update $G^m$ or $\gamma$  
| Sample $v \sim \text{Multinomial}(\xi_1, \ldots, \xi_L)$  
| Depending on the value of $v$ propose $G^{m(i)} \sim q(G^{m(i)}|G^{m(i-1)})$ or $\gamma^{(i)} \sim q(\gamma^{(i)}|\gamma^{(i-1)})$  
| if $G^{m}$ updated then  
| | Train xgboost for proposed centroid $G^{m(i)}$ as per (1)  
| end |
| **Draw new IS sample of networks:** $G^{IS(1)}_1, \ldots, G^{IS(K)}_K \sim \text{CER}(\hat{\gamma}, \hat{\gamma}^m)$.  
| **Predict HS distance:** Calculate $d_{\text{Hamm}}(G^{IS(i)}_k, G^{m(i)}), d_{\text{Jacc}}(G^{IS(i)}_k, G^{m(i)})$ and $d_{\text{centr}}(G^{IS(i)}_k, G^{m(i)})$ and predict $d_{\text{symm}}(G^{IS(i)}_k, G^{m(i)})$ using the trained xgboost of iteration $(i)$, for $k \in \{1, \ldots, K\}$  
| **Estimate Z:** Use equation (7) to estimate normalising constant in posterior $P(G^{m(i)}, \gamma^{(i)}|G_1, \ldots, G_N)$  
| **Calculate MH ratio:** $r = \min\left(1, \frac{P(G^{m(i)}, \gamma^{(i)}|G_1, \ldots, G_N)q(G^{m(i)}|G^{m(i-1)}, \gamma^{(i-1)})q(\gamma^{(i)}|G^{m(i-1)}, \gamma^{(i-1)})}{P(G^{m(i-1)}, \gamma^{(i-1)}|G_1, \ldots, G_N)q(G^{m(i-1)}|G^{m(i-1)}, \gamma^{(i-1)})q(\gamma^{(i-1)}|G^{m(i-1)})}\right)$  
| $u \sim \text{Bernoulli}(r)$  
| if $u = 1$ then  
| | Accept proposals $G^{m(i)}, \gamma^{(i)}$  
| else  
| | Reject proposals $G^{m(i)}, \gamma^{(i)}$  
| end |

6 Simulation study

We empirically evaluate our methodology in a simulated example similar to our Ecological study. Namely, we simulate $N = 5$ network samples sharing $n = 20$ nodes, consider two values of $\gamma = \{0.06, 0.6\}$ and simulate a centroid as seen in Figure 3. The two alternative sizes of $\gamma$ indicate two different levels of variability of the simulated networks from the centroid, as can be seen from the boxplots in Figure 16 in Supplementary material Section 4.1.
We compare the performance of our proposed MCMC algorithm with approximated HS distance and compare its results to those obtained from the MCMC with the exact calculation of the HS. Moreover, we highlight the computational time benefit from applying the xgboost algorithm. For each simulation regime we run our MCMC for 5,000 iterations and obtain an IS sample of $K = 6,000$ networks within each iteration.

Figure 4 presents posterior summaries for $\gamma$ for networks simulated with $\gamma = 0.06$. We see the posterior draws for $\gamma$ are similarly distributed for both the exact and xgboost predictions of the HS distance. For the latter, we note that the posterior distribution covers a wider range of values, and the 50% credible interval encloses the true value of 0.06. This is also seen from the traceplots in Figure 4 that show the posterior samples for $\gamma$ using the predicted HS distance covering a greater range than samples using the exact HS distance.

Figure 5 presents similar summaries for the second simulation with $\gamma = 0.6$. Here, the posterior samples with the exact HS distance are generally closer to the true value of $\gamma$. However, the traceplot shows the chains for the exact and the xgb schemes both have some mixing and stationarity issues. An explanation for the chains’ behaviour here is possible by examining the EDA boxplots obtained in Figure 16 in Supplementary material Section 4.1. We see when the true value of $\gamma$ is in the range $(0.3, 0.8)$, the MCMC chains all propose networks with a similar distribution in their distance from the centroid. This may affect convergence of MCMC chains, due to non-distinguishable regimes of $\gamma$ being explored.

A common result from both MCMC implementations, is that the centroids inferred under each scheme are different from the true centroid by approximately 40 edges as measured by...
Figure 5: Boxplots (left) and traceplots (right) for posterior samples of $\gamma$ in simulation $\gamma = 0.6$ resulting from MCMC using the exact HS distance (red) versus MCMC using the xgboost predicted HS distance (blue). Red dashed line indicates the true value of $\gamma$.

Figure 6: Hamming distance between the posterior mode centroid and the true centroid (y axis) versus the posterior mass of the posterior mode centroid (x axis) for each simulation regime (shapes) and MCMC implementation (colours).

the Hamming distance, and they concentrate low masses for both simulation regimes, as presented in Figure 6.

Lastly, we highlight the significant computational gains using xgboost to predict the HS distance over its exact calculation. Notably, 5,000 iterations of the MCMC with xgboost predictions requires 7 hours to complete, while 5,000 iterations of the MCMC with exact calculation of the HS distance requires 5 days. Thus, the MCMC with xgboost prediction is 16 times faster than the MCMC with the exact calculation of HS distance.

In Supplementary material Section 4.2, we further consider a simulation study for small network sizes with 5 nodes. This allows calculation of the true normalising constant, and so we are able to investigate the performance of our method to an MCMC using the true normalising constant.

Based on our findings here we believe the MCMC framework involving xgboost predictions is an appropriate model to apply to the Ecological data example. In particular, the substantive computational savings make this approach appealing over other methods that would be impractical to use in these settings.
7 Ecological Study

We now analyse the Ecological study data collected at Christmas Island in the Indian Ocean (Keith et al. (2018)). Each network observation represents the aggressive interactions between 18 species of fish at 3 different reefs. Thus our data set consists of $N = 3$ undirected network observations that share the same set of $n = 18$ nodes, as shown in Figure 2 of Section 3. In Supplementary material Section 5 we list the fish species together with their node labels.

We fit the SNF model to obtain posterior draws for the centroid network $G^n_m$ and the dispersion parameter $\gamma$, assuming the HS distance metric that captures information about the networks’ cycles. To fit the SNF model with HS distance, we first tune the prior distributions of the parameters and the IS density. We centre the prior for the centroid at the network observation that minimises the distance from the other network data, being the right network in Figure 2 of Section 3, following Lunagómez et al. (2020). We also specify a Gamma prior distribution for the dispersion parameter $\gamma$. We specify the CER model as the IS density of our algorithm, and sample from it using MCMC sampling. The size of each IS sample is $K = 6,000$ networks, after a burn-in of 1,000 networks.

We run our MCMC with xgboost prediction for 5,000 iterations and obtain the traceplot and histogram of the posterior samples for $\gamma$ in Figure 7. The 5 networks with highest posterior mass for the centroid are shown in Figure 8. We highlight in pink which edges of these posterior samples are also present in the network data, to indicate which inferred edges are also observed in the data.

![Traceplot and Histogram](image)

Figure 7: Left: Traceplot of posterior samples for $\gamma$; Right: Histogram of posterior samples for $\gamma$, when applying the proposed model to make inferences from the ecological data using MCMC with IS and xgboost to predict the HS distance. The red solid line indicates the posterior mean 0.0085, and red dashed lines indicate the 95% credible interval (0.0028, 0.017).

In Figure 7, we observe good mixing of the MCMC chain for $\gamma$. We further notice that the sizes of the posterior draws for $\gamma$ are small, indicating a high dispersion of the data from the posterior centroids inferred. Moreover, the 5 most commonly drawn centroids involve edges that are not observed in the network data, and concentrate small posterior masses. The challenge of making inferences with a single centroid here is due to many not in common cycles amongst the network data. Notably, the middle network in Figure 2 in Section 3 has 1834 cycles while the other two networks contain 0 and 12 cycles only.

To investigate the cycle information captured from the centroid inference, we obtain the 10 most common cycles observed from the posterior centroid draws along with the proportion...
of the posterior centroid samples containing each cycle, and detect whether these cycles are also observed in the network data. The results for the centroids’ cycles are in the left sub-table of Table 1 below. We see most of these cycles are inferred rather than observed in the network data except for the cycle between nodes 1, 15, and 8, which is observed in 16% of the posterior centroid samples. Interestingly, the inferred cycles are present in a high proportion of the posterior samples, indicating that those cycles might be meaningful and merit further investigation.

For comparison we fit the CER model, that only considers the Hamming distance, to the data, to obtain posterior draws for the centroid $G_{CER}^m$ and the dispersion $\alpha$. In Figure 9 we present the posterior centroid $G_{CER}^m$ with highest posterior mass equal to 0.15 and the histogram of posterior samples of $\alpha$. The posterior mean of $\alpha$ is equal to 0.07, indicating low dispersion of the data from the centroid inferred, contrary to what was observed when using the HS distance.

Figure 8: Five highest posterior mass centroids with, from top left to bottom right, 0.027, 0.025, 0.023, 0.021 and 0.019 mass. Pink edges indicate edges also present in the data.

Figure 9: Left: Posterior modal centroid inferred under the CER model Right: Histogram of posterior samples for $\alpha$ with red solid line indicating the posterior mean 0.072, and red dashed lines indicating the 95% credible interval (0.05,0.096).
The high posterior mass of the centroid and the small dispersion inferred indicate that identifying a representative for the fish networks at the Christmas island is not challenging when we only consider information on the edges. In contrast, identifying a representative for the Christmas island data under the SNF model with the HS distance, is more challenging due to the variability in the networks with respect to their cycles.

| SNF model with HS distance | CER model |
|---------------------------|-----------|
| 8-15-14-8                 | 10-15-17-10 | 0.98 | observed |
| 3-12-4-3                  | 1-8-15-1 | 0.95 | observed |
| 5-16-15-10-5              | 5-15-10-11-16-5 | 0.86 | observed |
| 8-17-11-8                 | 5-15-17-10-11-16-5 | 0.85 | inferred |
| 5-17-11-5                 | 10-11-15-10 | 0.7 | observed |
| 9-14-12-9                 | 10-11-15-17-10 | 0.68 | observed |
| 1-15-8-1                  | 5-15-11-16-5 | 0.58 | observed |
| 4-15-10-12-4              | 5-11-10-15-5 | 0.12 | observed |
| 6-18-8-15-13-6            | 5-11-16-5 | 0.12 | inferred |
| 1-8-17-3-1                | 5-11-10-17-15-5 | 0.12 | observed |

Table 1: 10 most common cycles in posterior centroid samples, proportion of times each cycle detected in posterior draws and presence (observed) or absence (inferred) of cycle in the data under the SNF model with HS distance (Left) and the CER model (Right).

To facilitate comparisons with the SNF model with HS distance, in the right sub-table of Table 1, we present the 10 most common cycles detected in the posterior centroid samples drawn under the CER model. We observe that most of these cycles are also observed in the data, in contrast to the SNF model with HS distance where the cycles were inferred. This demonstrates the additional information concerning network cycles that the HS distance captures in the SNF model over the CER model that ignores this property. In addition, under the CER model, the most common cycles are detected in high proportions of the posterior centroid samples which can be attributed to the convergence of the MCMC to a centroid. Under the SNF with HS distance, the most common cycles are detected in lower proportions among the posterior centroid samples, but considering the space of cycles in an 18-node network, these proportions are still significant and more plausible than the implausibly high proportions obtained with the CER model.

Lastly, under the CER model we observe that specific fish species are repeatedly identified in the most common cycles, which are also species associated with the majority of the edges of the data. In contrast, there are a range of species identified in the most common cycles under the SNF model with HS distance, which suggests the model reveals new information from the data. To further investigate, we obtain the contingency table of the counts of each species observed in the most common cycles from the posterior centroid samples under the CER and the SNF model, and perform Fisher’s exact test to investigate any association between the species involved in these cycles and the network model used. The p-value obtained is 0.01 suggesting that at a 5% level there is evidence the occurrence of species in the most common cycles of the posterior centroids is not independent of the model used.
Modelling multiple network data is essential to addressing many applied research questions. Being able to appreciate cyclical properties of networks is of particular interest in ecological studies of aggressive interactions between different species. In this article we proposed a metric that explicitly incorporates networks’ cycles, denoted as the HS distance. We incorporated this metric within the SNF model and developed a computational framework to allow posterior inferences in practical ecological settings, hitherto not possible with the original implementation of the model. We applied our modelling framework to make inferences from ecological data studying aggressive interactions between species of fish and were able to infer cyclical properties that were not possible to detect using a simpler CER model that does not account for cycle information.

While our approach has been shown to have benefits in the analysis of ecological studies, cycles are of interest in many other applied fields such as Neuroscience or Genetics. The HS distance can thus be an informative measure of dissimilarity in a range of other network applications. A key challenge in these settings is dealing with the larger size of networks (number of nodes). Dealing with cycles is already a substantial computational endeavour, and this issue will be exacerbated in large networks. In our setting, we addressed this through machine learning models to approximate the number of cycles based on other network properties easier to calculate. This direction may continue to offer advantages in reducing the computational burden and allowing practical implementation of the model. It would be interesting to explore how our model could be scaled to deal with larger networks and how well the approximation of cycles performs here. Considering alternative strategies to deal with the computational burden of calculating cycles would also be of interest.

The ecological study representing the species interactions also contained edges weights, corresponding to the multiple interactions observed between species of fish. It would be interesting to consider how this feature could be incorporated within our modelling framework. A modification of the Hamming distance in the HS metric would be required to quantify dissimilarities between weighted graphs, with the Frobenius distance an alternative. We would also need to adapt the computational framework to permit sampling of networks from a weighted space of graphs. This would be necessary for both sampling network representatives in the MCMC as well for approximating the normalising constant through Importance Sampling. There is no straightforward solution to addressing this, but if a model could be developed and implemented practically, it would open up the possibility to model a wide range of weighted networks previously not possible with existing methods.

There have been various techniques developed to approximate intractable normalising constants. We implemented an IS that offered substantial advantages over the original Auxiliary Variable method proposed for the SNF model in Lunagómez et al. (2020). It would be interesting to explore whether other approximations might also confer advantages and develop an appreciation for which methods are best suited for the particular setting being considered.

As our desire to analyse more complex data structures increases so do the modelling and computational challenges. Our methodology for incorporating network cycles for statistical modelling and inference of ecological data has opened up an exciting new area within analysis of multiple networks to explore. Accordingly, there is the potential to build on this and address a number of important questions in the field, both theoretical and applied.
SUPPLEMENTARY MATERIAL

The supplement to “Bayesian modelling and computation utilising cycles in multiple network data” contains additional details about our proposed distance metric, methodological framework developed, the simulations performed, and the real data application.

Acknowledgments

The authors gratefully acknowledge Sally Keith for providing the data for this study.

References

Alquier, P., Friel, N., Everitt, R. and Boland, A. (2016), ‘Noisy monte carlo: Convergence of markov chains with approximate transition kernels’, Statistics and Computing 26(1-2), 29–47.

Andrieu, C. and Roberts, G. O. (2009), ‘The pseudo-marginal approach for efficient monte carlo computations’, The Annals of Statistics 37(2), 697–725.

Arroyo, J., Athreya, A., Cape, J., Chen, G., Priebe, C. E. and Vogelstein, J. T. (2019), ‘Inference for multiple heterogeneous networks with a common invariant subspace’, arXiv preprint arXiv:1906.10026.

Atchadé, Y. F., Lartillot, N. and Robert, C. (2013), ‘Bayesian computation for statistical models with intractable normalizing constants’, Brazilian Journal of Probability and Statistics 27(4), 416–436.

Beaumont, M. A. (2003), ‘Estimation of population growth or decline in genetically monitored populations’, Genetics 164(3), 1139–1160.

Biau, G. (2012), ‘Analysis of a random forests model’, The Journal of Machine Learning Research 13, 1063–1095.

Chen, M.-H. and Shao, Q.-M. (1997), ‘On monte carlo methods for estimating ratios of normalizing constants’, The Annals of Statistics 25(4), 1563–1594.

Chen, T. and Guestrin, C. (2016), Xgboost: A scalable tree boosting system, in ‘Proceedings of the 22nd acm sigkdd international conference on knowledge discovery and data mining’, pp. 785–794.

Chen, T., He, T., Benesty, M., Khotilovich, V., Tang, Y., Cho, H., Chen, K., Mitchell, R., Cano, I., Zhou, T., Li, M., Xie, J., Lin, M., Geng, Y. and Li, Y. (2021), xgboost: Extreme Gradient Boosting. R package version 1.3.2.1.

URL: https://CRAN.R-project.org/package=xgboost

Csardi, G. and Nepusz, T. (2006), ‘The igraph software package for complex network research’, InterJournal Complex Systems, 1695.

URL: https://igraph.org
Delmas, E., Besson, M., Brice, M.-H., Burkle, L. A., Dalla Riva, G. V., Fortin, M.-J., Gravel, D., Guimarães Jr, P. R., Hembry, D. H., Newman, E. A. et al. (2019), ‘Analysing ecological networks of species interactions’, *Biological Reviews* **94**(1), 16–36.

Donnat, C. and Holmes, S. (2018), ‘Tracking network dynamics: A survey using graph distances’, *The Annals of Applied Statistics* **12**(2), 971–1012.

Durante, D., Dunson, D. B. and Vogelstein, J. T. (2017), ‘Nonparametric bayes modeling of populations of networks.’, *Journal of the American Statistical Association* .

Everitt, R. G., Johansen, A. M., Rowing, E. and Evdemon-Hogan, M. (2017), ‘Bayesian model comparison with un-normalised likelihoods’, *Statistics and Computing* **27**(2), 403–422.

Everitt, R. G., Prangle, D., Maybank, P. and Bell, M. (2017), ‘Marginal sequential monte carlo for doubly intractable models’, *arXiv preprint arXiv:1710.04382*.

Fan, T., Lü, L. and Shi, D. (2019), ‘Towards the cycle structures in complex network: A new perspective’, *arXiv preprint arXiv:1903.01397*.

Friedman, J., Hastie, T., Tibshirani, R. et al. (2001), *The elements of statistical learning*, Vol. 1, Springer series in statistics New York.

Gelman, A. and Meng, X. (1994), ‘Path sampling for computing normalizing constants: identities and theory’, *University of Chicago Department of Statistics Technical Report* .

Ginestet, C. E., Li, J., Balachandran, P., Rosenberg, S., Kolaczyk, E. D. et al. (2017), ‘Hypothesis testing for network data in functional neuroimaging’, *The Annals of Applied Statistics* **11**(2), 725–750.

Gollini, I. and Murphy, T. B. (2016), ‘Joint modeling of multiple network views’, *Journal of Computational and Graphical Statistics* **25**(1), 246–265.

Han, D., Li, J., Wang, H., Su, X., Hou, J., Gu, Y., Qian, C., Lin, Y., Liu, X., Huang, M. et al. (2017), ‘Circular rna circmto1 acts as the sponge of microrna-9 to suppress hepatocellular carcinoma progression’, *Hepatology* **66**(4), 1151–1164.

Keith, S. A., Baird, A. H., Hobbs, J.-P. A., Woolsey, E. S., Hoey, A. S., Fadli, N. and Sanders, N. J. (2018), ‘Synchronous behavioural shifts in reef fishes linked to mass coral bleaching’, *Nature Climate Change* **8**(11), 986–991.

Kolaczyk, E., Lin, L., Rosenberg, S. and Walters, J. (2017), ‘Averages of unlabeled networks: Geometric characterization and asymptotic behavior’, *arXiv preprint arXiv:1709.02793*.

Koutrouli, M., Karatzas, E., Paez-Espino, D. and Pavlopoulos, G. A. (2020), ‘A guide to conquer the biological network era using graph theory’, *Frontiers in bioengineering and biotechnology* **8**, 34.

Le, C. M., Levin, K., Levina, E. et al. (2018), ‘Estimating a network from multiple noisy realizations’, *Electronic Journal of Statistics* **12**(2), 4697–4740.
Liang, F. (2010), ‘A double metropolis–hastings sampler for spatial models with intractable normalizing constants’, *Journal of Statistical Computation and Simulation* **80**(9), 1007–1022.

Lunagómez, S., Olhede, S. C. and Wolfe, P. J. (2020), ‘Modeling network populations via graph distances’, *Journal of the American Statistical Association* pp. 1–18.

Mallows, C. L. (1957), ‘Non-null ranking models. i’, *Biometrika* **44**(1/2), 114–130.

Mantziou, A., Lunagomez, S. and Mitra, R. (2021), ‘Bayesian model-based clustering for multiple network data’, *arXiv preprint arXiv:2107.03431*.

Mardia, K. and Dryden, I. (1999), ‘The complex watson distribution and shape analysis’, *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* **61**(4), 913–926.

Maugis, P.-A. G., Olhede, S. C. and Wolfe, P. J. (2017), ‘Topology reveals universal features for network comparison’, *arXiv preprint arXiv:1705.05677*.

Meng, X.-L. and Wong, W. H. (1996), ‘Simulating ratios of normalizing constants via a simple identity: a theoretical exploration’, *Statistica Sinica* pp. 831–860.

Mittelbach, G. G. and McGill, B. J. (2019), Species interactions in ecological networks, in ‘Community Ecology’, Oxford University Press, pp. 179–205.

Møller, J., Pettitt, A. N., Reeves, R. and Berthelsen, K. K. (2006), ‘An efficient markov chain monte carlo method for distributions with intractable normalising constants.’, *Biometrika*.

Murray, I., Ghahramani, Z. and MacKay, D. (2012), ‘Mcmc for doubly-intractable distributions’, *arXiv preprint arXiv:1206.6848*.

Newman, M. E. (2018), ‘Estimating network structure from unreliable measurements’, *Physical Review E* **98**(6), 062321.

Nielsen, A. M. and Witten, D. (2018), ‘The multiple random dot product graph model’, *arXiv preprint arXiv:1811.12172*.

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

Peixoto, T. P. (2018), ‘Reconstructing networks with unknown and heterogeneous errors’, *Physical Review X* **8**(4), 041011.

Robert, C. and Casella, G. (2013), *Monte Carlo statistical methods*, Springer Science & Business Media.

Sizemore, A. E., Giusti, C., Kahn, A., Vettel, J. M., Betzel, R. F. and Bassett, D. S. (2018), ‘Cliques and cavities in the human connectome’, *Journal of computational neuroscience* **44**(1), 115–145.

Sokhn, N., Baltensperger, R., Bersier, L.-F., Hennebert, J. and Ultes-Nitsche, U. (2012), Identification of chordless cycles in ecological networks, in ‘International Conference on Complex Sciences’, Springer, pp. 316–324.
Song, Y.-Y. and Ying, L. (2015), ‘Decision tree methods: applications for classification and prediction’, *Shanghai archives of psychiatry* 27(2), 130.

Vitelli, V., Sørensen, O., Crispino, M., Frigessi, A. and Arjas, E. (2017), ‘Probabilistic preference learning with the mallows rank model.’, *The Journal of Machine Learning Research*.

Wang, S., Arroyo, J., Vogelstein, J. T. and Priebe, C. E. (2019), ‘Joint embedding of graphs’, *IEEE transactions on pattern analysis and machine intelligence*.

Yan, X. and Su, X. (2009), *Linear regression analysis: theory and computing*, World Scientific.
Supplement to ”Bayesian modelling and computation utilising cycles in multiple network data”

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*Keywords:* Doubly intractable distributions, Importance Sampling, Object data analysis, Relational data.
In this document we provide supplementary material to the article "Bayesian modelling and computation utilising cycles in multiple network data". In Section 1 we provide more details about our proposed metric introduced in Section 3 of the main article. In Section 2 we provide additional results for the mixing issue arising with the implementation of the Auxiliary Variable technique for the SNF model, and how our methodology overcomes that issue, as discussed in Sections 3 and 4 of the main article. In Section 3, we provide additional details for our proposed MCMC with Importance Sampling (IS) step introduced in Section 5 of the main article. In Section 4 we provide additional details for the simulation study presented in Section 6 of the main article, as well as an additional simulation study for small network sizes. Lastly, in Section 5 we provide additional information about the data discussed in Section 7 of the main article.

1 Additional details for the Proposed HS distance

In this section we prove the HS distance satisfies the properties to be a distance metric. We also illustrate the behaviour of the HS distance through synthetic data experiments.

1.1 Proof HS is a distance metric

The HS measure is the weighted sum of the Hamming distance and the symmetric difference of cycles between two graphs. The Hamming distance is a well-known distance metric, thus, to prove that the HS measure is also a distance metric, we need to prove that the symmetric difference of cycles is a distance metric.

Let $C_n$ be the set of cycles for graphs of size $n$, and each $C_{G_i}, C_{G_j}, C_{G_k} \in C_n$ be the subset of cycles found in graphs $G_i, G_j$ and $G_k$ respectively. Thence, the symmetric difference of the cycles of two graphs is $d_{symm} = |C_{G_i} \Delta C_{G_j}|$. The function $d_{symm} : C_n \times C_n \to [0, \infty)$ is a distance metric if the following conditions are satisfied:

1. $d_{symm}(C_{G_i}, C_{G_j}) = 0 \iff C_{G_i} = C_{G_j}$
2. $d_{symm}(C_{G_i}, C_{G_j}) = d_{symm}(C_{G_j}, C_{G_i})$
3. $d_{symm}(C_{G_i}, C_{G_j}) \leq d_{symm}(C_{G_i}, C_{G_k}) + d_{symm}(C_{G_k}, C_{G_j})$

Conditions 1 and 2 are clearly satisfied. Thus, we need to prove that the triangle inequality holds for the symmetric difference of cycles. The symmetric difference has the following property,

$$C_{G_i} \Delta C_{G_j} = (C_{G_i} \Delta C_{G_k}) \Delta (C_{G_k} \Delta C_{G_j}).$$

It follows that

$$C_{G_i} \Delta C_{G_j} \subseteq (C_{G_i} \Delta C_{G_k}) \cup (C_{G_k} \Delta C_{G_j}) \Rightarrow |C_{G_i} \Delta C_{G_j}| \leq |C_{G_i} \Delta C_{G_k}| + |C_{G_k} \Delta C_{G_j}|.$$

Thus condition 3 is satisfied for the symmetric difference of cycles between graphs.
1.2 Synthetic data experiments for HS distance metric

Inspired by the study of Donnat and Holmes (2018), who explore the properties of various network distance metrics from the network literature, in this simulation study we explore the properties of the HS distance through its application on a set of network observations with diverse structures. Specifically, we simulate network data characterised by different topologies, and obtain distance matrices containing the pairwise distances between the simulated networks. Thence, we analyse the distance matrices obtained in the following ways:

- We map the pairwise distances of the networks in a two dimensional space through a Multidimensional scaling (MDS) projection. This representation allow us to observe whether networks with similar characteristics are identified to be closer to each other with respect to the distance metric specified.

- We obtain the minimum spanning tree graph and apply a Friedman-Rafsky test, as presented in Donnat and Holmes (2018). This hypothesis testing framework allows us to examine whether the distance metric under consideration captures similarities between networks with respect to their structure.

First, we generate network observations under three well-known network models that exhibit diverse structures, similar to the synthetic data experiments presented in Donnat and Holmes (2018). In our study, we consider networks with \( n = 20 \) nodes, motivated by the network sizes of the ecological application. The network models used to simulate network data, along with their parameterisations, are the following:

1. The Erdős-Rényi (ER) model with probability of connection \( p = 0.1 \).
2. The Preferential Attachment (PA) model with power equal to 1.
3. The Stochastic Block Model (SBM) with two equally sized communities of nodes and probability matrix \[
\begin{pmatrix}
0.2 & 0.01 \\
0.01 & 0.3
\end{pmatrix}
\].

For each network model specification, we simulate 10 independent network observations, resulting in a set of \( N = 30 \) networks. We further fix the density of the graphs to be equal to 0.1, so that the variability of the simulated networks originates only from the networks’ structure.

As presented in Section 3 of the main article, the HS distance metric involves a weighting factor \( \lambda \) indicating the importance of the symmetric difference on the overall distance between two networks. In this respect, we consider a range of values for the weighting factor \( \lambda = \{0.1, 0.25, 0.5, 0.75, 1, 1.5, 2, 4, 8\} \), to explore its impact on the distance metric performance. To further understand the behaviour of the HS distance, we also consider two widely used network distance metrics, the Hamming and the Jaccard distance, to serve as a reference for comparing the results obtained from the HS distance. Lastly, we obtain the Symmetric difference distance solely, to observe its behaviour when we do not combine it with the Hamming distance in the HS distance metric.

Figure 1 shows the MDS projections for each distance metric considered, where each dot corresponds to a network observation and the colour of the dots correspond to the network model used to simulate the networks. For both the Hamming and the Jaccard MDS projections, we notice that the networks simulated from the same model are positioned closer...
in the 2-d plane, while for the Symmetric difference of the cycles, the networks are clustered
together irrespectively of the network structure, with some networks placed away from that
center. This finding indicates that it is hard to identify similarities among networks with
respect to their structure, considering solely the Symmetric difference distance.

Figure 1: MDS for the Hamming distance matrix (left), the Jaccard distance matrix (middle)
and Symmetric difference distance matrix (right), for networks generated under the Erdős-
Rényi (ER), the Preferential Attachment (PA) and the Stochastic Block Model (SBM).

Figure 2: MDS for the HS distance matrix for varying sizes of $\lambda$, for networks generated
under the Erdős-Rényi (ER), the Preferential Attachment (PA) and the Stochastic Block Model (SBM)

In Figure 2, we show the MDS projections for the HS distance, for different $\lambda$ weights for
the Symmetric difference part of the metric. We notice that as the impact of the Symmetric difference distance increases over the Hamming distance, the networks tend to cluster together in one group. This is an anticipated result considering the behaviours of the Hamming and Symmetric difference distance independently, as seen in MDS projections in Figure 1. It is worth noting that as $\lambda$ increases, the first networks that start to form a cluster are those simulated from the ER and PA models, while the SBM networks differentiate from that cluster, even for greater $\lambda$ values. This result highlights the importance of combining the Hamming distance with the Symmetric difference to form the HS distance metric, as the Hamming distance captures information about the overall structure of the networks. In addition, the illustration in Figure 2 shows the importance of the weight factor $\lambda$ in the overall behaviour of the HS distance.

We further identify other characteristics of the simulated networks, to investigate whether the distance metrics considered are able to detect similarities among networks with similar characteristics. Network characteristics summarise information about structural properties of the networks on both node and edge level. Maugis et al. (2017) show that two dominant network features that reveal information about a network’s topology are trees and cycles. The latter is also a network characteristic that we aim to capture with the HS distance metric formulated. In this regard, we calculate the number of cycles of all sizes and star-trees of size 4 in the simulated networks, and illustrate the results through the MDS projections obtained from the distance metrics.

Figures 3 and 4 show the MDS projections for the networks, where colours correspond to the number of cycles identified in the networks and shapes correspond to the network model used to simulate the networks. In Figure 3, we observe that the Hamming and the Jaccard distance identify similarities among networks that have less cycles, while networks having between 5 to 25 cycles are not distinguishable. On the other hand, the Symmetric difference is able to distinguish the networks with the largest number of cycles from the rest of the networks. We further notice that the networks with the fewest cycles are those simulated under the PA model, as expected due to their tree-like shape, while the networks simulated under the ER and the SBM enclose varying number of cycles.

For the HS distance metric in Figure 4, we notice that as we increase the size of $\lambda$ the networks with less cycles start to group together, while the networks involving a large number of cycles are still identified as dissimilar to the other networks, as seen from the three networks consistently positioned away from all other networks in the 2-d plane. This is a sensible result if we consider that the more cycles networks have, the greater the possibility for not in common cycles.

We now detect the 4-node star-tree motifs (Figure 5) formed in the simulated networks, and present the results through the MDS projections in Figures 6 and 7. We observe that the Hamming and the Jaccard distance display a similar behaviour with respect to the similarities identified among the networks enclosing varying numbers of star-trees. Overall, we observe that both metrics do not strongly group together networks with similar amount of star-trees. However, we notice that the networks with the largest number of star-trees tend to be identified as more similar, and they are distinguishable from the networks with less star-trees. Instead, the Symmetric difference identifies the networks with the largest number of stars to be very similar, as can be deduced by their overlapping positions in the 2-d plane. This can also be seen with the HS distance metric in Figure 7, where we observe that increasing $\lambda$ leads to the identification of the networks with the largest number of star motifs as very similar, as opposed to the rest of the networks which are more dispersed in the
Figure 3: MDS for the Hamming distance matrix (left), the Jaccard distance matrix (middle) and Symmetric difference distance matrix (right), for networks generated under the Erdős-Rényi (ER), the Preferential Attachment (PA) and the Stochastic Block Model (SBM), with colours corresponding to number of cycles.

Figure 4: MDS for the HS distance matrix for varying sizes of $\lambda$, for networks generated under the Erdős-Rényi (ER), the Preferential Attachment (PA) and the Stochastic Block Model (SBM), with colours corresponding to number of cycles

2-d plane. This finding suggests that the HS distance can detect similarities among networks characterised by many star-tree motifs.

Another informative summary about networks’ topology is the networks’ transitivity which expresses the probability that connected triples in a graph close to form triangles. In Figures 8 and 9, we present the MDS projections with respect to the networks’ transi-
Figure 5: 4-node star-tree motif.

Figure 6: MDS for the Hamming distance matrix (left), the Jaccard distance matrix (middle) and Symmetric difference distance matrix (right), for networks generated under the Erdős-Rényi (ER), the Preferential Attachment (PA) and the Stochastic Block Model (SBM), with colours corresponding to number of stars.

We notice that the Hamming and the Jaccard distance tend to detect similarities between networks having close transitivity probability. However, the Symmetric difference distance does not consistently group together graphs with close transitivity probability, as seen by the networks positioned away from the group of networks forming a cluster.

Alternatively, the HS distance metric appears to identify similarities among graphs with close transitivity probabilities as seen in Figure 9. Specifically, increasing the importance of the Symmetric difference on the overall metric, assists in identifying similarities between networks with small transitivity probability, while simultaneously networks with moderate to higher transitivity also group together. This becomes more prominent for $\lambda = 0.75$ for which we can clearly see networks grouping according to their transitivity.

We now describe the Friedman-Rafsky test performed on the minimum spanning tree induced by the distance matrices, as presented in Donnat and Holmes (2018). Under this framework we want to test whether the distance metrics are able to identify groups of networks with respect to their structure. Thus, in our case we have three different groups corresponding to the three different network models used to simulate the networks. By performing this test we are able to quantify the uncertainty of what we observed from the MDS projections.

As commented above, to perform the Friedman-Rafsky test we first obtain the minimum
Figure 7: MDS for the HS distance matrix for varying sizes of $\lambda$, for networks generated under the Erdős-Rényi (ER), the Preferential Attachment (PA) and the Stochastic Block Model (SBM), with colours corresponding to number of stars.

Figure 8: MDS for the Hamming distance matrix (left), the Jaccard distance matrix (middle) and Symmetric difference distance matrix (right), for networks generated under the Erdős-Rényi (ER), the Preferential Attachment (PA) and the Stochastic Block Model (SBM), with colours corresponding to transitivity measure.

spanning tree (MST) resulting from a distance matrix. The minimum spanning tree is a connected graph with nodes representing networks, and edges connecting networks with the greatest similarities, such that no cycles are being formed. Figures 10 and 11 show the minimum spanning trees obtained for the Hamming, the Jaccard, the Symmetric difference and the HS distance matrices, for $\lambda = \{0.25,1,2\}$ indicatively. The colours of the graphs’
Figure 9: MDS for the HS distance matrix for varying sizes of $\lambda$, for networks generated under the Erdős-Rényi (ER), the Preferential Attachment (PA) and the Stochastic Block Model (SBM), with colours corresponding to transitivity measure.

nodes correspond to the three different network models. We observe that the minimum spanning trees obtained for the Hamming, the Jaccard and the HS distance, mostly connect graphs simulated under the same network model, while this is clearly not the case for the Symmetric difference distance.

We further investigate this by performing a Friedman-Rafsky test in the following way. First, we derive the test statistic for our sample, which is the number of edges connecting graphs of the same group (network model), for each minimum spanning tree. Then, we construct the sampling distribution of the test statistic by obtaining 50,000 permutations of the node labels of each minimum spanning tree graph, while keeping the graph’s topology fixed. Thence we obtain 50,000 graphs from the node label permutation, and for each graph we calculate the number of edges connecting graphs of the same group. This give us the probability of seeing a test statistic at least as extreme as the one observed, namely the p-value of our test. If the p-value is significantly small, then we can claim that there is evidence suggesting that the corresponding distance metric groups together graphs simulated from the same network model.

In Table 1, we report the p-values obtained under the Friedman-Rafsky test, formulated for the minimum spanning trees of the Hamming, the Jaccard and the HS distance for $\lambda = \{0.25, 1, 2\}$. We comment here that it is not meaningful to obtain the Friedman-Rafsky test for the minimum spanning tree of the Symmetric difference distance, as any label permutation would result in the same test statistic due to the graph’s topology seen in Figure 10 (right). We observe that the p-values derived for all the distance metrics are statistically significant, except for the HS distance with $\lambda = 2$. This result supports the findings from the MDS projections which showed that the Hamming and the Jaccard are able to detect similarities among networks of the same group. Moreover, the p-values obtained for various $\lambda$ values of
Figure 10: MST for the Hamming distance matrix (left), the Jaccard distance matrix (middle) and the Symmetric difference distance matrix (right).

Figure 11: MST for the HS distance matrix with $\lambda = 0.25$ (left), $\lambda = 1$ (middle) and $\lambda = 2$ (right).

the HS distance indicate the impact of the weight on the overall behaviour of the HS distance. Notably, we observe that the HS distance with $\lambda = 0.25$ and 1 is able to detect similarities among networks belonging in the same group.

| Distance metric | FR p-values |
|-----------------|-------------|
| Hamming         | 0.0000      |
| Jaccard         | 0.0000      |
| HS $\lambda = 0.25$ | 0.0001 |
| HS $\lambda = 1$  | 0.0732      |
| HS $\lambda = 2$  | 0.2584      |

Table 1: p-values for Friedman-Rafsky test applied on the MSTs for the Hamming, the Jaccard and the HS distance.
2 Additional details for Auxiliary Variable Technique for the SNF model

In this Section we demonstrate the mixing issue that arises with MCMC chains using the Auxiliary Variable method (Møller et al. (2006)) for the SNF model with HS distance, through the use of a specific simulated data example. We further demonstrate the improvement in the mixing of the chain after the implementation of our proposed MCMC scheme with IS step, for the same simulated data example.

To illustrate the mixing issue, we first simulate a population of $N = 50$ networks, with $n = 5$ nodes from the SNF model with HS distance and parameters $\gamma = 0.6$ and centroid $G^m$ as seen in Figure 12.

![Figure 12: 5-node centroid $G^m$ generated for simulated data example.](image)

We apply the MCMC scheme with Auxiliary Variable method proposed in Lunagómez et al. (2020) on the simulated network data to make inferences for the SNF model parameters. Figure 13 shows the traceplot for the dispersion parameter $\gamma$, after running the MCMC for 10,000 iterations with no burn-in.

![Figure 13: Traceplot of $\gamma$ for 10,000 iterations of the MCMC with Auxiliary Variable method applied on the simulated population of 5-node networks.](image)

To facilitate comparisons, we apply our MCMC scheme with IS step on the same simulated network data, and present the traceplot for the dispersion $\gamma$ for 10,000 iterations of the MCMC and no burn-in in Figure 14. From the figures we notice a significant improvement in the mixing of the MCMC chain for $\gamma$ under our proposed MCMC scheme with IS step.
3 Additional details for Proposed Bayesian inference framework for the SNF model using Importance Sampling

In this section we present additional details for the proposed methods discussed in Section 5 of the main article.

3.1 Sampling network data from the CER model

To sample networks from the CER model with fixed parameters $\tilde{A}_G$ and $\tilde{\alpha}$, we use a MH algorithm similarly to the SNF sampling scheme proposed in Lunagómez et al. (2020). In every iteration of the algorithm, we propose a new network with adjacency $A_g^{(prop)}$ by perturbing the edges of the current network with adjacency $A_g^{(curr)}$ in the following way:

$$A_g^{(prop)}(i, j) = \begin{cases} 1 - A_g^{(curr)}(i, j), \text{ with probability } \omega \\ A_g^{(curr)}(i, j), \text{ with probability } 1 - \omega \end{cases},$$

and accept it with probability,

$$\min \left\{ 1, \frac{\tilde{\alpha}^{d_H(A_g^{(prop)}, \tilde{A}_G)}(1 - \tilde{\alpha})^{n(n-1)} - d_H(A_g^{(prop)}, \tilde{A}_G)}{\tilde{\alpha}^{d_H(A_g^{(curr)}, \tilde{A}_G)}(1 - \tilde{\alpha})^{n(n-1)} - d_H(A_g^{(curr)}, \tilde{A}_G)} \right\}.\tag{2}$$

We note here that under this proposal scheme the proposal distribution cancels from the MH ratio. Thus, in the nominator and denominator of the MH ratio we only have the density of the CER model, being our target distribution.

3.2 MCMC scheme with IS step

We now present additional details on the inferential scheme used to obtain draws from the posterior distributions of the parameters of the SNF model, as discussed in Section 5.2 of the main article. Notably, we update the adjacency matrix of the centroid $A_G$ using either of the following two proposals,
(I) We perturb the edges of the current centroid $A_{G_m}^{(curr)}$ as follows:

$$
A_{G_m}^{(prop)}(i,j) = \begin{cases} 
1 - A_{G_m}^{(curr)}(i,j), & \text{with probability } \omega \\
A_{G_m}^{(curr)}(i,j), & \text{with probability } 1 - \omega
\end{cases}
$$

(II) We propose a new network representative $A_{G_m}^{(prop)}$, with each edge of the proposed representative being drawn independently from a Bernoulli distribution with parameter $\frac{1}{N} \sum_{i=1}^{N} A_{G_i}(i,j)$, where $\{A_{G_i}\}_{i=1}^{N}$ denoting the $N$ observed networks.

Under case (I), we accept the proposed network representative $A_{G_m}^{(prop)}$ with probability

$$
\min \left\{ 1, \frac{\exp \left\{-\gamma_0 d_G(A_{G_m}^{(prop)}, A_{G_0})\right\}}{\exp \left\{-\gamma_0 d_G(A_{G_m}^{(curr)}, A_{G_0})\right\}} \cdot \frac{\sum_{i=1}^{N} exp\{-\gamma(A_{G_i}, A_{G_m}^{(prop)})\}}{\sum_{i=1}^{N} exp\{-\gamma(A_{G_i}, A_{G_m}^{(curr)})\}} \cdot \frac{\frac{1}{N} \sum_{i=1}^{N} d_G(A_{G_i}, A_{G_m}^{(prop)})}{\frac{1}{N} \sum_{i=1}^{N} d_G(A_{G_i}, A_{G_m}^{(curr)})} \cdot Q(A_{G_m}^{(curr)} | A_{G_m}^{(prop)}) \right\},
$$

while under case (II), we accept the proposed network representative $A_{G_m}^{(prop)}$ with probability

$$
\min \left\{ 1, \frac{\exp \left\{-\gamma_0 d_G(A_{G_m}^{(prop)}, A_{G_0})\right\}}{\exp \left\{-\gamma_0 d_G(A_{G_m}^{(curr)}, A_{G_0})\right\}} \cdot \frac{\sum_{i=1}^{N} exp\{-\gamma(A_{G_i}, A_{G_m}^{(prop)})\}}{\sum_{i=1}^{N} exp\{-\gamma(A_{G_i}, A_{G_m}^{(curr)})\}} \cdot \frac{\frac{1}{N} \sum_{i=1}^{N} d_G(A_{G_i}, A_{G_m}^{(prop)})}{\frac{1}{N} \sum_{i=1}^{N} d_G(A_{G_i}, A_{G_m}^{(curr)})} \cdot Q(A_{G_m}^{( propel)} | A_{G_m}^{(curr)}) \right\},
$$

We note here that the proposal distribution under case (I) is symmetric, and thus it cancels out from the Metropolis ratio, while under case (II) the proposal distribution $Q(A_{G_m}^{(prop)} | A_{G_m}^{(curr)})$ does not cancel.

Accordingly, we use a mixture of $K$ random walks to propose values for the dispersion parameter $\gamma$, as follows:

1. Draw a uniform random variable $u \sim \text{Unif}(-\nu_k, \nu_k)$, with k indicating the $k^{th}$ proposal.

2. Perturb the current state $\gamma^{(curr)}$ by the uniform random variable drawn, $y = \gamma^{(curr)} + u$.

3. The newly proposed value for $\gamma$ is $\gamma^{(prop)} = \begin{cases} y, & \text{if } y > 0 \\
- y, & \text{if } y < 0
\end{cases}$

which we accept with probability

$$
\min \left\{ 1, \frac{\sum_{i=1}^{N} exp\{-\gamma(A_{G_i}, A_{G_m}^{(prop)})\}}{\sum_{i=1}^{N} exp\{-\gamma(A_{G_i}, A_{G_m}^{(curr)})\}} \cdot P(\gamma^{(prop)} | \alpha_0) \right\},
$$

Under this scheme, in each iteration of the MCMC algorithm, we draw a new sample from the IS density to calculate $\hat{Z}$ in the nominator and denominator of the MH ratio, as detailed in Sections 5.2 and 5.3 of the main article.
3.3 Other network distance metrics

We now present the Jaccard and the centrality-betweenness distances considered as covariates for the xgboost algorithm presented in Section 5.3 of the main article, to predict the HS distance between graphs in each iteration of the MCMC.

The **Jaccard distance** counts the not in common edges and non-edges between two graphs, accounting for the number of edges present in the graphs under comparison, using a normalisation with respect to the union of their edges, defined as:

\[
d_J(G, \tilde{G}) = \frac{\sum_{i,j} |A_G(i, j) - A_{\tilde{G}}(i, j)|}{\sum_{i,j} \max(A_G(i, j), A_{\tilde{G}}(i, j))}.
\]

As discussed in Donnat and Holmes (2018), the centrality-betweenness dissimilarity measure for two graphs $G$ and $\tilde{G}$, quantifies changes between graphs with respect to the betweenness of the graphs’ nodes, i.e. the centrality of the nodes in each graph. Specifically, the centrality-betweenness of node $i$, denoted by $c_i$, measures the number of shortest paths going through node $i$. Thus, the centrality-betweenness distance between graphs $G$ and $\tilde{G}$ is

\[
d(G, \tilde{G}) = \sqrt{\sum_{i=1}^{n} (c_i^G - c_i^{\tilde{G}})^2}.
\]

4 Additional details for Simulation study

In this section we discuss additional details for the simulation study presented in Section 6 of the main article. We further present a simulation study for 5-node networks that allows the comparison of our methods to the case under which the true normalising constant is known.

4.1 Behaviour of SNF model with HS distance

We now explore the behaviour of the SNF model when specifying the HS distance metric by conducting Exploratory Data Analysis (EDA). In this respect, we simulate network populations from the SNF model with centroid $G^0$ presented in Figure 15 and various sizes of $\gamma_0$, and obtain the distances between the simulated networks and the centroid. To simulate the network populations we use an MH algorithm, as proposed in Lunagómez et al. (2020). Figure 16 shows the distribution of the distance obtained for each size of $\gamma_0$.

From the functional form of the SNF model we expect that as the dispersion $\gamma_0$ increases, the distance between the simulated network data and the centroid $G^0$ will decrease. Nonetheless, different distance metric specifications will reveal different relationships between the expected distance $\mathbb{E}[d(G, G^0)]$ and the dispersion $\gamma_0$. For the case of the HS distance, the boxplots reveal that for $\gamma_0$ ranging from 0.2 to 1, there is not a significant change in the distribution of the distance.
4.2 Simulation study for 5-node networks

In this section we investigate the performance of our algorithm in inferring the model parameters, for small networks sizes. Specifically, we consider networks with 5 nodes, as the space of graphs for this size of networks $\{G_n\}$ encompasses $2^{10} = 1024$ graphs, rendering the calculation of the true normalising constant feasible. This is an important condition in order to investigate the performance of our MCMC algorithm with the IS step, as it enables us to compare its results against the results obtained from the implementation of an MCMC algorithm with the true normalising constant calculated within the MH ratio.

Similarly to the previous section, we conduct EDA by sampling networks from the SNF model with HS distance for various $\gamma_0$ sizes and fixed centroid $G^0$ as seen in Figure 12.

Under the HS distance metric specification in Figure 17, we observe that the distances between the simulated network data and the centroid are close to 0 for $\gamma = 1.6$. Thus, network data simulated for $\gamma_0 > 1.6$ are very close to the centroid, resulting in limited variability in the network population generated for those regimes. Considering the EDA results, we set up our simulation study for $\gamma = \{0.01, 0.6, 1.1, 1.6\}$, to investigate the performance of our method in inferring the model parameters for a range of network populations, with respect to their variability from the centroid. In addition, we consider two sample sizes $K$ for the IS step, equal to 2000 and 4000, to explore the effect of the IS sample size when making inferences for the 5-node network scenario. In Table 2, we present the simulation regimes considered for the HS distance metric for the 5-node networks.

We generate network data for each simulation regime specified and fit them to the SNF model under two different MCMC schemes, (i) our proposed MCMC scheme with IS step,
Figure 17: Distribution of the HS distance between networks generated from the SNF($\mathcal{G}^0, \gamma_0$) for various sizes of $\gamma_0$, for 5-node networks.

Table 2: Simulation regimes for 5 node networks for the HS distance metric.

| n | N   | K       | $\gamma$ |
|---|------|---------|----------|
| 5 | 5    | 2000    | 0.01     |
| 5 | 5    | 4000    | 0.01     |
| 5 | 5    | 2000    | 0.6      |
| 5 | 5    | 4000    | 0.6      |
| 5 | 5    | 2000    | 1.1      |
| 5 | 5    | 4000    | 1.1      |
| 5 | 5    | 2000    | 1.6      |
| 5 | 5    | 4000    | 1.6      |
explore the same region of values for $\gamma$, close to its true value.

Figure 18: Posterior distribution of $\gamma$ for simulation regimes presented in Table 2, after the MCMC scheme with IS step and the MCMC scheme with the calculation of the true normalising constant. Red dashed lines indicate the true values of $\gamma$.

We investigate the performance of the MCMC with IS step in inferring the centroid network $G^m$, by obtaining the posterior mode from the MCMC draws for $G^m$, calculating the posterior mass that the mode concentrates, and computing the Hamming distance between the posterior mode and the true centroid to detect how accurately the centroid has been inferred. We summarise the results in Figure 20.

Firstly, we note that both our proposed MCMC scheme with IS step, and the MCMC with the true normalising constant calculated, perform similarly for all size of $\gamma$. However, for $\gamma = 1.6$ we observe a difference in the posterior masses that the modes concentrate under each MCMC scheme. For the regime of $\gamma = 0.01$ corresponding to the populations of networks with the greatest variability from the centroid, we notice that the centroid is not fully identified and the posterior modes concentrate low masses for both MCMC schemes. On the other hand, for the remaining simulation regimes of $\gamma$, the true centroid is accurately inferred, with the posterior modes having a Hamming distance from the true centroid equal to 0 and 1.
Figure 19: Traceplots for $\gamma$ for simulation regimes presented in Table 2 with sample size $N = 5$, after the MCMC scheme with IS step and the MCMC scheme with the calculation of the true normalising constant.

Figure 20: Hamming distance between the posterior mode centroid and the true centroid (y axis) versus the posterior mass of the posterior mode centroid (x axis) for various $\gamma$ sizes, number of importance samples $K = 2000$, network population size $N = 5$, and two alternative MCMC schemes.
5 Additional details for Real data

In Table 3, we present the 18 fish species recorded at three different reefs of Christmas Island, considered in Section 7 of the main article, along with their node labels.

| Fish Species | Label |
|--------------|-------|
| auriga       | 1     |
| baronessa    | 2     |
| citrinellus  | 3     |
| ephippium    | 4     |
| guttatissimus| 5     |
| kleinii      | 6     |
| lineolatus   | 7     |
| lunula       | 8     |
| lunulatus    | 9     |

| Fish Species | Label |
|--------------|-------|
| meyeri       | 10    |
| ornatissimus | 11    |
| punctatofasciatus | 12 |
| rafflesii    | 13    |
| speculum     | 14    |
| trifascialis | 15    |
| trifasciatus | 16    |
| unimaculatus | 17    |
| vagabundus   | 18    |

Table 3: Node labels assigned to species of fish at Christmas Island.

References

Donnat, C. and Holmes, S. (2018), ‘Tracking network dynamics: A survey using graph distances’, *The Annals of Applied Statistics* **12**(2), 971–1012.

Lunagómez, S., Olhede, S. C. and Wolfe, P. J. (2020), ‘Modeling network populations via graph distances’, *Journal of the American Statistical Association* pp. 1–18.

Maugis, P.-A. G., Olhede, S. C. and Wolfe, P. J. (2017), ‘Topology reveals universal features for network comparison’, *arXiv preprint arXiv:1705.05677*.

Møller, J., Pettitt, A. N., Reeves, R. and Berthelsen, K. K. (2006), ‘An efficient markov chain monte carlo method for distributions with intractable normalising constants.’, *Biometrika*.