Inference for the stochastic block model with unknown number of blocks and non-conjugate edge models

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Abstract

The stochastic block model (SBM) is a popular model for capturing community structure and interaction within a network. There is increasingly a range of network data with non-binary edges becoming commonplace. However, existing methods for inferring parameters of an SBM are commonly restricted to models for edges which yield a conjugate prior distribution. This paper introduces an effective reversible jump Markov chain Monte Carlo sampler for estimating the parameters and the number of blocks for a general network model allowing for a non-conjugate prior distribution on the edge model. Keywords: network, stochastic block model, statistical analysis of network data, non-conjugate analysis

1 Introduction

Statistical analysis of networks has seen much growth in recent years with the increasing availability of network data. The term “network” is used in a broad range of research fields. In this paper, a network consists of a set of nodes, which can form pairwise interactions. Each possible interaction is referred to as an edge, with the value of that interaction being denoted as an edge-state. In similar work, these are referred to as possible edges and edge-weights. By referring to each possible pair of nodes as an edge, the terminology is more succinct. The aim of statistical network modelling is to describe the edge-states with a probabilistic model, potentially performing inference for model parameters. Such models include the exponential random graph (Snijders et al., 2006), the class of latent space models (Hoff et al., 2002) and the stochastic block model (SBM) (Holland et al., 1983). Under the SBM, the set of nodes is partitioned into blocks such that the edge-state between two nodes depends on their block memberships. For example, an assortative block structure in a network with binary edge-states is formed when nodes in the same block are more likely to have an edge-state of one than between nodes in different blocks.

Previous work on the SBM has focused on binary edge-states starting with Holland et al. (1983); Frank and Harary (1982). Attention turned to non-binary edge-states in the 2000s Jiang et al. (2009); Mariadassou et al. (2010); Ambroise and Matias (2012). There is a rich literature on the SBM including both Bayesian and Frequentist treatments. Extensions to the SBM include restricting the SBM to only within-block and between-block edge-state distributions in the affiliation network.
(Snijders and Nowicki, 1997; Nowicki and Snijders, 2001; Copic et al., 2009), multiple-block memberships in the mixed-membership SBM (Airoldi et al., 2008), degree-corrected SBM (Karrer and Newman, 2011), and the infinite relational model (IRM), (Kemp et al., 2006) where the number of blocks is treated as unknown. For a thorough review of the SBM and inference methods, see Matias and Robin (2014).

This article aims to identify network structure via an extension of the stochastic block model for networks with general edge-states in a Bayesian framework. Research has extended the SBM to edge-state models with conjugate prior distributions, for example Mørup and Schmidt (2012, 2013) and McDaid et al. (2013). The inference algorithms presented in this paper allow much more flexible modelling than previous work on networks with general edge-states. Relaxing the restriction to conjugate edge-state models allows for more flexibility in the choice of prior. This is key in incorporating prior knowledge in applications. Furthermore, flexible edge-state models can be used within the presented framework that could not previous be used. For example, in Section 5.2 a negative binomial model is applied to the edge-states within an email network. Such a model cannot be fit using existing methodology since no conjugate prior distribution exists for the negative binomial. This greatly broadens the applicability of the stochastic block model to general network data with arbitrary edge-states.

Not only does the sampling method facilitate the fitting of general models to edge-states, it also performs inference on the number of blocks. Various methods have been considered to estimate the number of blocks within a network. Such methods fall into two main approaches: (1) a post-hoc analysis of multiple models (using model selection methodology) or (2) incorporating the number of blocks as a random variable. The model selection techniques in likelihood based methods using the Bayesian information criteria and its derivatives (Daudin et al., 2008; Latouche et al., 2012; Wang et al., 2017; Saldana et al., 2017), information-based methods using minimum description lengths (Peixoto, 2013), sequential testing by embedding successive block models with an increasing number of blocks (Lei, 2016) and cross validation (Chen and Lei, 2016). These methods all fit multiple SBM models with differing numbers of blocks, then do a post-hoc analysis to choose a final number. Alternatively, treating the number of blocks as a random variable allows inference on the joint distribution of number of blocks, block membership of nodes and model parameters. Extending the SBM by allowing the number of blocks to vary leads to the IRM (Mørup and Schmidt, 2013). The IRM extends the model hierarchy of the SBM by placing a Chinese Restaurant Process (CRP) prior (Gershman and Blei, 2012) on the number of blocks. On top of this, the parameters $\theta$ can be integrated out of the SBM model, leading to efficient collapsed Gibbs sampling algorithms (Mørup et al., 2011; Mørup and Schmidt, 2012, 2013; McDaid et al., 2013).

In this paper, the number of blocks is estimated under the latter paradigm. An algorithm is presented to sample from the posterior distribution of the block parameters, block memberships and number of blocks in a stochastic block model. The sampling algorithm is inspired by Green and Richardson (2001) – a reversible jump Markov chain Monte Carlo (RJMCMC) (Green, 1995) scheme using split and merge proposals to explore the posterior by either combining two blocks, or splitting a block into two. Nobile and Fearnside (2007); McDaid et al. (2013) make use of a split-merge proposal, although due to the conjugate models considered, they do not require parameter values $\theta'$. The difficulty in designing an effective split-merge algorithm rests on ensuring that parameter values are “matched” when changing dimension. Previous authors have proposed sampling algorithms, such as the collapsed Gibbs sampler of McDaid et al. (2013) – for a given node $i$, the posterior probability of belonging to block $k$ is computed with all other parameters fixed. Under the collapsed regime, considering assigning $i$ to a new block $k^*$ is simple, since the
parameters $\theta$ have been integrated from the model. In the case of non-conjugate mixture models, the parameter $\theta_{k^*}$ is required to evaluate the likelihood of node $i$ belonging to block $k^*$.

The remainder of the paper is organised as follows: in Section 2 the specifics of the SBM are presented. Section 3 introduces the split-merge sampling algorithm. In Section 4 the sampler is applied to simulated data, whilst in Section 5 the split-merge sampler is used to analyse some real networks. Finally, closing remarks and extensions to the model and sampler are discussed in Section 6.

2 Model

The canonical SBM (Holland et al., 1983; Fienberg et al., 1985; Wasserman and Anderson, 1987) considers a network with a fixed number of nodes and blocks denoted as $N$ and $\kappa$ respectively. The nodes are then partitioned into blocks, with each node belonging to only one block. Let $z$ be the block indicator matrix with $z_{ik} = 1$ if node $i$ belongs to block $k$ and 0 otherwise. As such, $z_i$ is a one-of-$\kappa$ indicator vector. It is assumed that $z_i$ is drawn from a Multinomial distribution with parameter $\omega$. The parameter $\omega$ governs the block memberships, with $\omega_k$ being the probability that a node joins block $k$.

For each pair of blocks, there is an associated parameter $\vartheta_{kl}$ which governs the probability of an edge-state between nodes in blocks $k$ and $l$. These parameters can be arranged into a matrix, with diagonal elements $\vartheta_{kk}$ governing edge-states between nodes both in block $k$. In the case of undirected edges, the parameter matrix is symmetric with $\vartheta_{kl} = \vartheta_{lk}$. Finally, the edge-states are modelled as independent Bernoulli random variables with probability of success based on the block membership of the nodes. Specifically, the edge-state for edge $ij$, denoted $E_{ij}$, is drawn from a Bernoulli distribution with probability $\vartheta_{kl}$ where $z_{ik} = z_{jl} = 1$. Notice that this can be written in a quadratic form as $z_i' \vartheta z_j$. This model is summarised in Equation (1); first the nodes are assigned to blocks, then – given these block memberships – the edge-states are drawn with parameters depending on the block membership of the end-nodes.

$$
\begin{align*}
    z \mid \omega &\sim \text{Multinomial}(\omega, \kappa) \\
    E_{ij} \mid \vartheta, z &\sim \text{Bernoulli}(z_i' \vartheta z_j)
\end{align*}
$$

(1)

Given a data set consisting of the edge-states in a network, recovery of the block memberships is of interest. However, when performing inference, the values for parameters $\vartheta$ are likely to be unknown. In the case of binary edge-states, a natural extension to Equation (1) is to allow $\vartheta_{kl}$ to be a Beta random variable. Therefore, inference must be performed on both $z$ and $\vartheta$ in applications of the SBM where only the edge-states are observed.

The structure of the SBM can be applied to non-binary edge-states, such as count data or a continuous value. In this way, the parameters $\vartheta$ apply to some edge-state distribution other than the Bernoulli. As such, a prior distribution other than the Beta is required for the parameters in order to perform inference. A further extension allows $\omega$ to be treated as unknown by assigning it a Dirichlet prior. Letting $G$ and $G_0$ be the distribution on the edges-states and parameters respectively yields the model in Equation (2).
\[
\omega \sim \text{Dirichlet}(\gamma) \\
z|\omega \sim \text{Multinomial}(\omega, \kappa) \\
\vartheta_{kl} \sim G_0(\alpha_{kl}) \\
E_{ij}|\vartheta, z \sim G(\vartheta_{z_i}z_j)
\]  

(2)

The IRM treats the number of blocks as unknown. Multiple authors have considered Bayesian inference for the IRM with conjugate models for the edge-states. In this case, the parameters governing the edge-states can be integrated out of the likelihood, resulting in a collapsed Gibbs sampler (McDaid et al., 2013). Such an approach is reliant on the conjugate assumptions; hence, only a limited number of edge-state models can be fit using such algorithms.

In the canonical SBM, there are \(\kappa\) blocks. When considering the block membership of the end-nodes, there are \(\binom{\kappa+1}{2}\) possibilities: the end nodes can be in the same block (\(\kappa\) possibilities) or in different blocks (\(\binom{\kappa}{2}\) possibilities). For example, if every pair of blocks \(k, l\) is governed by different parameters \(\vartheta_{kl}\), then the number of parameters grows quadratically in \(\kappa\). The affiliation model (Snijders and Nowicki, 1997; Nowicki and Snijders, 2001; Copic et al., 2009) only has two parameters: one for edges between nodes in the same block and another for edges between nodes in different blocks. Therefore, the number of parameters is always two, no matter how many blocks there are. This paper considers a parameterisation between these two extremes: letting \(\theta_k\) be the parameters governing edges between nodes in the same block \(k\) (of which there are \(\kappa\)), and a global parameter \(\theta_0\) for edge-states between nodes in different blocks. In this way, the number of parameters is \(\kappa + 1\), and grows linearly in the number of blocks. This model is appropriate for networks where between block connections are relatively homogeneous; for example, in ecological contact networks, where herds of animals remain close together for most of the time, with some interactions between herds. For comparison to the generic SBM from Equation (2), let \(\theta\) be the matrix with parameters \(\theta_{kl} = \theta_0\) and \(\theta_{kk} = \theta_k\), then the quadratic form \(z_i'\theta z_j\) picks the parameter governing the edge-state \(E_{ij}\). This may be extended to edge-state distribution \(G\) with multiple parameters. Note that \(\theta_k\) is a vector of parameters for the edge-state distribution for edges in block \(k\) (or between blocks if \(k = 0\)). For example, if \(G\) represents the Gaussian distribution, then \(\theta_k = (\mu_k, \sigma_k^2)\) represents the mean and variance of the edge-states in block \(k\). In this case, an additional subscript is required on \(\theta_{kp}\) such that \(\theta_{kp}\) is the \(p^{th}\) parameter for block \(k\). In the Gaussian example, \(\theta_{k1}\) is the mean value of edges in block \(k\).

Since the number of blocks \(\kappa\) is considered to be unknown, a prior must be placed on both the number of blocks and block memberships. Choices for this prior are discussed in Section 2.1. Prior parameters \(\alpha\) are assigned to the block parameters \(\theta\). Let \(F\) be a joint distribution for \((\kappa, z)\) with parameters \(\gamma\), hence the restricted form of the SBM considered in this paper is shown in Equation (3).

\[
\kappa, z \sim F(\gamma, \delta) \\
\theta_k \sim G_0(\alpha) \\
E_{ij}|\theta, z \sim G(z_i\theta z_j)
\]  

(3)

2.1 Prior for block structure

Under the canonical SBM, the number of blocks \(\kappa\) is assumed known. In this case, the standard prior to place on the block allocations \(z\) is a \(\text{Multinomial}(\omega)\). In the case where \(\kappa\) is unknown,
this can be extended by setting a prior on both $\kappa$ and $z$. A hierarchical prior distribution can be achieved by first setting an arbitrary prior distribution $F_0$ for $\kappa$, and then setting a prior for $z$ given $\kappa$. One approach is to let $z \sim \text{Multinomial}(\omega)$; where $\omega$ follows a symmetric Dirichlet distribution on the $\kappa - 1$ simplex denoted by $\text{Dirichlet}(\gamma, \kappa)$. Such a hierarchical prior is referred to as a Dirichlet Multinomial Allocation (DMA) prior (Green and Richardson, 2001). Since a symmetric Dirichlet distribution with parameter $\gamma$ is used, the parameter $\omega$ can be marginalised out to obtain a prior density for block memberships depending only on $\kappa$ and $\gamma$ as shown in Equation (4).

\[
f(z|\gamma, \kappa) = \int_{\omega} f(z|\omega) \pi_0(\omega|\gamma) d\omega
\]

\[
= \int_{\omega} \prod_{k=1}^{\kappa} \prod_{i=1}^{N} \omega_{k, i}^{z_{ik}+\gamma+1} \frac{\Gamma(\kappa \gamma)}{\Gamma(\gamma)} d\omega
\]

\[
= \frac{\Gamma(\kappa \gamma)}{\Gamma(\gamma)^\kappa} \prod_{k=1}^{\kappa} \Gamma(\sum_{i=1}^{N} z_{ik} + \gamma)
\]

where $N_k$ is the number of nodes in block $k$ and $\Gamma(a) = \int_{0}^{\infty} x^{a-1} e^{-x} dx$ is the gamma function.

By taking the limits $\kappa \to \infty, \gamma \to 0$ while $\kappa \gamma \to \hat{\gamma}$, the Dirichlet process (DP) named the Chinese Restaurant Process (CRP) is obtained (Aldous, 1985). This has the interpretation of a block model with infinitely many blocks, while the sum of the Dirichlet parameters remains equal to $\hat{\gamma}$. For further discussion on the connections between DMA and DPs, see Green and Richardson (2001).

The CRP is a popular choice of prior for the SBM (Mørup et al., 2011; Mørup and Schmidt, 2012; Cha and Cho, 2012), used in topic modelling (Blei et al., 2003; Broderick et al., 2013) and includes extensions such as the Indian Buffet Process (Ghahramani and Griffiths, 2006). It is appealing since it jointly models the number of blocks and block memberships via one parameter $\gamma$. The expected number of blocks is available in closed form in Equation (5) where $\Psi$ is the digamma function.

\[
E[\kappa] = \gamma (\Psi(\gamma + N) - \Psi(\gamma))
\]

However, the marginal distribution on the number of blocks, $p(\kappa)$, depends on the Stirling numbers of the first kind. The computation of Stirling numbers is non-trivial (Antoniak, 1974).

One downside to using the CRP is that generated blocks structures are skewed towards one large block with multiple smaller blocks. By keeping an explicit DMA prior, the possible block structures are more flexible and interpretation of parameters is easier, since they are independent features of the model. Firstly, by choosing a specific prior distribution $F_0$ for $\kappa$, much more can be said about the number of blocks; this allows more informative priors when modelling. Secondly, explicit choices can be made for the distribution of nodes to these blocks via $\gamma$. Therefore, for flexible modelling, the DMA is preferred. In this work, the DMA prior is used with $F_0$ the distribution obtained by adding one to a Poisson random variable. As a consequence, $f_0(K = \kappa) = \frac{\kappa^{-1} \exp(-\kappa)}{(k-1)!}$ for $\kappa = 1, 2, \ldots \ldots$. A comparison of block structures generated under each model is shown in Figure 1. In each diagram, five block structures have been generated for 100 nodes from two settings in each of the CRP and DMA model. Each structure is represented as a bar split into cells, with one cell for each block. The area of a cell is proportional to the number of nodes assigned to a block; hence, the cells have very different areas for when uneven block structures are considered. In all cases, the blocks have been sorted by size. As such, notice that the CRP generates uneven block structures, especially for smaller $\gamma$. However, to generate more even block sizes, a higher value for $\gamma$ is required; this also increases the probability of generating more blocks. This is due to the low probability of generating
even blocks under the CRP. In both cases for the DMA, the expected number of blocks is 5, with
\( \gamma \) set as 1 or 5. The sizes of the blocks in the case that \( \gamma = 1 \) are drawn uniformly across all block
sizes with the given number of blocks. In the case that \( \gamma = 5 \), the block sizes are drawn from
a symmetric Dirichlet(5) distribution – this concentrates the block size distribution to more even
blocks, yielding cells of equal area.

Considering the points raised in this section, prior specification is more precise under the DMA
and will therefore be used throughout this paper. Both the prior density and prior marginal densities
for a single node belonging to a block are required in the sampler presented in Section 3 – these
are available in Equation (6) for the DMA.

\[
f(z_i = l | z_{-i}, \eta) = \sum_{\kappa = \eta}^{\eta + M_l} \frac{f(z|\kappa^*) \pi_0(\kappa^*|\eta)}{\pi_0(z_{-i}|\eta)}
= \frac{\Gamma(\gamma)^n}{\Gamma(\gamma \eta)} \prod_{k=1}^{\eta-1} \Gamma(\gamma + M_k)
\times \left[ \frac{\Gamma(\gamma \eta) \prod_{k=1}^{\eta-1} \Gamma(\gamma + M_k + z_{ik})}{\Gamma(\gamma \eta + M + 1)} \pi_0(\eta|\eta) \right. \\
+ \frac{\Gamma(\gamma \eta + \gamma) \prod_{k=1}^{\eta+1} \Gamma(\gamma + M_k + z_{ik})}{\Gamma(\gamma \eta + \gamma + M + 1)} \pi_0(\eta + 1|\eta) \right]
= \begin{cases} \\
\pi_0(\eta + 1|\eta) \frac{B(\gamma + 1, M + \eta \gamma)}{B(\gamma, \eta \gamma)} & \text{if } l = \eta + 1 \\
\pi_0(\eta|\eta) \frac{M_l + \gamma}{M + \eta \gamma} + \pi_0(\eta + 1|\eta) \frac{B(\gamma + 1, M + \eta \gamma)}{B(\gamma, \eta \gamma)} (1 + \frac{M_l}{\gamma}) & \text{o.w.} \\
\end{cases}
\]

where \( B(x, y) = \Gamma(x) \Gamma(y) / \Gamma(x + y) \) is the beta function, \( z_{-i} \) is the set of nodes without node \( i \),
\( M = N - 1 \) is the number of nodes without \( i \), \( \eta \) is the number of blocks defined by the set \( z_{-i} \) and
\( M_k \) is the number of nodes in block \( k \) from the set \( z_{-i} \).

3 Split-merge sampler

In this section a split-merge RJMCMC sampler is proposed for the SBM: this algorithm draws
samples from the posterior distribution of \( (\kappa, z, \theta) \). Before introducing the algorithm, the benefit of
split-merge steps over Gibbs samplers (Mørup and Schmidt, 2012; McDaid et al., 2013) is discussed.

3.1 Benefit over Gibbs sampling

Consider two “true” blocks \( k \) and \( l \) with \( n_k \geq n_l \) nodes and a state \( s \) of a Gibbs sampler with a
block \( k^s \) consisting of all nodes in true blocks \( k \) and \( l \). For the Gibbs sampler to separate the nodes
in \( k^s \) into blocks \( k \) and \( l \), it will require at least \( n_l \) steps, each of which takes a node assigned to \( k^s \)
and assigns it to a new block \( l^s \). Each of these moves is quite unlikely, especially if the parameters
\( \theta_k, \theta_l \) are close to \( \theta_0 \). On the other hand, if all nodes could be moved at once, then the proposal
would be more likely to be accepted. This is a common problem with Gibbs sampling algorithms:
the one-at-a-time nature of the algorithm means large changes in posterior space are unlikely, even
if the combined changes increase the posterior considerably. This phenomenon can cause Gibbs
samplers to get “stuck” in local modes of the posterior: One way to address this problem is to use
a split-merge sampler.
Figure 1: Comparison of block structures on 100 nodes. For each model, five example block structures are drawn. Each network is represented as a bar divided into cells. Each cell represents the relative size of the blocks. Top left: CRP(1), top right: CRP(5), bottom left: DMA(1,5), bottom right: DMA(5,5).

3.2 Comparison to mixture models

Split-merge samplers have been developed for general mixture models (Green and Richardson 2001), with emphasis on the canonical mixture of normal densities. In a standard parametric mixture model, each data point is drawn from a component of the mixture. Each component has a different form, either different distributions or different parameter values. A split-merge
sampler applied to such a data set explores the possible assignments of data points to components by successively proposing to either merge two components together or split one component in two. Care must be taken when designing such proposals: it must be an isomorphism and differentiable to ensure the validity of the underlying Markov chain. Furthermore, to be efficient, the proposal must ensure that a proposed structure has similar posterior support to the current structure to ensure a reasonable acceptance probability. Notice that, since each data-point belongs to one component, a split move which assigns a data-point to a new cluster will be penalised by the prior on the number of components but the likelihood will increase if the parameter for new component is a good fit for the assigned data-point.

Notice that for the SBM, the latent block membership is a mixture model. Difficulty arises when compared to the standard mixture model, since reassigning a node to a new block does not affect only that node – it affects the edges incident to the node. This implies that the prior will penalise the split move for adding a block for the new node, and the likelihood will penalise based on the \((N-1)\) edge-states. Therefore, when considering split-merge samplers for the SBM, multiple edge-states are affected by changing the block membership of one node.

### 3.3 Split-merge for the restricted SBM

The remainder of this section introduces the split-merge sampler for the restricted SBM. The sampler consists of four moves:

- resampling parameter values,
- splitting or merging blocks,
- reassigning nodes to the current set of blocks.
- adding or deleting an empty block,

Let \((\kappa^s, z^s, \theta^s)\) be the current state of the parameters in step \(s\) of the sampler. Values for parameter \(\theta\) given the block structure can be sampled using any MCMC techniques. In this work, each \(\theta_i\) is resampled using a random walk on a transformed scale. The difficult proposals are trans-dimensional: merging and splitting blocks. These are described in the follow subsections. The full split-merge algorithm is given in Algorithm 1.

#### 3.4 Merge move

The merge proposal takes a state \((\kappa^s, z^s, \theta^s)\) and proposes a new state \((\kappa', z', \theta')\). Such a move will reduce the number of blocks by one: \(\kappa' = \kappa^s - 1\). Firstly, two blocks \(k\) and \(l\) are sampled to merge – possible mechanisms include choosing blocks proportional to block size, inversely proportional to block size, at random, etc. In this paper, for simplicity, \(k\) and \(l\) are chosen at random. Secondly, the block membership \(z'\) is updated. This is deterministic: any node which is a member of block \(k\) or \(l\) in \(z^s\) is assigned to block \(k'\) in \(z'\). All other nodes keep their block assignment. Next, the parameter values are updated. Following the recommendations of Green and Richardson (2001), proposing a value \(\theta'_{k'}\) with similar explanatory power as \(\theta_k\) and \(\theta_l\) should ensure that \(\theta'_{k'}\) is well supported in the posterior. A simple approach is to take the mean value: \(\theta'_{k'} = \theta_k/2 + \theta_l/2\). However, to allow more flexibility in the sampler, an uneven merge is considered with a sampler parameter \(w \in [0, 1]\), giving a weighted mean of parameter values. Since the split move will invert the merge move, a
Algorithm 1 Reversible jump Markov Chain Monte Carlo sampler for the restricted SBM with unknown $\kappa$: split-merge algorithm.

**Inputs:** Edge-states $E$, prior parameters $\alpha, \gamma, \delta$.

1. Draw $\kappa^0, z^0 \sim F_0(\cdot|\gamma, \delta)$.
2. Draw $\theta^0 \sim G_0(\cdot|\alpha)$.

for $s = 1, \ldots, S$ do

3. Draw $\theta^s \sim \text{Update}(\cdot|E, \kappa^{s-1}, z^{s-1}, \theta^{s-1}, \alpha)$
4. Let $\kappa^s = \kappa^{s-1}$
5. if $\kappa^s=1$ then

   - Propose a split

   else with probability $1/2$ propose a split or a merge

   end if

6. if There are no empty blocks then

   - Propose adding an empty block

   else with probability $\frac{N_{\emptyset}}{N + \rho}$ attempt deleting an empty block.

   or with probability $\frac{\rho}{N_{\emptyset} + \rho}$ attempt adding an empty block.

   end if

7. for $i = 1, \ldots, N$ do

   for $k = 1, \ldots, \kappa^s$ do

   - Let $p_k = g(E_i, z_{-i}, z_{ik} = 1, \theta) f(z_{ik} = 1|z_{-i})$

   end for

   Draw $z_i' \sim \text{Multinomial}(p)$

   end for

8. Store sample $(z^s, \theta^s, \kappa^s)$.

end for
matching function $m$ is required to ensure that parameters lie in the correct space. For example, a rate parameter must be positive, whereby a suitable choice for $m$ is the exponential function. Possible matching functions for a given parameter space are shown in Table 1. The merge move is show in Equation (7):

$$m(\theta_k') = wm(\theta_k) + (1 - w)m(\theta_l)$$

Finally, the acceptance probability $\alpha$ is computed (see Appendix A Equation 16) and the next state of the sampler $(\kappa^{s+1}, z^{s+1}, \theta^{s+1})$ is taken as $(\kappa', z', \theta')$ with probability $\alpha$.

Table 1: Possible matching functions to ensure parameters lie in the correct space.

| Range for $\theta$ | Possible matching function $m$ |
|---------------------|--------------------------------|
| $(\infty, \infty)$  | $m(x) = x$                      |
| $[0, \infty)$       | $m(x) = \log(x)$               |
| $[0, 1]$            | $m(x) = \log(x) - \log(1 - x)$ |

3.5 Split move

The split proposal takes a state $(\kappa^s, z^s, \theta^s)$ and proposes a new state $(\kappa', z', \theta')$ with $\kappa' = \kappa^s + 1$. Firstly, the block to split is chosen at random – again there is flexibility in the choice here, but in this paper the block is chosen uniformly amongst the $\kappa^s$ blocks. To mirror the notation of the merge move, the block to split is labelled $k'$, and the proposed new blocks are $k$ and $l$.

Next, the method for simulating new block parameters is described. This requires the inverse of Equation (7). On top of this, an auxiliary variable $u'$ is needed to match the dimension of the parameter space. In this work, $u' \sim N(0, \sigma^2)$ and represents the weighted difference of the mapped parameters $m(\theta_k)$ and $m(\theta_l)$. The parameter split is thus:

$$m(\theta_k) = \frac{m(\theta_k') + u'}{2w'}$$

$$m(\theta_l) = \frac{m(\theta_l') - u'}{2(1 - w')}$$

Note that the dimension-matching criterion of RJMCMC [Green 1995] is achieved since the vectors $(\theta_k', u', w')$ and $(\theta_l, \theta_l, w)$ have the same cardinality.

It remains to describe the method to reassigned the nodes in $z^s$. In a similar fashion to [Green and Richardson 2001], nodes are assigned sequentially to block $k$ or $l$ proportional to the model likelihood. However, that it is not possible to compute the full likelihood during this procedure for the restricted SBM because edge-states exist between all nodes. Specifically, let $i$ and $j$ be the only nodes in block $k'$. Choosing to assign $i$ to block $k$ or $l$ proportional to the likelihood requires knowledge of the block membership of $j$, which does not yet exist. The quantity can be calculated in principle by looking at all the possible allocations of the nodes in block $k$ to $k'$ and $l'$. This operation is expensive; instead, it is estimated by the following sequential process:

First, all nodes in block $k'$ are unassigned and placed in a holding set $\mathcal{I}$. The set of remaining nodes is labelled $\mathcal{J}$. Take a permutation $\sigma(\mathcal{I})$ of $\mathcal{I}$ – this is the order in which nodes will be assigned.

When assigning node $i$, the following can be calculated:

$$q(z_i' = k) = \frac{f(\mathcal{E}|z_i' = k, z_{\mathcal{J}}', \theta')}{f(\mathcal{E}|z_i' = k, z_{\mathcal{J}}', \theta') + f(\mathcal{E}|z_i' = l, z_{\mathcal{J}}', \theta')}$$

10
Node \( i \) is then assigned to block \( k \) with probability \( q(z_i' = k) \) and block \( l \) otherwise. Once assigned, \( i \) is moved from \( I \) to \( J \) for the net assignment.

The total proposal probability of the new block assignment is thus:

\[
q(z') = \prod_{i \in \sigma(I)} q(z_i' = k) \left[ (1 - q(z_i' = k)) \right]^{|z_i' = l|} \tag{11}
\]

Finally, the proposed split is accepted as the next state of the sampler with probability \( A_{\text{split}} \) as in Equation (16), Appendix A.

### 3.6 Gibbs reassignment move

To allow the sampler to explore the parameter space, an additional two moves are included: a Gibbs-like move (which allocates each node to a block proportional to the posterior density) and a move that allows the addition and deletion of empty blocks.

The Gibbs-like allocation move takes a node \( i \) and computes the marginal posterior for \( i \) being a member of each of the \( \kappa \) blocks in the current state of the sampler. Since \( \kappa \) is finite in any given step of the sampler, a vector \( p_i \) can be calculated with \( p_{ik} \) the probability that node \( i \) is proposed to move to block \( k \). Thanks to the structure of the restricted SBM, \( p_{ik} \) can be written as the product of two densities: the posterior density of edge-states to nodes in the block \( k \) and the posterior density of edge-states to nodes in other blocks as in Equation (12).

\[
p_{ik} = \pi(z_{ik} = 1|z_{-i}, E, \theta) \propto f(z_{ik} = 1|z_{-i}) \prod_{j \neq i} g(E_{ij}|z_j, b_{zik} = 1, \theta) \tag{12}
\]

Note that proposing to assign \( i \) back to the block to which it currently belongs is allowed. Furthermore, since \( \kappa \) is finite, dividing by the sum of \( p_i \) is trivial to obtain a probability vector.

### 3.7 Add or delete empty blocks

The second extension allows the deletion and addition of empty blocks. Notice that the split or Gibbs allocation moves can leave empty blocks. Waiting for the sampler to merge an empty block with another block can leave empty blocks in the sampler state for some time. Furthermore, such merge moves may be unsuccessful due to the parameter averaging as in Equation (7). Therefore, a delete empty block proposal is included. To ensure the steady-state properties of the sampler, the inverse add empty block proposal is required. During the delete empty block move, a candidate block is chosen at random from the current set of empty blocks. When an empty block is added, it is simply labelled \( \kappa + 1 \). For simplicity, when an add/delete move is attempted, the probability of adding a block is chosen proportional to an algorithm parameter \( \rho \). The probability of choosing to delete an empty block is proportional to the number of empty blocks in the current state, \( N_0 \). Note that the likelihood of the edge-states does not change with the addition of empty blocks since the entire node structure remains unaffected. When a block is added, a parameter \( \theta^* \) is drawn from the prior distribution. The acceptance probabilities of the add and delete empty block moves are be calculated as in Equation (13).
4 Simulated data

In this section, the split-merge sampler of Section 3 is demonstrated on simulated data. The R package “SBMSplitMerge” Matthew Ludkin (2019) was used to perform the inference. The package also contains scripts to generate these example networks and produce the figures.

4.1 Example networks

In this section, two example data sets are considered: one with Bernoulli edge-state distributions and the other using a negative binomial distribution. The generalised negative binomial distribution is parameterised by the real-valued “number of failures” \( r > 0 \) and success probability \( p \). Therefore, if \( X \) follows a negative binomial distribution with parameters \( r \) and \( p \), it has probability mass function:

\[
P(X = x) = \frac{\Gamma(x + r)}{\Gamma(r) x!} p^r (1 - p)^x, \quad \text{for } x = 0, 1, \ldots, r > 0 \text{ and } p \in (0, 1]
\]

Notice that the Bernoulli distribution admits a conjugate prior; therefore, existing samplers, such as those introduced by Mørup and Schmidt (2012) and McDaid et al. (2013), could be applied. However, for the negative binomial with both parameters unknown, no conjugate model exists. Each of these networks are formed on the same block-structure of 100 nodes. The block sizes are 19, 23, 27 and 31.

In each network, the split-merge sampler was implemented with vague prior distributions applied to each parameter \( \theta \). As for the prior on \( \kappa \) and \( z \), a DMA(1, 10) prior was used with a Poisson distribution on \( \kappa - 1 \). As discussed in Section 2.1, this ensures that the support for \( \kappa \) is the positive integers, hence, the prior expected number of blocks is nine. The parameter values used for each of the edge-state models is given in Table 2. For the network with Bernoulli-distributed edge-states, the uniform prior Beta(1, 1) was applied to each parameter \( \theta \). In the negative binomial case with both parameters unknown, a Beta(1, 1) distribution is placed on the probability parameter \( p \) and a Gamma(1, 1) distribution for \( r \) is used.

Table 2: Simulated data parameter values for each edge-state distribution

| Parameter           | \( \theta_0 \) | \( \theta_1 \) | \( \theta_2 \) | \( \theta_3 \) | \( \theta_4 \) |
|---------------------|----------------|----------------|----------------|----------------|----------------|
| Bernoulli(\( p \))  | 0.05           | 0.4            | 0.5            | 0.6            | 0.7            |
| Negative binomial(\( p, r \)) | (0.5, 1) | (0.5, 1) | (0.5, 4) | (0.5, 5) | (0.5, 6) |

The split-merge sampler was run for 10,000 iterations with 5000 discarded as burn-in. Notice that at each iteration, a single split or merge move is proposed which can affect multiple nodes and
a Gibbs step is taken to update the membership of each node to the available blocks. Therefore, new blocks can be created with multiple nodes by splitting a current block into two new blocks. In all cases, a random walk Metropolis-Hastings step was used on the transformed parameters with variance equal to 0.1. A draw from the prior is taken as the starting state.

To evaluate the algorithm’s performance, the joint probabilities that two nodes belong to the same block are calculated after burn-in, as:

\[ p_{ij} = \frac{1}{|S|} \sum_{s \in S} \mathbb{I}[z_{is} = z_{js}] , \]  

where \( S \) are the indices of samples remaining after burn-in. The posterior joint probability that two nodes are in the same block (after burn-in) is displayed for the Bernoulli network in Figure 2a and for the the negative binomial network in Figure 3a.

Another point to consider when evaluating the performance of the sampler is the estimated parameter values. The posterior modes of the parameters are shown in Table 3 together with the 5% and 95% quantiles. Notice that the posterior modal values of \( \theta_k \), for \( k = 0, \ldots, 4 \) are close estimates to the true values in Table 2.

The Bernoulli case is rather easy; the parameter values within blocks are quite different to the between-block parameter \( \theta_0 \) and as such, the algorithm performs well here. The sampler also performs well in the network with negative binomial distributed edge-states. Note that the simulated block 1 has \( \theta_0 = \theta_1 \). The sampler is able to explore regions where the nodes in simulated block 1 are separate from the other nodes, as seen by the low probability region in Figure 3a. This corresponds to inferred block 4, where \( \hat{\theta}_4 \) is poorly estimated (the posterior quantiles are wide). This is due in part to there being little data (simulated block 1 consists of only 19 nodes) and since \( \theta_0 = \theta_1 \) it is hard to identify block 1.

Table 3: Mode, 5% and 95% posterior quantiles for parameters in example networks.

|             | Bernoulli(\( p \)) | NegBin(\( p \)) | NegBin(\( r \)) |
|-------------|---------------------|-----------------|-----------------|
| \( \theta_0 \) | 0.052 (0.046, 0.058) | 0.471 (0.446, 0.495) | 0.909 (0.828, 0.983) |
| \( \theta_1 \) | 0.505 (0.452, 0.556) | 0.532 (0.464, 0.600) | 5.45 (4.15, 7.28) |
| \( \theta_2 \) | 0.676 (0.640, 0.715) | 0.469 (0.397, 0.539) | 3.19 (2.37, 4.13) |
| \( \theta_3 \) | 0.641 (0.598, 0.678) | 0.475 (0.421, 0.546) | 5.46 (4.34, 7.21) |
| \( \theta_4 \) | 0.427 (0.367, 0.487) | 0.443 (0.173, 0.897) | 0.708 (0.05, 1.680) |

4.2 Assessing convergence

Assessing the convergence of a reversible jump Markov chain is non-trivial. Two techniques are applied in this section: (1) applying the Rubin-Gelman convergence statistic (Gelman and Rubin, 1992) to a summary statistic and (2) starting two independent samplers from extreme block configurations – one with all nodes assigned to one block and the other with each node assigned to different blocks.

In the first case, the mean and variance of the parameter values are used as summary statistics of the sampler performance, which are recorded at every iteration of the sampler. The Rubin-Gelman (Gelman and Rubin, 1992) statistics for the sampler for each model are shown in Table 4.
based on 30 independent chains. These values are mostly close to 1, indicating that convergence looks to have occurred during the first 10,000 iterations in the example networks of Section 4.1.

The second technique for assessing convergence is inspired by perfect simulation: considering two samplers starting at opposite extremes and observing both converging to the same area gives
Table 4: Rubin-Gelman statistics (and upper bound of 95% confidence interval) for each model with 30 independent chains of 10000 iterations.

| Model          | Bernoulli          | Negative binomial |
|----------------|--------------------|-------------------|
| Mean           | 1.0005 (1.0007)    | 1.0098 (1.0153)   |
| Variance       | 1.0005 (1.0006)    | 1.0069 (1.0106)   |

an indication that the underlying Markov chains have converged. This process was used for the simulated data sets; trace plots for the number of blocks in each case are shown in Figure 4.

![Trace plots for number of blocks](image)

(a) Bernoulli: Perfect simulation trace plot for $\kappa$
(b) Negative binomial: Perfect simulation trace plot for $\kappa$

Figure 4: Trace plots for number of blocks $\kappa$ in example networks. Two chains are simulated in each case: the “lower chain” with all nodes initially in one block (orange line) and the “upper chain” with all nodes initially assigned to different blocks (blue line).

5 Real data

The split-merge sampler is demonstrated on real networks: a network of brain connectivity with binary edge-states in Section 5.1 and a network of emails with edge-state consisting of counts is analysed in Section 5.2. In both cases, the edge-states are directed, therefore in Equation (2), $\vartheta_{kl} \neq \vartheta_{lk}$, allowing for different sender-receiver behaviour between blocks. For example, in the macaque network with binary edge-states, an edge from a node block $k$ to a node in block $l$ may be more likely than an edge pointing in the opposite direction.

5.1 Macaque

The first data set analysed concerns the brain of a macaque monkey (Négyessy et al., 2006). Regions of the cortex were deemed connected, or not, during a sensory task. In total, 45 regions of the brain were analysed as a network. Figure 5a shows the data set as an adjacency matrix.

A block model is proposed to partition the regions of the brain. This model assigns regions of the brain to the same block if their neural activity is similar. Since the data only provides binary
edge-states, a Bernoulli SBM is applied. A Beta(1,1) prior was placed on the edge probability parameters $\theta_k$. The split-merge algorithm was run for 15,000 iterations to provide samples from the posterior distribution of both block membership and parameter values. 1000 samples were discarded as burn-in. A DMA(1,6) prior for block memberships is used, thus the prior expected number of blocks is five.

Figure 5 displays posterior summaries for the split-merge sampler. Figure 5b shows four blocks with high posterior probability. There is some uncertainty around some nodes belong to block one or two (from the lower left) indicated by the paler shading. A trace plot for the number of blocks is shown in Figure 5c. This shows that the sampler quickly settles on between 4 and 6 blocks. Model parameter estimates are shown in Table 5, together with the 5% and 95% quantiles and the effective sample size. Note that parameter $\theta_4$ is more uncertain; this is due in part because the block is small (4 to 6 nodes).

![Figure 5](image.png)

(a) Edge-states sorted by most likely block assignments
(b) Posterior joint block membership
(c) Trace plot for $\kappa$

Figure 5: Posterior summaries for block membership in macaque brain network using Dirichlet process sampler after burn-in.

Table 5: Modal Parameter estimates, 95% posterior quantiles and effective sample sizes for macaque network.

| Parameter | 5% quantile | Mode | 95% quantile | Effective Sample Size |
|-----------|-------------|------|--------------|-----------------------|
| $\theta_0$ | 0.079 | 0.091 | 0.10 | 1700 |
| $\theta_1$ | 0.650 | 0.700 | 0.75 | 1000 |
| $\theta_2$ | 0.620 | 0.720 | 0.80 | 360 |
| $\theta_3$ | 0.400 | 0.480 | 0.58 | 530 |
| $\theta_4$ | 0.230 | 0.540 | 0.87 | 170 |

5.2 Enron

The Enron corporation was declared bankrupt in 2001 and later multiple employees were found guilty of accounting fraud. As a result of the trial, a corpus of emails leading up to the closure of the company were released as a public data set (Klimt and Yang, 2004). Aggregate counts of
emails between any two employees are analysed over the entire period available. Note that these are directed and contain self-loops (since some emails are sent to mailing lists, to which the sender belongs). Therefore, the edge-states are from the set of non-negative integers. Two edge-state models are considered: (i) a Poisson with a Gamma(1,1) prior and (ii) a negative binomial with a Gamma(1,1) prior for $r$ and a Beta(1,1) prior for $p$. On a first analysis, the mean number of emails sent by any one employee is 3.7, whilst the variance is 4753, so a Poisson model seems a bad fit a priori. The split-merge algorithm of Section 3 was applied with 10,000 steps with both a negative binomial and Poisson edge-state model. In both cases a DMA(1,10) joint prior is placed on $\kappa, z$.

The resulting modal block structure under the Poisson model is shown in Figure 6(b). The adjacency matrix is plotted with the same ordering of nodes in Figure 6(a) (on a log scale). The corresponding results for the negative binomial are shown in Figure 7. The negative binomial model shows more uncertainty in the block membership of nodes (Figure 7b) compared to the Poisson model (Figure 6b). In both models, the large group (corresponding to $\lambda_3$ and $r_3, p_3$) has a low incidence of sent emails. This large group is smaller under the negative binomial indicating that the negative binomial has found more structure. This is due in part to the lack of flexibility in the Poisson model. The modal parameter values for each model are given in Table 6 together with the 5% and 95% quantiles.

![Figure 6](image-url)

(a) Poisson: log(edge-states) permuted by the modal block membership under the posterior

(b) Poisson: Joint block membership posterior

(c) Poisson: Trace plot for $\kappa$

Figure 6: Posterior summaries for block membership in Enron network with Poisson edge-state model (after burn-in).

6 Concluding remarks

This paper has considered a restricted form of the stochastic block model (SBM) with arbitrary edge-state distributions and an unknown number of blocks. A Bayesian inference algorithm was proposed: a split-merge algorithm facilitated by a reversible jump Markov chain Monte Carlo sampler in Section 3. Unlike previous Bayesian treatments of the stochastic block model with an unknown number of blocks (Mørup and Schmidt 2012, 2013; McDaid et al. 2013), the proposed algorithm handles edge-state distributions without conjugate priors. This allows for more flexible modelling of network data, as demonstrated in Section 5.2 on the Enron email network. In this

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Table 6: Parameter mode, 5% and 95% posterior quantiles for the Enron data with edge-state model: (i) Possion(\(\lambda\)) and (ii) NegativeBinomial(\(r, p\))

|       | 5%   | Mode | 95%   |
|-------|------|------|-------|
| \(r_0\) | 0.0150 | 0.0160 | 0.0170 |
| \(r_1\) | 0.1300 | 0.2000 | 0.2800 |
| \(r_2\) | 0.1500 | 0.1800 | 0.2100 |
| \(r_3\) | 0.0071 | 0.0088 | 0.0110 |
| \(r_4\) | 0.2800 | 0.3200 | 0.3600 |
| \(r_5\) | 0.0410 | 0.1400 | 0.5900 |
| \(r_6\) | 0.1300 | 0.1500 | 0.1600 |
| \(r_7\) | 0.1000 | 0.1300 | 0.1500 |
| \(p_0\) | 0.0110 | 0.0120 | 0.0140 |
| \(p_1\) | 0.0030 | 0.0058 | 0.0100 |
| \(p_2\) | 0.0016 | 0.0023 | 0.0030 |
| \(p_3\) | 0.0240 | 0.0380 | 0.0520 |
| \(p_4\) | 0.0057 | 0.0072 | 0.0091 |
| \(p_5\) | 0.0015 | 0.0080 | 0.2300 |
| \(p_6\) | 0.0020 | 0.0026 | 0.0055 |
| \(p_7\) | 0.0041 | 0.0055 | 0.0077 |
| \(\lambda_0\) | 2.90 | 2.90 | 3.00 |
| \(\lambda_1\) | 640.00 | 640.00 | 660.00 |
| \(\lambda_2\) | 100.00 | 100.00 | 110.00 |
| \(\lambda_3\) | 0.36 | 0.37 | 0.38 |
| \(\lambda_4\) | 99.00 | 100.00 | 110.00 |
| \(\lambda_5\) | 130.00 | 130.00 | 140.00 |
| \(\lambda_6\) | 81.00 | 84.00 | 86.00 |
| \(\lambda_7\) | 5.70 | 85.00 | 350.00 |

example, a negative binomial model (with both parameters unknown) was fit to the edge-states, allowing for a higher variance of edge-states within a block than under the Poisson model. In the Enron data set, the negative binomial explored the parameter space better than the Poisson model since it visited posterior states with more structure.

The algorithm presented here is general and can be applied to the stochastic block model with any edge-state distributions from which samples can be taken and densities evaluated. This can easily include co-variate information in either the edge-state distribution, \(G\), or the block membership distribution, \(F\). The model as presented here assumes that all edge-states are observed. This could be relaxed by including a sparsity parameter as in Matias and Miele (2017) which could be inferred within the SBM framework (since it treats edges as a mixture of a density and a Dirac mass at zero). Alternatively, for truly missing data, a data augmentation scheme could be applied within the proposed sampler to infer the missing edge-states together with the block memberships and model parameters.
Figure 7: Posterior summaries for block membership in Enron network with Nbinson edge-state model (after burn-in).

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A Acceptance probability calculations

Since a merge move is the inverse of a split move, \( A_{\text{merge}} = 1/A_{\text{split}} \), hence only \( A_{\text{split}} \) is derived. The acceptance probability can be split into the following parts: posterior density ratio, proposal density ratio, ratio of densities of auxiliary variables, and the Jacobian; as such \( A_{\text{split}} \) has the general form:

\[
A_{\text{split}} = \frac{\pi(\kappa + 1, z', \theta'|E) q(\kappa, z, \theta|\kappa + 1, z', \theta') q(w)}{\pi(\kappa, z, \theta|E) q(\kappa + 1, z', \theta|\kappa, z, \theta) q(u', w')} J_{\text{split}}
\]

\[
= \frac{\pi(\kappa + 1, z', \theta'|E) q(\text{merge}|\kappa + 1) q(k', l') q(w)}{\pi(\kappa, z, \theta|E) q(\text{split}|\kappa) q(k) q(w')} \frac{1}{J_{\text{split}}}
\]

where \( q(\text{split}|\kappa) \) and \( q(\text{merge}|\kappa) \) are the probabilities of proposing a split or merge move given that the current state of the sampler contains \( \kappa \) blocks. These are chosen as \( 1/2 \) where possible. That is \( q(\text{split}|\kappa = 1) = 1 \) and \( q(\text{merge}|\kappa = 1) = 0 \) since merging is impossible when there is only one block. Note that in the examples: \( w, w' \sim \text{Unif}(0, 1) \), \( u' \sim \mathcal{N}(0, 1) \), \( k' \) and \( k, l \) are sampled at random amongst the set of available blocks.

Finally, \( J_{\text{split}} \) is the Jacobian of the split proposal given in Equation (17) and \( p \) is the dimensionality of each \( \theta_k \).

\[
J_{\text{split}} = \left| \begin{array}{cc}
\frac{\partial \theta'_k}{\partial u'} & \frac{\partial \theta'_l}{\partial u'} \\
\frac{\partial \theta'_k}{\partial u'} & \frac{\partial \theta'_l}{\partial u'}
\end{array} \right| = \left| \frac{\nabla m(\theta'_k) \nabla m(\theta'_l)}{\nabla m(\theta_k) (2w(1-w))^p} \right|
\]

Therefore, in the examples, where specific choices for \( u', w', w \) and \( q(\text{merge}), q(\text{split}) \) have been made, the acceptance probabilities reduce to:

\[
A_{\text{split}} = \frac{\pi(\kappa + 1, z', \theta'|E) 1}{\pi(\kappa, z, \theta|E) 1 + \mathbb{I}[\kappa = 1] \frac{\kappa + 1}{2}} \frac{1}{\phi(u'|0, \sigma^2) q(z'|\theta')} \frac{1}{\nabla m(\theta'_k) \nabla m(\theta'_l) (2w(1-w))^p}
\]

\[
A_{\text{merge}} = \frac{\pi(\kappa - 1, z', \theta'|E)}{\pi(\kappa, z, \theta|E) (1 + \mathbb{I}[\kappa = 2]) \frac{\kappa}{2}} \phi(u|0, \sigma^2) q(z|\theta) \frac{\nabla m(\theta'_k) (2w(1-w))^p}{\nabla m(\theta_k) \nabla m(\theta_l)}
\]