Inferring community characteristics in labelled networks

Lawrence Tray
Department of Engineering
University of Cambridge
lpt30@cam.ac.uk

Ioannis Kontoyiannis
Statistical Laboratory, DPMMS
University of Cambridge
ik355@cam.ac.uk

Abstract

Labelled networks form a very common and important class of data, naturally appearing in numerous applications in science and engineering. A typical inference goal is to determine how the vertex labels (called features) affect the network's graph structure. A standard approach has been to partition the network into blocks grouped by distinct values of the feature of interest. A block-based random graph model – typically a variant of the stochastic block model (SBM) – is then used to test for evidence of asymmetric behaviour within these feature-based communities. Nevertheless, the resulting communities often do not produce a natural partition of the graph. In this work we introduce a new generative model, the feature-first block model (FFBM), which is more effective at describing vertex-labelled undirected graphs and also facilitates the use of richer queries on labelled networks. We develop a Bayesian framework for inference with this model, and we present a method to efficiently sample from the posterior distribution of the FFBM parameters. The FFBM's structure is kept deliberately simple to retain easy interpretability of the parameter values. We apply the proposed methods to a variety of network data to extract the most important features along which the vertices are partitioned. The main advantages of the proposed approach are that the whole feature-space is used automatically, and features can be rank-ordered implicitly according to impact. Any features that do not significantly impact the high-level structure can be discarded to reduce the problem dimension. In cases where the vertex features available do not readily explain the community structure in the resulting network, the approach detects this and is protected against over-fitting. Results on several real-world datasets illustrate the performance of the proposed methods.

1 Introduction

A somewhat surprising property of many real-world networks is that they exhibit strong community structure. In other words, each node will often belong to a cluster of densely connected nodes. There is high interest in recovering the latent communities from the observed graphs. The inferred communities can be exploited for compression algorithms [1] or used for link prediction in incomplete networks [4] to name but a few applications.

We restrict our analysis to labelled networks. These are graphs where we additionally have information about the properties of each vertex. We shall refer to these vertex properties as features. One of the most common questions we can ask of labelled networks is whether a given vertex feature has an impact on the structure of the graph. To answer this question from a Bayesian perspective we must use a random graph model; the most common form is the stochastic block model (SBM) [10]. This is a latent variable model where each vertex belongs to a single block and the probability two nodes are connected depends only on the block memberships of each. There have been many variants to this model; the most popular are the mixed-membership stochastic block model (MMSBM) [2] and the

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overlapping stochastic block model (OSBM) [20]. Effectively, these just extend the model to allow each vertex to belong to multiple blocks simultaneously.

However, a major drawback of these graphical models as applied to labelled networks is that they do not automatically include vertex features in the random graph generation process. Approaches based on graph neural networks [9] that utilise vertex features have been developed but these lack the easy interpretability of the simpler models.

To analyse a labelled network using one of the simple SBM variants, a typical inference procedure would be to partition the graph into blocks grouped by distinct values of the feature of interest. The associated model can then be used to test for evidence of heterogeneous connectivity between the feature-grouped blocks. Nevertheless, this approach is limited in that it can only consider one feature at a time; this leaves any conclusions drawn highly vulnerable to the presence of confounding variables. Furthermore, considering each feature separately makes it difficult to rank order the features by magnitude of impact. Lastly, the feature-grouped blocks are often an unnatural partition of the graph, leading to a poor model fit. We would instead prefer to partition the graph into its most natural blocks and then find which of the available features – if any – best predict the resulting partition.

With these desiderata in mind, we present a novel framework for modelling labelled networks, which we call the feature-first block model (FFBM). This can be thought of as an extension of the SBM to labelled networks. In the FFBM, we use the features first to generate the latent block membership for each vertex. The latent block membership is therefore a stepping stone rather than a starting point in our model. We go on to present an efficient algorithm for sampling from the parameters of the feature-to-block generator. We can interpret the sampled FFBM parameters to determine which features have the largest impact on overall graphical structure. Any features found to be irrelevant can be discarded as a form of dimensionality reduction.

2 Preliminaries

We first need a model for community-like structure in a network. For this we adopt the stochastic block model (SBM) - widely used across academia. The premise is that each node in the graph belongs to a unique community called a block. The probability that two nodes are connected depends only on the block memberships of each. Graphs drawn from the SBM ensemble exhibit community structure. Specifically, we will use the microcanonical variant of the SBM, proposed by Peixoto [15]. To allow for degree-variability between members of the same block, we must choose the degree-corrected formulation of the SBM (DC-SBM).

Definition 2.1 (Microcanonical DC-SBM) *Let $N \in \mathbb{Z}^+$ denote the number of vertices in an undirected graph. The block memberships are encoded by a vector $b \in [B]^N$,[1] where $B \in \mathbb{Z}^+$ is the number of non-empty blocks. Let $e \in (\mathbb{Z}_0^+)^{N\times N}$ be the matrix of edge counts between blocks. e_{rs} is then the number of edges from block r onto block s – or twice that number if $r = s$. For undirected graphs, e is symmetric. Let $k \in (\mathbb{Z}_0^+)^N$ be a vector denoting the degree sequence of the graph. k_i is then the degree of vertex i.*

For the degree-corrected stochastic block model (DC-SBM), we say that the graph's adjacency matrix $A \in \{0,1\}^{N\times N}$ is generated as follows:

$$A \sim \textit{DC-SBM}_{MC}(b, e, k) \tag{1}$$

Where edges are placed uniformly at random but respecting the constraints imposed by e, b and k – hence why this formulation is given the microcanonical moniker. Specifically, A must satisfy the following:

$$e_{rs} = \sum_{i,j\in[N]} A_{ij}\mathbb{1}\{b_i = r\}\mathbb{1}\{b_j = s\} \quad \forall r, s \in [B] \quad \textit{and} \quad k_i = \sum_{j\in[N]} A_{ij} \quad \forall i \in [N] \tag{2}$$

The additional parameters N and B are omitted as they can be inferred from the shapes of b and e.

[1] We introduce the notation $[K] \coloneqq \{1, 2 \dots K\}$ to compactly define a set of K indices. Clearly, $[K]$ is only defined for $K \in \mathbb{Z}^+$.

3 Feature-first block model

In this section we propose a novel generative model for labelled networks. As before, we let N denote the number of nodes. We define the vector $x_i \in \mathcal{X}^D$ as the feature vector for the i'th vertex. Each vertex has D total features and we assume all entries take values from the same set $\mathcal{X}$. For the datasets we analyse, we deal with binary feature flags so $\mathcal{X} = \{0, 1\}$. The feature vectors $\{x_i\}_{i=1}^N$ may be compactly subsumed into the feature matrix $X \in \mathcal{X}^{N \times D}$.

The proposed generative model (which we call the feature-first block model - FFBM) is given in figure 1. First, we start with the feature matrix X and probabilistically generate a vector of block memberships b. The parameters of this step are encapsulated by θ. Each feature vector x_i is treated independently and used to generate the corresponding block membership b_i. Each entry $b_i \in [B]$ where B is the number of blocks and a constant in our model. We choose a single softmax layer to model $p(b_i|x_i, \theta)$. More complex models are possible but then deriving meaning from the inferred parameter distributions is more difficult. Summarising, we write $p(b|X, \theta)$ as follows:

$$p(b|X,\theta) = \prod_{i=1}^{N} p(b_i|x_i,\theta) = \prod_{i=1}^{N} \phi_{b_i}(x_i;\theta) = \prod_{i=1}^{N} \frac{\exp\left(w_{b_i}^T \tilde{x}_i\right)}{\sum_{k=1}^{B} \exp\left(w_k^T \tilde{x}_i\right)} \tag{3}$$

Where $\tilde{x} \coloneqq [x_1, x_2, \dots x_D, 1]^T$ is an augmented version of x that allows for a bias term. The parameter vector θ for this stage contains of the all the weight vectors $\theta = \{w_k\}_{k=1}^B$. Each w_k has dimension $D + 1$. We could instead write the parameters θ as a $B \times (D + 1)$ matrix of weights W; this form has computational benefits as then $z_i \coloneqq W\tilde{x}_i$ is the input to the softmax activation function.

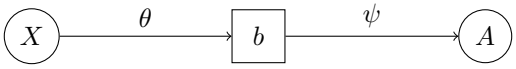


Figure 1: Feature-first block model

Once the block memberships b have been generated, we then draw the graph A from the microcanonical DC-SBM (equation 4) with additional parameters encapsulated by $\psi = \{e, k\}$. In a slight abuse of notation we denote the inter-block edge count matrix with $e = \psi_e$ and the degree sequence $k = \psi_k$ to make explicit that these parameters are contained in ψ.

$$A \sim \text{DC-SBM}_{\text{MC}}(b, \psi_e, \psi_k) \tag{4}$$

3.1 Prior selection

Before performing any inference, we must specify priors on θ and ψ. For θ it seems sensible to choose a Gaussian prior, with zero mean and variance matrix $\sigma_\theta^2 I$ such that each element of θ is independent and distributed like $\sim \mathcal{N}(0, \sigma_\theta^2)$. In vector form, the prior for θ is therefore:

$$p(\theta) = \mathcal{N}\left(\theta; 0, \sigma_\theta^2 I\right) \tag{5}$$

We will see that this form of prior is equivalent to a regularisation term in neural network training that penalises extreme weight magnitudes. For $\sigma_\theta^2 \to \infty$ this becomes an uninformative uniform prior.

In our model, the block memberships vector b is an intermediate latent variable and so we are not free to choose a prior for it. Nevertheless, as far as inference on the right-hand-side of figure 1, we regard $p(b|X)$ as a pseudo-prior on b. We can show (appendix A.2) that our choice of prior for $p(\theta)$ in equation 5 leads to a uniform $p(b|X)$ in equation 6.

$$p(b|X) = \int p(b|X,\theta)p(\theta)d\theta = B^{-N} \tag{6}$$

This is a uniform distribution that only depends on the number of blocks B. This is an enormously important simplification as evaluating $p(b|X)$ does not require knowing the exact value X takes and can be performed without an expensive Monte-Carlo integration over the θ-domain. Peixoto [15] proposes careful choices for the additional microcanonical SBM parameters ψ which we adopt. Peixoto's idea is to write the joint prior on (b, e, k) as a product of conditionals $p(b, e, k) =$

$p(b)p(e|b)p(k|e,b) = p(b)p(\psi|b)$. For our purposes we must insert a conditioning on X, to form our pseudo-prior for b and ψ, to give equation 7.

$$p(b, \psi|X) = p(b|X)p(\psi|b, X) = p(b|X)p(\psi|b) \tag{7}$$

Where the simplification is made apparent by noting $(\psi \perp\!\!\!\perp X)|b$. We then borrow the priors proposed by Peixoto [15] for $p(\psi|b)$ to complete our model. Please refer to appendix A.1 for the exact form of $p(\psi|b)$. All that concerns us is that we have a form which is computable.

4 Inference

Now that we have defined the FFBM, we wish to leverage it to perform inference. Suppose we are presented with a vertex-labelled graph (A, X); the goal is to draw samples for θ according to the posterior given the observed data:

$$\theta^{(t)} \sim p(\theta|A, X) \tag{8}$$

These samples allow us to approximate the posterior distribution for θ as well as compute a predictive distribution $p(b^*|x^*, A, X) = \int p(b^*|x^*, \theta)p(\theta|X, A)d\theta \approx \frac{1}{T}\sum_{t=1}^{T} p(b^*|x^*, \theta^{(t)})$. However, generating these samples is not easily done in practice.

We propose an iterative approach. We first draw samples $b^{(t)}$ from the block membership posterior (equation 9). We then use each $b^{(t)}$ to draw samples for θ as in equation 10.

$$b^{(t)} \sim p\Big(b|A, X\Big) \tag{9}$$

$$\theta^{(t)} \sim p\Big(\theta|X, b^{(t)}\Big) \tag{10}$$

Both of these sampling steps can be implemented with a Markov Chain through the Metropolis-Hastings algorithm [5]. We just need to define a proposal distribution $q(x, x')$ for proposing a move $x \to x'$ and be able to evaluate an un-normalised form of the target distribution, denoted $\pi(\cdot)$, point-wise. The proposed move is then accepted with probability α (equation 11) else it is rejected and we stay at x.

$$\alpha = \min\left(\frac{\pi(x')q(x', x)}{\pi(x)q(x, x')}, 1\right) \tag{11}$$

This accept-reject step ensures the resulting Markov Chain is in detailed balance with the target distribution $\pi(\cdot)$. What we propose in equations 9 and 10 is therefore implemented through a 2-level Markov chain. The resulting samples for $\theta^{(i)}$ are unbiased in the sense that the expectation of their distribution is the posterior we are targeting in equation 8.

$$\mathbb{E}_{b^{(t)}}\left[p\left(\theta|X, b^{(t)}\right)\right] = \sum_{b\in[B]^N} p(\theta|X, b)p(b|A, X) = \sum_{b\in[B]^N} p(\theta, b|A, X) = p(\theta|A, X) \tag{12}$$

This is an example of a pseudo-marginal approach. Indeed, Andrieu and Roberts [3] show that the unbiased result in equation 12 is sufficient to prove that for sufficient samples, $\theta^{(t)} \sim \mathbb{E}_{b^{(i)}}\left[p(\theta|X, b^t)\right] = p(\theta|A, X)$ which is exactly the distribution we are targetting (equation 8).

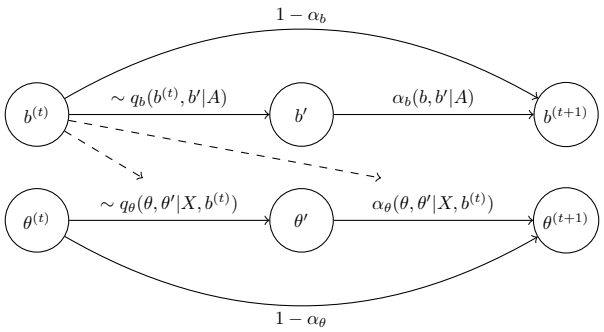


Figure 2: Sampling sequence

The reason we split the Markov chain into two stages is because the summation over all latent states $b \in [B]^N$ required to directly compute the likelihood $p(A|X,\theta) = \sum_{b\in[B]^N} p(A|b)P(b|X,\theta)$ is intractable $O(B^N)$.

Figure 2 shows an overview of the proposed method. We have introduced subscripts and conditionings to make explicit what parameters each step utilises. We note the power of the simplification given by equation 6. As $p(b|X) = B^{-N}$ does not depend on the exact value of X, we do not need to know the value of X to perform the sampling on b. Conversely, for the $\theta^{(t)}$ samples, we use only $b^{(t)}$ but not A as $(\theta \perp\!\!\!\perp A)|b$.

4.1 Sampling block memberships

Peixoto [13] proposes a Monte Carlo method which we will base our approach on. It relies on writing the posterior in the following form:

$$p(b|A,X) \propto p(A|b,X)\cdot p(b|X) = \pi_b(b) \tag{13}$$

Now $\pi_b(\cdot)$ is the un-normalised density we wish to sample from for the b-chain. In other words, we wish to construct a Markov chain that has $\pi_b(\cdot)$ as its invariant distribution. We can break π_b down as follows:

$$\pi_b(b) = p(b|X)\sum\nolimits_{\psi} p(A,\psi|b,X) = p(b|X)p(A,\psi^*|b,X) = p(A|b,\psi^*)\cdot p(\psi^*|b)\cdot p(b|X) \tag{14}$$

Since we are using the microcanonical SBM formulation, there is only one value of ψ that is compatible with the given (A,b) pair (given in equation 2). We denote this value $\psi^* = \{\psi_k^*, \psi_e^*\}$. Therefore, the summation over all ψ reduces to just the single ψ^* term; this is the power of the microcanonical formulation. We also define the microcanonical entropy of the configuration as.

$$S(b) = -\log \pi_b(b) = -\Big(\log p(A|b,\psi^*) + \log p(\psi^*, b|X)\Big) \tag{15}$$

This entropy can equally be thought of as the description length of the graph – the minimum amount of information required to store the graph and its parameters. The exact form of the proposal distribution and accept-reject step is explored thoroughly by Peixoto [13] and not repeated here. There is a widely used library for Python made available under LGPL called `graph-tool` [14], which implements this algorithm. The only modification we make is in the block membership prior $p(b)$ which we replace with $p(b|X) = B^{-N}$ which is a uniform distribution and so cancels out in the MH accept-reject step.

4.2 Sampling feature-to-block classifier parameters

The invariant distribution we wish to target for the θ samples is the posterior of θ given the values of the pair (X,b). We write this as follows:

$$p(\theta|X,b) \propto p(b|X,\theta)p(\theta) = \pi_\theta(\theta) \propto \exp\left(-U(\theta)\right) \tag{16}$$

$$\therefore U(\theta) = -\left(\log p(b|X,\theta) + \log p(\theta)\right) + \text{const} \tag{17}$$

Where we have introduced $U(\theta)$ equal to the negative log posterior. Each of the constituent terms of $U(\theta)$ are easily computed (equation 18). Similarly, we define $y_{ij} \coloneqq \mathbb{1}\{b_i = j\}$ and $a_{ij} \coloneqq \phi_j(x_i;\theta)$.

$$\log p(b|X,\theta) = \sum_{i\in[N]}\sum_{j\in[B]} y_{ij}\log a_{ij} \quad \text{and} \quad \log p(\theta) = -\frac{(D+1)(B)}{2}\log 2\pi - \frac{1}{2\sigma_\theta^2}||\theta||^2 \tag{18}$$

Discarding constant terms, we write $U(\theta)$ as in equation 19. Note that $||\theta||^2 = \sum_i \theta_i^2 = \sum_{j=1}^B ||w_j||^2$ is the Euclidean norm of the vector of parameters θ.

$$U(\theta) = \left(\sum_{i=1}^{N}\sum_{j=1}^{B} y_{ij}\log\frac{1}{a_{ij}}\right) + \frac{1}{2\sigma_\theta^2}||\theta||^2 = N\cdot\mathcal{L}(\theta) + \frac{1}{2\sigma_\theta^2}||\theta||^2 \tag{19}$$

$U(\theta)$ in equation 19 appears a typical objective function for neural network training. The first term – which we collect into $N\cdot\mathcal{L}(\theta)$ – is the cross-entropy between the graph-predicted and feature-predicted block memberships summed over all vertices. The second term of equation 19 – introduced

by the prior – brings a form of regularisation, guarding against over-fitting. In traditional applications we only seek the value of θ that minimises the objective function $U(\theta)$, which in our case would yield the maximum a posteriori (MAP) estimate. This is often done through some kind of gradient descent as ∇U is easily computable (equation 22).

However, our goal is not to find the MAP estimate but to draw samples from the posterior $\pi_\theta(\cdot) \propto \exp(-U(\cdot))$. It is sufficient to specify a proposal distribution and then apply a MH accept-reject step to ensure detailed balance with $\pi_\theta(\cdot)$. However, we can use ∇U as a useful heuristic to bias our proposal towards regions of higher target density. We therefore adopt the Metropolis Adjusted Langevin Algorithm (MALA) – first proposed by Roberts and Tweedie [16] – which leverages the ∇U information. Given the current sample θ, we propose a new sample θ' according to:

$$\theta' = \theta - h\nabla U(\theta) + \sqrt{2h} \cdot \xi \tag{20}$$

Where $\xi \sim \mathcal{N}(0, I)$ and h is a step-size parameter – which may vary with the sample index (appendix A.4 explores this more fully). Without the injected noise term, MALA is equivalent to gradient descent. We require the noise term ξ to fully explore the parameter space. We can write the proposal distribution simply as:

$$q_\theta(\theta, \theta') = \mathcal{N}\left(\theta'; \theta - h\nabla U(\theta), 2hI\right) \tag{21}$$

The term ∇U has an easy to compute analytic form (derived in Appendix A.3). By noting that $\theta = \{w_k\}_{k=1}^B$, we write the derivative with respect to each w_k as:

$$\frac{\partial U}{\partial w_k} = -\left(\sum_{i=1}^{N}\left\{\tilde{x}_i(y_{ik} - a_{ik})\right\} - \frac{w_k}{\sigma_\theta^2}\right) \tag{22}$$

After a proposed move is generated, in typical Metropolis-Hastings fashion we accept the move with probability α_θ:

$$\alpha_\theta(\theta, \theta') = \min\left(\exp\left(U(\theta) - U(\theta')\right)\frac{q_\theta(\theta', \theta)}{q_\theta(\theta, \theta')}, 1\right) \tag{23}$$

4.3 Sampling sequence

Up to this point, each $\theta^{(t)}$ update uses its corresponding $b^{(t)}$ sample. This means that the evaluation of $U(\theta)$ and $\nabla U(\theta)$ has high variance. This may lead to longer burn-in for the resulting Markov Chain. The only link between $b^{(t)}$ and $\theta^{(t)}$ is in the evaluation of $U(\theta)$ and $\nabla U(\theta)$ which depends only on the matrix $y^{(t)}$ with entries $y_{ij}^{(t)} \coloneqq \mathbb{1}\{b_i^{(t)} = j\}$. We would rather deal with the expectation of each $y_{ij}^{(t)}$:

$$\mathbb{E}\left[y_{ij}^{(t)}\right] = \mathbb{E}_{b^{(t)}}\left[\mathbb{1}(b_i^{(t)} = j)\right] = p(b_i = j|A, X) \tag{24}$$

We can obtain an unbiased estimate for this quantity using the block membership samples $\left\{b^{(t)}\right\}$. However, as with all MCMC methods, we must only uses samples after burn-in and thinning have been applied. We introduce $\mathcal{T}_b$ to denote the retained set of indices for the b-samples and $\mathcal{T}_\theta$ similarly for the θ-chain. An in-depth discussion of how these sets are chosen is given in appendix A.5. The unbiased estimate for $y_{ij}^{(t)}$ using the restricted sample set $\mathcal{T}_b$ is denoted $\hat{y}_{ij}$ and has form:

$$\hat{y}_{ij} \coloneqq \frac{1}{|\mathcal{T}_b|}\sum_{t\in\mathcal{T}_b} y_{ij}^{(t)} = \frac{1}{|\mathcal{T}_b|}\sum_{t\in\mathcal{T}_b}\mathbb{1}\{b_i^{(t)} = j\} \tag{25}$$

We therefore, choose to feed each $\theta^{(t)}$ update step the same matrix $\hat{y}$ for all t rather than the corresponding $y^{(t)}$. This means we no longer need to run the b and θ Markov chains concurrently. Instead, we run the b-chain to completion and use it to generate $\hat{y}$. This is an estimate of $p(b|A, X)$ that we use for every iteration of the θ Markov chain.

This affords us the flexibility to vary the number of samples we draw for the b and θ-chains; we denote the total number of samples generated T_b and T_θ henceforth. Note that due to burn-in and thinning, $|\mathcal{T}_b| < T_b$ and $|\mathcal{T}_\theta| < T_\theta$. Furthermore, this changeover from $y^{(t)}$ to $\hat{y}$ reduces the burn-in time for the θ-chain by reducing the variance in our evaluation of U and ∇U. A description of the overall algorithms is given in appendix A.7.

4.4 Dimensionality reduction

Once we have the samples $\{\theta^{(t)}\} \sim p(\theta|A, X)$, we can compute the empirical mean and standard deviation of each component of θ. Switching back to matrix notation we define $\theta = W$, such that W_{ij} is the weight component for block i and feature j, we can define:

$$\hat{\mu}_{ij} \coloneqq \frac{1}{|\mathcal{T}_\theta|} \sum_{t \in \mathcal{T}_\theta} W_{ij}^{(t)} \qquad \text{and} \qquad \hat{\sigma}_{ij} \coloneqq \frac{1}{|\mathcal{T}_\theta|} \sum_{t \in \mathcal{T}_\theta} \left(W_{ij}^{(t)} - \hat{\mu}_{ij} \right)^2 \tag{26}$$

A simple heuristic to discard the least important features requires specifying a cutoff $c > 0$ and a multiplier $k > 0$. We define the function $\mathcal{F}_i(j)$ as in 27 then only keep features with indices $d \in \mathcal{D}'$, where $\mathcal{D}'$ is constructed as in equation 28.

$$\mathcal{F}_i(j) \coloneqq (\hat{\mu}_{ij} - k\hat{\sigma}_{ij}, \hat{\mu}_{ij} + k\hat{\sigma}_{ij}) \cap (-c, +c) \tag{27}$$

$$\mathcal{D}' \coloneqq \{j \in [D] : \exists i \in [B] \text{ s.t. } \mathcal{F}_i(j) \neq \emptyset\} \tag{28}$$

Intuitively, this means discarding any feature for which $\hat{\mu}_{ij} \pm k\hat{\sigma}_{ij}$ lies within or spans the null region $(-c, c)$ for all block indices. If we were to use the Laplace approximation for the posterior $p(W_{ij}|A, X) \approx \mathcal{N}(W_{ij}; \mu_{ij}, \sigma_{ij})$, then this is effectively a hypothesis test on the value of W_{ij} (equation 29). $\mathcal{D}'$ then comprises all features i for which H_1 is accepted at least once for some $j \in [B]$.

$$H_0 : |\mu_{ij}| \leq c \qquad H_1 : |\mu_{ij}| > c \tag{29}$$

The multiplier k determines the degree of significance of the result. However, as the Laplace approximation is not exact we will only treat this dimensionality reduction method as a useful heuristic and not an exact method.

Conversely, we could fix $k = k_0$ and the dimension of our reduced feature set $|\mathcal{D}'| = D'$. We would then like to find the largest value of c such that $|\mathcal{D}'| = D'$ given $k = k_0$. This is summarised in equation 30. This approach is often preferred as it fixes the number of reduced dimensions.

$$c^* = \arg\max_{c>0}(c : |\mathcal{D}'| = D', k = k_0) \tag{30}$$

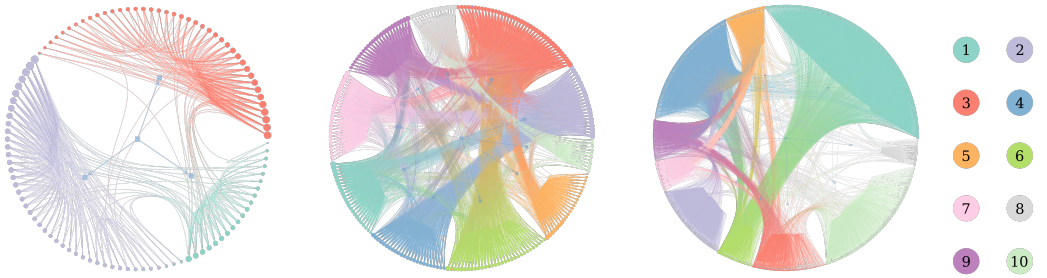
5 Experiments

We apply the developed methods to a variety of datasets. Datasets are chosen to span a range of node counts N, edge counts E and feature space dimension D. We consider the following datasets:[2]

- **Political books** [11] ($N = 105, E = 441, D = 3$) – network of Amazon book sales about U.S. politics, published close to the presidential election in 2004. Two books are connected if they were frequently co-purchased by the same customer. Vertex features encode the political affiliation of the author (liberal, conservative or neutral).
- **Primary school dynamic contacts** [18] ($N = 238, E = 5539, D = 13$) – network of face-to-face contacts amongst students and teachers at a primary school in Lyon, France. Two nodes are connected if the two parties shared a face-to-face interaction over the course of the day. Vertex features include class membership (one of 10 values 1A-5B), gender and whether or not the individual is a teacher or pupil. These data were collected on consecutive days in October 2009. We choose to analyse just the second day.
- **Facebook egonet** [7] ($N = 747, E = 30025, D = 480$) – an assortment of Facebook egonets. These are networks of a particular user's friends list and all the connections within that. Vertex features are extracted from each user's profile and are fully anonymized. They include information about education history, languages spoken, gender, home-town, date of birth, name to give a few examples. We focus on the egonet with id 1912.

We require metrics to assess performance. This can be split into two separate components: the microcanonical SBM fit (concerned with the b-samples) and the fit of the feature-to-block generator

[2]For information as to how these data were collected and how personally identifiable information was removed, please refer to the cited papers.



(a) Polbooks (b) School (c) Facebook egonet (d) Legend

Figure 3: Networks laid out and coloured according by inferred block memberships $\hat{y}$ for a given experiment iteration. Visualisation performed using *graph-tool* [14]

(concerned with the θ-samples). Starting with the SBM, $S(b)$ (equation 15) can be interpreted as the description length of the partition imposed by b. It is only natural to divide this quantity by the number of entities (nodes and edges) in our graph $N + E$ to allow for rough comparison between graphs. This defines a simple metric to gauge the fit of the SBM: the description length per entity averaged over the b-samples (equation 31):

$$\bar{S}_e := \frac{1}{(N+E)|\mathcal{T}_b|} \sum_{t \in \mathcal{T}_b} S\left(b^{(t)}\right) \tag{31}$$

However, to assess the performance of the feature-to-block predictor, we must partition the vertex set $[N]$ into training and test sets: $\mathcal{G}_0$ and $\mathcal{G}_1$ respectively.[3] The b-chain is run using the whole network but we only use vertices $v \in \mathcal{G}_0$ to train the θ-chain. As $|\mathcal{G}_0| \neq |\mathcal{G}_1|$ sets, we cannot use the un-normalised log target U (equation 19) for comparison; the total cross-entropy loss is scaled by the size of each set but the prior term stays constant. We therefore must use the average cross-entropy loss over each set (equation 32):

$$\bar{\mathcal{L}}_\star := \frac{1}{|\mathcal{T}_\theta|} \sum_{t \in \mathcal{T}_\theta} \mathcal{L}_\star\left(\theta^{(t)}\right) \qquad \text{where} \qquad \mathcal{L}_\star\left(\theta^{(t)}\right) := \frac{1}{|\mathcal{G}_\star|} \sum_{i \in \mathcal{G}_\star} \sum_{j \in [B]} \hat{y}_{ij} \log \frac{1}{\phi_j\left(x_i; \theta^{(t)}\right)} \tag{32}$$

Where $\star \in \{0, 1\}$ has been introduced to toggle between training and test sets. Table 1 summarises the results for each experiment.[4]

We also apply the dimensionality reduction method on the two higher dimensional datasets (the school and FB egonet). For this we leverage equation 30, to reduce the dimension from D to D' with $k = 1$ to yield c^*. We then retrain the feature-block predictor using just the retained feature set $\mathcal{D}'$ and report the loss over the training and test sets for the reduced classifier – denoted $\bar{\mathcal{L}}'_0$ and $\bar{\mathcal{L}}'_1$ respectively. These values are also included in table 1.

Table 1: Experimental results averaged over $n = 10$ iterations (mean $\pm$ standard deviation)

Dataset	B	D	D'	$\bar{S}_e$	$\bar{\mathcal{L}}_0$	$\bar{\mathcal{L}}_1$	c^*	$\bar{\mathcal{L}}'_0$	$\bar{\mathcal{L}}'_1$
Polbooks	3	3	–	2.250 ± 0.001	0.584 ± 0.033	0.557 ± 0.061	–	–	–
School	10	13	10	1.894 ± 0.006	0.793 ± 0.096	0.914 ± 0.112	1.112 ± 0.230	0.791 ± 0.096	0.864 ± 0.139
FB egonet	10	480	10	1.626 ± 0.003	1.305 ± 0.034	1.539 ± 0.087	0.942 ± 0.042	1.496 ± 0.093	1.578 ± 0.104

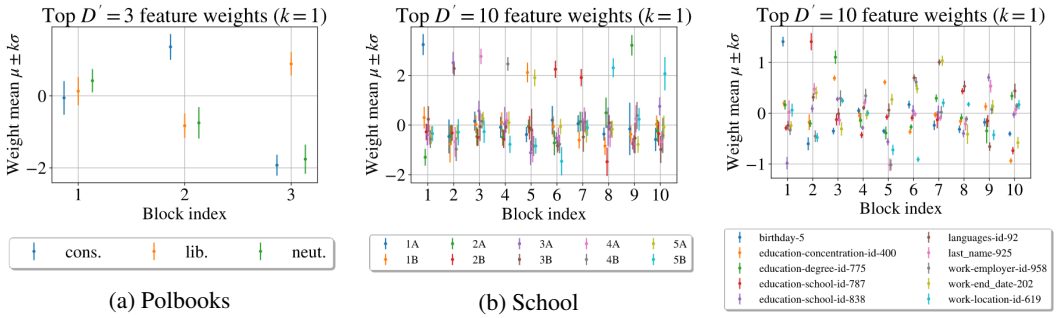
Table 1 already highlights some general trends in the results. Firstly, the variance of the test loss $\bar{\mathcal{L}}_1$ tends to be higher than the training loss $\bar{\mathcal{L}}_0$. This is expected as our test set is smaller than the training set and so more susceptible to variability in its construction. Indeed, much of the variance in the evaluation of $\bar{\mathcal{L}}_0$ and $\bar{\mathcal{L}}_1$ comes from the random partitioning of the graph into training and test sets $\mathcal{G}_0$ and $\mathcal{G}_1$. Secondly, it can be seen that the dimensionality reduction procedure brings the training and test losses closer together. This implies that the features we keep are indeed correlated with the underlying graphical partition.

[3] We choose to randomly create the partition on each experiment run such that a constant fraction f of the available vertices go to form our training set $\mathcal{G}_0$ and the remaining vertices are held out to form our test set $\mathcal{G}_1$. For all the experiments $f = 0.7$.

[4] For a comprehensive list of the hyper-parameters used for each experiment please see appendix A.8

The average description length per entity of the graph $\bar{S}_e$ has very low variance implying the detected communities can be found reliably (to within an arbitrary relabelling of blocks). For reference we plot an inferred partition for each of the graphs on figure 3. The polbooks graph yields the cleanest separation between blocks but nonetheless the inferred partitions for the other datasets do succeed at partitioning the graph into densely connected clusters.

On figure 4 we give the sampled feature weights for the reduced feature-set $\mathcal{D}'$ for a given experiment iteration (or just the original $\mathcal{D}$ for the polbooks dataset). We go on to analyse each of these in turn.



(a) Polbooks

(b) School

(c) Facebook egonet

Figure 4: Reduced dimension feature-to-block generator weight samples

5.1 Political books

We wish to determine whether political affiliation is a good predictor of the overall network structure. We choose to partition the network into $B = 3$ communities as we only have this many distinct values for political affiliation (conservative, liberal or neutral).

From, figure 4a, we see that all 3 blocks have a distinct political affiliation as their largest positive component. This is strong evidence that political affiliation is indeed the axis which best predicts the 3-way natural partition of the graph into blocks.

From figure 3a, we note that there are very few edges between blocks 2 and 3 (the detected conservative and liberal blocks as per figure 4b). Block 1 effectively acts as a separator between blocks 2 and 3; very few readers venture all the way across the political aisle for their next book.

From table 1 we see that the training and test losses are very similar (the test loss mean is even below the training loss) and both are low in magnitude. This is very strong evidence that the features we have available (the author's political affiliation) are indeed the drivers of the high-level graphical structure at $B = 3$.

5.2 Primary school dynamic contacts

We must first choose the number of blocks B to define the coarseness of our analysis. A total of 10 school-classes would suggest that $B = 10$ is a natural starting point. We visualise the inferred block memberships in figure 3b.

As before, we sample the block-generator parameters θ and employ the dimensionality reduction technique with standard deviation multiplier $k = 1$ to pick out the top $D' = 10$ features. We then plot the weights for the surviving features $d \in \mathcal{D}'$ on figure 4b. Immediately, we see that only the pupils' class memberships have survived (1A-5B); gender and teacher/student status have been discarded meaning that these are not good predictors of overall macro-structure.

The vast majority of blocks are composed of a single class. However, some blocks have 2 comparably good classes as their predictor. For example, block 2 contains classes 3A and 3B as its 2 best predictors. This suggests that the social divide between classes is less pronounced for pupils in year 3. Conversely, some classes are found to extend over two detected blocks (class 2B spans blocks 6 and 7) but we nonetheless do not have a feature which explains the division. The most surprising block is number 5 - which has comparable weightings for classes 5A and 1B. Perhaps there was a joint event between those two classes on the day the data were collected.

As for the training and test losses of the original and reduced classifiers. We see that the training loss stays roughly constant between the original and reduced classifiers $\bar{\mathcal{L}}_0 \approx \bar{\mathcal{L}}'_0$ but the test loss of the reduced classifier is ever-so-slightly decreased (within margin of error). This improved generalisation implies that the features we have discarded (gender and teacher/student status) do not impact the high-level graphical structure and simply lead to over-fitting in the original classifier. The features we have available do not capture the entire picture but they do quite well (modestly low overall loss).

5.3 Facebook egonet

This dataset was chosen to showcase the power of the dimensionality reduction technique as the feature-space has high dimension ($D = 480$). We sample the b-chain, specifying $B = 10$ total blocks and use this to construct the θ-samples as before.

We again apply the dimensionality reduction technique with $k = 1$ to target $D' = 10$ features in the reduced set. The remaining features (figure 4c) are those that best explain the high-level community structure. The majority of the surviving features are education related. Nevertheless, for $D' = 10$ we only have good explanations for the makeup of some of the detected blocks.

When the feature dimension is very large, it becomes increasingly likely that a particular feature may uniquely identify a small set of nodes. If these nodes are all part of the same community then the classifier will overfit for that particular parameter. The regularisation term imposed by the prior goes some way to alleviating this problem. Nevertheless, we see in figure 4c that the feature `birthday-5` has a very high weight as it relates to block 1. It might be possible to shift the feature values such that they take values in $\{-1, 1\}$ rather than $\{0, 1\}$ but to accept more than one feature-group per block.

The training and test losses (table 1) are the highest of the considered networks but nonetheless still low. This suggests that the features we have available only partly explain the high-level structure. Promisingly, after reducing the problem dimension our test loss barely changes, suggesting that the features we do keep are the best from the ones we have available at explaining the overall network structure.

6 Conclusion

The FFBM was developed to address the shortcomings of other graphical models when testing how vertex features affect community structure. The idea is to divide the graph into its most natural partition and test whether the vertex features can accurately explain this partition. We therefore hope to avoid a common pitfall in data science: correlation does not imply causation. It is very easy to find vertex features that are in some way correlated with the graphical structure. Nonetheless, only when we find the feature that best describes the most pronounced partition do we have a stronger case for causation.

With the newly-defined FFBM, we go on to present an efficient inference algorithm to sample the parameters θ of the feature-to-block generator. This is introduced as two concurrent Markov chains to sample the block memberships b and block generator parameters θ. The key trick to make the b-chain efficient is the use of the microcanonical rather than the traditional SBM (as proposed by Peixoto [15]) which allows us to bypass an expensive summation over the latent memberships b. Additionally, we use the empirical mean of the b-samples as the input to our θ-chain, as this reduces the variance in our evaluation of the target distribution and thus shortens the burn-in and auto-correlation times of our θ-chain.

The overall method is shown to be effective at extracting and describing the most natural communities in a labelled network. Nevertheless, the approach can only currently explain the structure at the macro-scale. We cannot explain structure within each community. Future work will benefit from extending the FFBM to be hierarchical in nature. That way, the structure of the network can be explained at all length-scales of interest. This work may be built upon to develop better methods of analysing structure in networks and drawing evidence-backed conclusions. So long as data collection techniques remain ethical and care is taken to respect personal privacy, such empowered decision-making can only help humankind.

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References

[1] Emmanuel Abbe. Graph compression: The effect of clusters. In *2016 54th Annual Allerton Conference on Communication, Control, and Computing (Allerton)*, pages 1–8, 2016. doi: 10.1109/ALLERTON.2016.7852203.

[2] Edo M Airoldi, David Blei, Stephen Fienberg, and Eric Xing. Mixed membership stochastic blockmodels. In D. Koller, D. Schuurmans, Y. Bengio, and L. Bottou, editors, *Advances in Neural Information Processing Systems*, volume 21. Curran Associates, Inc., 2009. URL https://proceedings.neurips.cc/paper/2008/file/8613985ec49eb8f757ae6439e879bb2a-Paper.pdf.

[3] Christophe Andrieu and Gareth O. Roberts. The pseudo-marginal approach for efficient Monte Carlo computations. *The Annals of Statistics*, 37(2):697 – 725, 2009. doi: 10.1214/07-AOS574. URL https://doi.org/10.1214/07-AOS574.

[4] Solenne Gaucher, Olga Klopp, and Geneviève Robin. Outliers detection in networks with missing links, 2020.

[5] W. K. Hastings. Monte carlo sampling methods using markov chains and their applications. *Biometrika*, 57(1):97–109, 1970. ISSN 00063444. URL http://www.jstor.org/stable/2334940.

[6] Matthew Kraatz, Nina Shah, and Emmanuel Lazega. The collegial phenomenon: The social mechanisms of cooperation among peers in a corporate law partnership. *Administrative Science Quarterly*, 48:525, 09 2003. doi: 10.2307/3556688.

[7] Jure Leskovec and Julian Mcauley. Learning to discover social circles in ego networks. In F. Pereira, C. J. C. Burges, L. Bottou, and K. Q. Weinberger, editors, *Advances in Neural Information Processing Systems*, volume 25. Curran Associates, Inc., 2012. URL https://proceedings.neurips.cc/paper/2012/file/7a614fd06c325499f1680b9896beedeb-Paper.pdf.

[8] Benjamin F. Maier and Dirk Brockmann. Cover time for random walks on arbitrary complex networks. *Phys. Rev. E*, 96:042307, Oct 2017. doi: 10.1103/PhysRevE.96.042307. URL https://link.aps.org/doi/10.1103/PhysRevE.96.042307.

[9] Nikhil Mehta, Lawrence Carin Duke, and Piyush Rai. Stochastic blockmodels meet graph neural networks. In Kamalika Chaudhuri and Ruslan Salakhutdinov, editors, *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pages 4466–4474. PMLR, 09–15 Jun 2019. URL http://proceedings.mlr.press/v97/mehta19a.html.

[10] Krzysztof Nowicki and Tom A. B Snijders. Estimation and prediction for stochastic blockstructures. *Journal of the American Statistical Association*, 96(455):1077–1087, 2001. doi: 10.1198/016214501753208735. URL https://doi.org/10.1198/016214501753208735.

[11] Boris Pasternak and Ivor Ivask. Four unpublished letters. *Books Abroad*, 44(2):196–200, 1970. ISSN 00067431. URL http://www.jstor.org/stable/40124305.

[12] Tiago P. Peixoto. Parsimonious module inference in large networks. *Physical Review Letters*, 110(14), Apr 2013. ISSN 1079-7114. doi: 10.1103/physrevlett.110.148701. URL http://dx.doi.org/10.1103/PhysRevLett.110.148701.

[13] Tiago P. Peixoto. Efficient monte carlo and greedy heuristic for the inference of stochastic block models. *Physical Review E*, 89(1), Jan 2014. ISSN 1550-2376. doi: 10.1103/physreve.89.012804. URL http://dx.doi.org/10.1103/PhysRevE.89.012804.

[14] Tiago P. Peixoto. The graph-tool python library. *figshare*, 2014. doi: 10.6084/m9.figshare.1164194. URL http://figshare.com/articles/graph_tool/1164194.

[15] Tiago P. Peixoto. Nonparametric bayesian inference of the microcanonical stochastic block model. *Physical Review E*, 95(1), Jan 2017. ISSN 2470-0053. doi: 10.1103/physreve.95.012317. URL http://dx.doi.org/10.1103/PhysRevE.95.012317.

[16] Gareth O. Roberts and Richard L. Tweedie. Exponential convergence of Langevin distributions and their discrete approximations. *Bernoulli*, 2(4):341 – 363, 1996. doi: bj/1178291835. URL https://doi.org/.

[17] Benedek Rozemberczki, Carl Allen, and Rik Sarkar. Multi-scale attributed node embedding, 2019.

[18] Juliette Stehlé, Nicolas Voirin, Alain Barrat, Ciro Cattuto, Lorenzo Isella, Jean-François Pinton, Marco Quaggiotto, Wouter Van den Broeck, Corinne Régis, Bruno Lina, and Philippe Vanhems. High-resolution measurements of face-to-face contact patterns in a primary school. *PLOS ONE*, 6(8):1–13, 08 2011. doi: 10.1371/journal.pone.0023176. URL https://doi.org/10.1371/journal.pone.0023176.

[19] Max Welling and Yee Whye Teh. Bayesian learning via stochastic gradient langevin dynamics. In *Proceedings of the 28th International Conference on International Conference on Machine Learning*, ICML'11, page 681–688, Madison, WI, USA, 2011. Omnipress. ISBN 9781450306195.

[20] Jun Zhu, Jiaming Song, and Bei Chen. Max-margin nonparametric latent feature models for link prediction, 2016.

Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes] See experiments section 5
   (b) Did you describe the limitations of your work? [Yes] See conclusion 6 and experiments 5 sections
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See conclusion 6
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] See inference section 4
   (b) Did you include complete proofs of all theoretical results? [Yes] See inference section 4
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] See supplementary code
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See appendix A.8
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] See table 1
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See appendix A.9
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes] See section experiments 5
   (b) Did you mention the license of the assets? [Yes] See section inference 4
   (c) Did you include any new assets either in the supplemental material or as a URL? [Yes] Supplementary material
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [Yes] Referred to original papers
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [Yes] Referred to original papers
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

A Appendix

A.1 SBM prior choice explanation

We have borrowed the priors proposed by Peixoto [15] for $p(\psi|b)$. These, are repeated here for reference:

$$p(\psi|b) = p(e|b)p(k|e,b) = \left[\left\{\begin{Bmatrix} B \\ 2 \end{Bmatrix}\right\}_{E}\right]^{-1} \cdot \left[\prod_r \frac{\prod_j \eta_j^r!}{n_r! q(e_r, n_r)}\right] \tag{33}$$

Where $\left\{{n \atop m}\right\}$ is shorthand for $\binom{n+m-1}{m} = \frac{(n+m-1)!}{(n-1)!(m)!}$ which can be thought of as the total number of distinct histograms with n bins under the constraint they sum to m. $E = \frac{1}{2}\sum_{r,s} e_{rs}$ is the total number of edges in the graph. Importantly, E is not allowed to vary and so $p(e|b)$ is uniform with respect to e. The variable η_j^r is introduced to denote the number of vertices in block r that have degree j. Formally, $\eta_j^r \coloneqq \sum_i \mathbb{1}\{b_i = r\}\,\mathbb{1}\{k_i = j\}$. Furthermore, $q(m,n)$ is the number of different histograms with at most n non-zero bins that sum to m. $q(m,n)$ is related to but different from $\left\{{n \atop m}\right\}$. Lastly, $e_r \coloneqq \sum_s e_{rs}$ is the total number of half edges in block r and $n_r \coloneqq \sum_i \mathbb{1}\{b_i = r\}$ is the number of vertices assigned to block r.

These were chosen carefully by Peixoto [15] to more closely match the structure of empirical networks than simple uniform priors. We do not repeat his arguments here.

A.2 Derivation of conditional block distribution given feature matrix

We wish to determine the form of $p(b|X)$. This can be done by integrating over the joint probability with respect to θ.

$$\begin{aligned} p(b|X) &= \int p(b,\theta|X,\theta)d\theta = \int p(b|X,\theta)p(\theta|X)d\theta \\ &= \int p(b|X,\theta)p(\theta)d\theta = \int \prod_{i\in[N]} \phi_{b_i}(x_i;\theta)p(\theta)d\theta \\ &= \prod_{i\in[N]} \int \frac{\exp(w_{b_i}^T \tilde{x}_i)\prod_{j\in[B]}\mathcal{N}(w_j;0,\sigma_\theta^2 I)}{\sum_{k\in[B]}\exp(w_k^T\tilde{x}_i)} dw_{1:B} \end{aligned}$$

We note that $b_i \in [B]$ and so the integral's value is unchanged with respect to b_i. The integrand has the same form no matter which value b_i takes as the prior is the same for each w_j. As such the integral can only be a function of at most $\tilde{x}_i$ and σ_θ^2 as it is symmetric with respect to b_i and all the various w_j are integrated out as they are dummy variables. Therefore, denoting the integral by the (unknown) function $f(\tilde{x}_i, \sigma_\theta^2)$, we write $p(b|X)$ as follows:

$$p(b|X) = \prod_{i=1}^{N} f(\tilde{x}_i, \sigma_\theta^2) = \text{const w.r.t } b = c$$

As this is a constant with respect to b we conclude that $p(b|X)$ must be a uniform distribution. $1/c$ is simply the size of the set of values that b can take. We know $b_i \in [B]$. Therefore, $b \in [B]^N$ and $|[B]^N| = B^N = 1/c$. Putting this all together we conclude that:

$$p(b|X) = B^{-N} \tag{34}$$

A.3 Derivation of U gradient with respect to feature parameters

The goal is to determine $\nabla U(\theta)$, the gradient of the negative log posterior with respect to the parameters. We repeat the form of $U(\theta)$ in equation 35.

$$U(\theta) = \left(\sum_{i\in[N]}\sum_{j\in[B]} y_{ij}\log\frac{1}{a_{ij}}\right) + \frac{1}{2\sigma_\theta^2}||\theta||^2 \tag{35}$$

Where y_{ij} is independent of θ and a_{ij} is the output from the softmax layer, with form as given in equation 36.

$$a_{ij} \coloneqq \phi_j(x_i;\theta) = \frac{\exp(w_j^T \tilde{x}_i)}{\sum_{r\in[B]} \exp(w_r^T \tilde{x}_i)} \tag{36}$$

We note that $\theta = \{w_k\}_{k=1}^B$, and as such we can write this in vector form $\theta = \left[w_1^T, w_2^T \dots w_B^T\right]^T$. Therefore, $\nabla U(\theta) = \left[{}^{\partial U}/_{\partial {w_1}^T}, {}^{\partial U}/_{\partial {w_2}^T} \dots {}^{\partial U}/_{\partial {w_B}^T}\right]^T$; to compute $\nabla U(\theta)$ it suffices to find the form of ${}^{\partial U}/_{\partial w_k}$ with respect to a general k.

To this end, we must first find partial derivatives of a_{ij} and $||\theta||$ with respect to w_k. Starting with a_{ij}:

$$\begin{aligned}\frac{\partial a_{ij}}{\partial w_k} &= \frac{\tilde{x}_i \exp(w_j^T \tilde{x}_i)\delta_{jk} \cdot \sum_{r\in[B]} \exp(w_r^T \tilde{x}_i) - \exp(w_j^T \tilde{x}_i) \cdot \tilde{x}_i \exp(w_k^T \tilde{x}_i)}{\left(\sum_{r\in[B]} \exp(w_r^T \tilde{x}_i)\right)^2} \\ &= \tilde{x}_i \left(a_{ij}\delta_{jk} - a_{ij}a_{ik}\right)\end{aligned} \tag{37}$$

Where $\delta_{jk} \coloneqq \mathbb{1}\{j = k\}$. Now moving onto the derivative of $||\theta||^2$:

$$\frac{\partial}{\partial w_k}||\theta||^2 = \frac{\partial}{\partial w_k}\left(\sum_{r\in[B]} ||w_r||^2\right) = 2w_k \tag{38}$$

We are ready to put this all together, to find the partial derivative of $U(\theta)$ with respect to each w_k:

$$\begin{aligned}\frac{\partial U}{\partial w_k} &= \sum_{i=1}^N \sum_{j=1}^B y_{ij} \left(\frac{-\tilde{x}_i}{a_{ij}} \left(a_{ij}\delta_{jk} - a_{ij}a_{ik}\right)\right) + \frac{w_k}{\sigma_\theta^2} \\ &= -\left(\sum_{i=1}^N \tilde{x}_i \left(y_{ik} - a_{ik}\sum_{j=1}^B y_{ij}\right) - \frac{w_k}{\sigma_\theta^2}\right) \\ &= -\left(\sum_{i=1}^N \left\{\tilde{x}_i (y_{ik} - a_{ik})\right\} - \frac{w_k}{\sigma_\theta^2}\right)\end{aligned} \tag{39}$$

This is the required result. This form can be computed efficiently through matrix operations. The only property of y_{ij} we have used in the derivation is the sum-to-one constraint $\sum_{j=1}^B y_{ij} = 1$ for all i.

A.4 Choosing the MALA step-size

For sampling from the θ-chain of the block membership generator parameters, we employed the Metropolis Adjusted Langevin Algorithm (MALA). At iteration t, the proposed sample is generated by:

$$\theta' = \theta^{(t)} - h_t \nabla U(\theta^{(t)}) + \sqrt{2h_t} \cdot \xi \tag{40}$$

There are two competing objectives when choosing the step-size h_t. On the one hand, we want the step-size to be large so that we arrive at a high density region quickly. However, too large a step-size will lead to a lower acceptance ratio and thus inefficient sampling. A solution to this problem would be to slowly decrease the step-size with t - often called simulated annealing. Therefore, we still have a short burn-in time but will not bounce around the mode for large t. As well as the trivial constraint for h_t to be strictly positive, we introduce two further constraints as outlined by Welling and Teh [19]:

$$\sum_{t=1}^\infty h_t = \infty \qquad \text{and} \qquad \sum_{t=1}^\infty h_t^2 < \infty \tag{41}$$

The first constraint ensures that we have cover sufficient distance to arrive at any arbitrary point in our domain, no matter the starting point. The second constraint ensures that once we converge to the mode rather than simply bouncing around it. Welling and Teh [19] propose the following form for a polynomially decaying step-size which we adopt:

$$h_t = \alpha(\beta + t)^{-\gamma} \tag{42}$$

Where α, β, γ are hyper-parameters to be chosen. We require $\alpha, \beta > 0$ and $\gamma \in (0.5, 1]$ to satisfy equation 41. To reduce the number of hyperparameters we set these to have values given by the equations 43.

$$\alpha = \frac{250 \cdot s}{N} \qquad \beta = 1000 \qquad \gamma = 0.8 \tag{43}$$

Where N is the number of data-points we are considering and now s is the only free variable which we call the step-size scaling. For approximate methods, we can choose to bypass the MH accept-reject entirely to speed up computation. If this is done, the algorithm is instead called stochastic gradient Langevin diffusion (SGLD) [19]. This speeds up computation at the expense of exactness of the method.

A.5 Burn-in and thinning

As with any MCMC method, we must deal with the issues presented by burn-in and thinning. We have introduced the notation $\mathcal{T}_b$ and $\mathcal{T}_\theta$ to denote the set of samples we keep from the b and θ chains respectively. Note that we generate T_b and T_θ samples total. The burn-in period refers to the time taken for the Markov Chain to converge to the stationary distribution. Sample thinning is necessary to ensure that neighbouring samples satisfy independence. However, as we do not leverage the independence property this is less important in our analysis. We can write the general set $\mathcal{T}_\star$ as:

$$\mathcal{T}_\star = \{T_\star \kappa_\star + i\lambda_\star : 0 \leq i \leq \lfloor T_\star(1 - \kappa_\star)/\lambda_\star \rfloor\} \tag{44}$$

Where the parameter $\kappa_\star \in (0, 1)$ controls our burn-in and $\lambda_\star$ controls our thinning. $\kappa_\star$ can be determined by plotting the log-target (either $S(b^{(t)})$ or $U(\theta^{(t)})$ with respect to the epoch t. $\kappa_\star$ is then chosen to encompass the region where the log-target has roughly equilibrated. As we do not leverage sample independence $\lambda_\star$ can be chosen less rigorously. We often just use $\lambda_b = 5$ and $\lambda_\theta = 10$.

A.6 Initializing the b-chain

For the purposes of our model (the FFBM), the number of blocks B is a constant which must be specified by the data scientist. We could however, allow our choice of B to be influenced by the observed data. This places us in the domain of empirical Bayes, which must be negotiated carefully. Prior beliefs must be determined a priori else they are not prior. However, as the number of blocks only specifies the coarseness of the analysis, it is fine to allow it to vary. Indeed, Peixoto [12] shows that for a fixed average degree the maximum number of detectable blocks scales as $O(\sqrt{N})$ where N is the number of vertices.

If we allow B to vary in the b-chain (i.e. new blocks can be created and we permit empty blocks) then it can be run until a minimum description length (MDL) solution is reached. We take the number of non-empty blocks at the MDL to be our fixed block number B for subsequent analysis. Indeed, it is prudent to start our b-chain at this MDL solution as then we can burn-in time is greatly reduced.

A.7 Algorithms

Algorithm 1 Block membership sample generation

$b^{(0)} \leftarrow \arg\min_b S(b|A)$ ▷ Implemented as greedy heuristic in *graph-tool* library
for $t \in \{0, 1 \dots T_b - 1\}$ **do**
  $b' \leftarrow\sim q_b(b^{(t)}, b'|A)$
  $\log \alpha_b \leftarrow \log \alpha_b(b^{(t)}, b'|A)$
  $\eta \leftarrow\sim \text{Unif}(0, 1)$
  if $\log \eta < \log \alpha_b$ **then**
    $b^{(t+1)} \leftarrow b'$
  else
    $b^{(t+1)} \leftarrow b^{(t)}$
  end if
end for
return $\{b^{(t)}\}_{t=1}^{T_b}$

Algorithm 2 FFBM parameter pseudo-marginal inference

$\hat{Y}_{ij} \leftarrow \frac{1}{|\mathcal{T}_b|} \sum_{t \in \mathcal{T}_b} \mathbb{1}\{b_i^{(t)} = j\} \quad \forall i, j$
$\theta^{(0)} \leftarrow\sim \mathcal{N}(0, \sigma_\theta I)$

for $t \in \{0, 1 \dots T_\theta - 1\}$ **do**
  $\xi \leftarrow\sim \mathcal{N}(0, I)$
  $\theta' \leftarrow \theta^{(t)} - h_t \nabla U(\theta^{(t)} | X, \hat{Y}) + \sqrt{2h_t} \cdot \xi$
  $\log \alpha_\theta \leftarrow \log \alpha_\theta(\theta^{(t)}, \theta' | A, \hat{Y})$
  $\eta \leftarrow\sim \text{Unif}(0, 1)$
  if $\log \eta < \log \alpha_\theta$ **then**
    $\theta^{(t+1)} \leftarrow \theta'$
  else
    $\theta^{(t+1)} \leftarrow \theta^{(t)}$
  end if
end for
return $\{\theta^{(t)}\}_{t=1}^{T_\theta}$

A.8 Hyperparameter values

Table 2: Hyper-parameter values for each experiment

Dataset	B	f	σ_θ	T_b	κ_b	λ_b	T_θ	κ_θ	λ_θ	s	k	D'	T'_θ	κ'_θ	λ'_θ	s'
Polbooks	3	0.7	1	1,000	0.2	5	10,000	0.4	10	0.05	–	–	–	–	–	–
School	10	0.7	1	1,000	0.2	5	10,000	0.4	10	0.2	1	10	10,000	0.4	10	0.2
FB Egonet	10	0.7	1	1,000	0.2	5	10,000	0.4	10	0.017	1	10	10,000	0.4	10	0.5

A.9 Implementation details

All data analysis and visualisation was implemented in Python. Full source code is available in the supplementary material. The scripts were run using a standard PC using the Windows Subsystem for Linux (WSL) environment. Specs are:

- **CPU**: Intel(R) Core(TM) i7-1065G7
- **RAM**: 8GB
- **GPU**: Intel(R) Iris(R) Plus Graphics

On this hardware each experiment iteration took the following amount of time to execute:

Table 3: Compute-time for each experiment

Dataset	b-chain	θ-chain	Reduced θ-chain	Overall compute time
Polbooks	$\sim$1s	$\sim$4s	–	$\sim$5s
School	$\sim$10s	$\sim$10s	$\sim$10s	$\sim$30s
FB Egonet	$\sim$20s	$\sim$180s	$\sim$10s	$\sim$210s