Mixed Membership Stochastic Blockmodels for the Human Connectome

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Abstract. Alzheimer's disease and other neurological diseases are often characterized by brain atrophy. It is hypothesized that such degradation directly affects connectivity as measured by whole brain tractographies and their derived connectivity networks. It is unclear, however, that current network construction methods provide either the most useful or efficient representation of the underlying connectivity structure. In the present work, we study the applications of a generative network model that can be used for automated cortical parcellation as well as network summary. We evaluate its performance through an independent classification task. In particular, we study whole brain tractographies from 96 subjects from the Alzheimer's Disease Neuroimaging Inititive (ADNI). We fit a Mixed Membership Stochastic Blockmodel (MMSB) to both an anatomically generated connectome as well as a larger, finely resolved connectome. We reduce each network to a much smaller block connectivity representation, and then use a generic Support Vector Machine to classify the resulting matrices by disease category. Our results suggest that mixed membership blockmodels produce parsimonious representations of existing anatomic connectomes, as well as useful parcellations of higher resolution networks.

Keywords: random networks, graph theory, human connectomics

1 Introduction

In recent literature, the brains of numerous organisms have often been modeled as a network [1]. These so-called "connectomes" provide a useful mathematical abstraction for understanding underlying patterns of brain connectivity. In particular, the construction of connectivity networks has opened the door to a variety of graph theoretic analytic tools. These include centrality measures, modularity, and spectral analyses [2, 3]. Important results stemming from these tools include the discovery of a strong core-periphery topology in brain connectivity networks (the "rich club") [4], and the importance of these topologies in neuro-degenerative diseases [5, 6]. These methods have mathematical connections to random network theory, an active area of research. It is useful to examine relatively new results and models in these fields in order to develop better methods.

In the present work, we propose the use of a variant of a well-known generative network model, the Stochastic Blockmodel (SBM), to produce parcellations and summary representations of human connectomes. Originally developed for social network analysis, SBMs associate each node with one of a fixed number of communities (blocks), and assume the probability of observing an edge between any two nodes is dependent on their respective communities. The Mixed Membership extension [7] of the Stochastic Blockmodel allows for nodes to be in multiple groups (i.e. to have a *distribution* of affiliations), an extension which better models the formation of rich clubs. Blockmodels also have a useful algebraic interpretation, providing a low rank assumption on the expectation of the random network. Finally, because this is a generative model, through the use of information criteria we are provided with principled methods of choosing model parameters, in this case specifically the number of clusters.

We validate the utility of Blockmodels for the human connectome in two cases, both of which involve an independent classification task between Alzheimer's Disease patients and a control group. We first fit models to a fairly coarse anatomical parcellation as a further graph clustering method, showing that it provides comparable classification accuracy with a fraction of the dimensions (nodes) compared to the original networks. We also fit block models to "continuous connectomes", which are very fine parcellations at the cortical mesh scale (~ 30000 nodes), in order to produce connectivity based parcellations of the whole cortex.

2 Mixed Membership Stochastic Blockmodels

The (non-mixture) Stochastic Blockmodel (SBM) is a latent variable generative model for binary directed graphs [8–10]. Defined for a random graph G composed of fixed nodes V and random binary edges E, it associates each node i with exactly one of K blocks using a hidden label z_i . Each block has some probability of interacting with another block (including itself). This interaction structure is captured by the block interaction matrix B, where the elements of B are the coefficients for Bernoulli random variables capturing the possible existence of edges. For the random edge between nodes i and j with associated labels z_i and z_j the edge exists with probability B_{z_i,z_j} .

The Mixed Membership Stochastic Blockmodel (MMSB) [7] is a flexible extension of the SBM that relaxes the assignment of nodes from a single group or cluster label to a distribution of group memberships; this is then expressed as labels for each of the possible edges of a node. Instead of one label per node in the SBM, the MMSB assigns one label per possible edge.

More formally, for every ordered pair of nodes $(i, j) \in V \times V$ we assign labels $z_{i \to j}$ and $z_{j \leftarrow i}$, which are the memberships of nodes *i* and *j* respectively in the context of the directed edge $i \to j$. Note that (i, j) and (j, i) may have distinct



Fig. 1: Diagram of the MMSB. The inner box in red is repeated for every entry in Adj. The priors for B are not pictured.

labels. It is helpful here to construct label vectors $\vec{z}_{i \to j}$ and $\vec{z}_{j \leftarrow i} \in \mathbb{R}^K$. Each label vector $\vec{z}_{i \to j} = \vec{e}_{z_{i \to j}} = [\dots \ 0 \ 1 \ 0 \ \dots]^T$, where $\vec{z}_{i \to j}$ has 1 in the $z_{i \to j}$ entry, and is zero elsewhere.

Each edge $i \to j$ then exists with probability $\vec{z}_{i \to j}^T B \vec{z}_{j \leftarrow i}$. We refer to the random network adjacency matrix associated with this model as Adj. Each independent realization of the random adjacency matrix is referred to as Adj^n , and is generated by the following process:

- 1. For each node $i \in \mathcal{V}$
- a) Draw a membership distribution vector $\pi_i \sim \text{Dirichlet}(\alpha)$
- 2. For each pair of nodes $(i, j) \in V \times V$
 - a) Draw a membership indicator $z_{i \to j} \sim \text{Multinomial}(\pi_i)$

 - b) Draw a membership indicator $z_{j\leftarrow i} \sim \text{Multinomial}(\pi_j)$ c) Sample their interaction $Adj_{i,j}^n \sim \text{Bernoulli}(\vec{z}_{i\rightarrow j}^T B \vec{z}_{j\leftarrow i})$ where B is the $K \times K$ matrix of block interaction probabilities, and where each entry $B_{i,j} \sim Beta(a_{i,j}, b_{i,j}).$

This provides the following joint distribution:

$$P(Adj^{n}, \{\pi_{i}\}, \{z_{i \to j}, z_{i \leftarrow j}\}, B | \alpha, a, b) = \prod_{i,j} P(Adj^{n}_{i,j} | z_{i \to j}, z_{j \leftarrow i}, B) P(z_{i \to j} | \pi_{i}) P(z_{j \leftarrow i} | \pi_{j}) \times \prod_{i} P(\pi_{i} | \alpha) \prod_{i} P(B | a, b)$$

Like many other simple generative mixture models (e.g. Latent Dirichlet Allocation), our overall objective is then to estimate the posterior distribution of hidden labels that maximizes the probability of the observed data.

In the context of human connectomes, the matrix Adj is the $N \times N$ connectivity matrix between ROIs, and the blocks are a form of "soft" clustering on the ROIs. We treat each subject as a realization Adj^n of the random network.

$\mathbf{2.1}$ **Estimation Methods**

For small networks, we sample from the posterior distribution via Collapsed Gibbs sampling, collapsing both priors. We provide the distributions below, using the following notation:

$N_{i \rightarrow}^{z}$	number of outward labels for node i assigned the label z
$N_{j\leftarrow}^z$	number of inward labels for node j assigned the label z
V^1	number of observed edges from label z_1 to z_2

$z_1 \rightarrow z_2$	number	or	UDSCI VCU	cuges	nom	laber	~1	10	~2
$Y_{z_1 \to z_2}$	number	of	possible	edges	from	label	z_1	to z	z_2

$$Y_{z_1 \to z_2}$$
 number of possible edges from label z_1 to z_2

$$P(z_{i \to j} = z | \{z_{k \to r}\}_{(k,r) \neq (i,j)}) \propto \frac{N_{i \to}^z + \alpha}{N + K\alpha} \frac{Y_{z \to z_{j \to i}}^1 + a}{Y_{z \to z_{j \to i}} + a + b}$$
(1)

$$P(z_{j\leftarrow i} = z | \{z_{r\leftarrow k}\}_{(k,r)\neq(i,j)}) \propto \frac{N_{j\leftarrow}^z + \alpha}{N + K\alpha} \frac{Y_{z\leftarrow z_{i\rightarrow j}}^1 + a}{Y_{z\leftarrow z_{i\rightarrow j}} + a + b}$$
(2)

Our Collapsed Gibbs Sampler scheme for the MMSB iterates over the set of all possible edges (all pairs of nodes), randomly reassigning labels according to Equations 1 and 2. In practice for small networks (e.g. the pre-parcellated FreeSurfer ROIs with 68 nodes), this converges quickly. For large networks however the size of each pass is much larger, and thus Gibbs Sampling is unfortunately too slow to be practical. We instead use Stochastic Variational Inference, a stochastic gradient descent method for mean field inference of the MMSB. The specifics of the method is described fully in [11], and we make use of their provided code, with minimal changes for our particular domain.

Given posterior estimates of the π_i membership vectors, the adjacency matrix of the expectation of the model has a succinct linear algebra form:

$$\mathbb{E}[Adj|\pi] = \pi^T B\pi$$

where π is a matrix with the membership vectors as columns. This can be approximated by substituting in posterior estimates of π and B. For our purposes we further define an empirical group connectivity matrix:

$$B_{emp} = \hat{\pi} A dj \hat{\pi}^T \tag{3}$$

which is interpreted as an estimate of a network realization's block connectivity. Note that here the diagonal is generally not zero, and represents the within-block connectivity.

2.2 Priors and Hyper-parameter Selection

In the MMSB generative process there are several hyper parameters and priors. The entries of B are Beta(a, b) distributed, using the conjugate prior of the Bernoulli distribution. The membership vectors π_i have an associated uniform mixing parameter α for their Dirichlet prior; while structure and information could be added to either of these distributions, our parameter choices keep the distributions symmetric and relatively uninformative (See Section 3).

Finally, the choice of the number of blocks is an important hyper-parameter controlling model specificity and complexity. Numerous models have been proposed placing a prior on the number of blocks [12, 13]. These models, which fall into a class of models known as Non-Parametric Bayes, have been particularly popular in previous works on probabilistic automated connectivity based segmentation [10, 13]. Due to the lack of hyper-parameter selection (i.e. selection of the number of blocks), inferences can easily be made on domains without *a priori* knowledge of the structures in the data.

However, this is not the only option for selecting the number of blocks in an uninformed manner. We can, instead, view each particular choice of K as an individual model. Through the use of an information criterion, we may then select an appropriate model (i.e. the block model with a "good" choice of the number of blocks). This allows us to fix the number of blocks across different realizations of the graph, yet still compare different choices of K in a principled manner.

Model selection remains an open area of research, including in the context of complex networks [14]. There is no dominant information criterion, but several are commonly accepted in the literature. The Bayesian Information Criterion (BIC) is one such criterion, and suggested by the original MMSB paper [7]. Another option is the Deviance Information Criterion (DIC) [15]. Both reward good fits to observed data with respect to log-likelihood while penalizing larger, more complex models, using the number of parameters as a measure of complexity.

BIC and DIC for this model are defined as follows:

$$BIC \approx 2 \log P(Adj|\{\pi_i\}, \{z_{i \to j}, z_{i \leftarrow j}\}, B, \alpha, a, b) - |2K^2 + K| \log(n^2)$$

$$DIC = 2\mathbb{E}[\log P(Adj|\{\pi_i\}, \{z_{i \to j}, z_{i \leftarrow j}\}, B, \alpha, a, b)] - P(Adj|\mathbb{E}[\{\pi_i\}, \{z_{i \to j}, z_{i \leftarrow j}\}, B|\alpha, a, b])$$

While BIC is linear in the number of parameters (and thus quadratic in the number of blocks, as seen here), DIC attempts to penalize the "effective number of parameters" [16]. DIC also usually requires sampling from the posterior distribution of parameters $(\{\pi_i\}, \{z_{i\to j}, z_{i\leftarrow j}\}, B)$. Though this could be accomplished simultaneously with the fitting of the blockmodel, here we sample even more for the DIC estimation, using 1000 posterior samples. Though not as universally accepted as BIC, DIC provides better results as measured by our predictive task.

3 Data and Procedure

Our data are taken from 96 subjects scanned as part of ADNI-2 [17], a continuation of the ADNI project in which Diffusion Imaging was added to the standard MRI protocol. The same dataset was used in Prasad et al. [18], in which the following description is featured. It is reproduced here for completeness, but both the data and its description are effectively the same, with the changes detailed below.

The dataset includes diffusion MRI scans from 50 cognitively normal controls, as well as 46 individuals with Alzheimer's Disease. Subjects were scanned on 3-Tesla GE Medical Systems scanners, which acquired both T1-weighted 3D anatomical spoiled gradient echo (SPGR) image volumes as well as diffusion weighted images (DWI).

The T1-weighted images were first cleared of extra-cerebral tissue, then corrected for inhomogeneity and registered to the Colin27 template using FSL FLIRT [19]. DWI images were corrected for head motion and eddy current distortion via FSL's eddy correct tool. Tractographies were generated for each subject through a global probabilistic tractography method based on the Hough transform [20] using 10,000 fibers (note that this number differs from [18], which used a lookup table accelerated method and 35,000 fibers).

3.1 Connectome Generation

In order to produce FreeSurfer anatomical regions of interest (ROI) connectivity networks, we segmented each subject's cortex into 34 ROIs per hemisphere. Each region was dilated using an isotropic box kernel to ensure its intersection with white matter. Weighted connectivity networks (connectomes) were then generated by counting for every pair of regions the number of fibers intersecting both regions at any point along the fibers.

High resolution connectomes were also computed on the full cortical mesh using a kernel based continuous connectivity framework [21]. Each kernel was sampled at approximately 32000 points and thresholded, providing an 8% sparse connectome which we treat as our graph adjacency matrix. Kernels were then registered to one control subject (which was not used in cross validation) by eigenvector matching.

Both these network generation methods produce weighted adjacency matrices Adj_n , which we treat as realizations of random networks. Note that two different groups of models are fit, one on the anatomical regions and one on the cortical mesh connectomes.

3.2 MMSB and SVM Fitting and Scoring

We fit a mixed membership stochastic blockmodel to one control subject for varying numbers of blocks. In the case of the FreeSurfer ROIs, we use $K \in \{8, 10, \ldots, 20\}$. In the case of the (sampled) Continuous Connectomes, we used $K \in \{40, 42, \ldots, 80\}$. We further computed results for an anatomically seeded

blockmodel, using the Freesurfer ROIs on the cortical mesh. This necessarily uses K = 70 (one region in each hemisphere is usually not connected to any streamlines using FreeSurfer, and thus is dropped unless using the regional seeds themselves).

Throughout the process we use $\alpha = 0.1$, $a = \mathbf{11}^T$, and $b = 5\mathbb{I} + \mathbf{11}^T$. Using the computed membership vectors π_i^{emp} we then construct the observed block connectivities B_{emp} for each subject's Adj matrix by the following:

$$B_{emp} = \hat{\pi} A dj \hat{\pi}^T$$

For each fitted block model we also calculate both BIC and DIC scores.

For both the empirical block connectivities B_{emp} as well as the full connectomes Adj we extract the upper triangular elements and vectorize them to form features. Since the original adjacency is symmetric, the block connectivities are symmetric as well. We train a kernel support vector machine (SVM) using the vectorized connectomes, tuning SVM parameters through an 8-fold validation step before calculating test accuracy on a held out set. We restrict these classifiers to linear kernels. This is repeated for 10 cross validation test folds, for each of which we measure performance in terms of precision, recall, and overall accuracy. We then report the mean of each measure across the folds.

As a means of fair comparison to a generic parcellation, we also generated regions from an ℓ_1 normalized uniform random vector, fixing the number of regions (blocks) to be the same as in the model selected by the BIC and DIC.

4 Results

After running our procedure we arrive at two distinct sets of classification accuracy scores, one for the anatomically generated parcellation and another for the cortical connectivity kernel. Performace results based on anatomical ROI networks are displayed in **Table 1**. For these networks, the optimal number of blocks K was chosen to be 6 by the BIC criterion, and 18 by DIC.

Type	Accuracy	Precision	Recall	F1 Score
Anatomic (68 regions)	0.831	0.883	0.780	0.828
MMSB (K = 6)	0.734	0.736	0.735	0.735
Random $(K = 6)$	0.693	0.699	0.735	0.717
MMSB (K = 18)	0.815	0.835	0.830	0.832
Random $(K = 18)$	0.797	0.854	0.71	0.775

Table 1: SVM performance using anatomical regions as initial network nodes.

Performance results for the continuous connectivity kernel are displayed for two different seeding choices (**Table 2**): one that is purely random, and one using the vertices corresponding to the anatomic parcellation. We compare this to the connectome generated by using the anatomic parcellation without running the MMSB. Note that this is generally not comparable to the anatomic parcellation without the kernel; due to the low number of streamlines compared to the number of nodes or regions (vertices in this specific case), using the same streamline counting technique on a dense cortical mesh model is not possible. The continuous kernel technique is itself an open area of research [21].

We here show results for the BIC suggested number of blocks, K = 40, the DIC suggested number of blocks, K = 78, the number of anatomic regions usually registered by FreeSurfer, K = 68, and the number of regions in the FreeSurfer atlas K = 70. We also display results for the fitted MMSB using seeded regions at the suggested anatomic parcellation, as well as treating the seeded regions as hard clusters (without fitting a MMSB).

Table 2: SVM performance using dense mesh vertices as initial network nodes. Please note that here the "Anatomic Seed" uses the FreeSurfer regions as a initialization for the MMSB, while "Anatomic" refers to their use without further blockmodel fitting.

Туре	Accuracy	Precision	Recall	F1 Score
Random Seed MMSB $(K = 40)$	0.635	0.673	0.530	0.593
Random Seed MMSB ($K = 68$)	0.718	0.755	0.645	0.696
Random Seed MMSB $(K = 70)$	0.630	0.651	0.550	0.596
Random Seed MMSB $(K = 78)$	0.665	0.740	0.600	0.662
Anatomic Seed MMSB $(K = 70)$	0.653	0.667	0.630	0.648
Anatomic	0.633	0.613	0.585	0.601

5 Discussion and Related Work

The results for the anatomically parcellated networks suggest that blockmodels accurately summarize connectomes. Unfortunately the set of linear SVM models for the larger network strictly contains that of the smaller network, so we would not expect a significant improvement in performance since the original case is tractable. However while accuracy scores do not increase, the DIC chosen MMSB representations are a little more than an order of magnitude smaller (a 68 node undirected network has 2278 possible edges, while an 18 node network with self edges has 175).

For the larger connectomes, the block connectivity matrices B_{emp} generated by the MMSB generally allow for much better classification than those generated by the anatomic labels. For both the large and small connectomes the



(a) Exemplar Block 1. Both hemispheres, lateral, anterior, and contralateral views



(b) Exemplar Block 2. Left hemisphere only, medial and lateral views

Fig. 2: Two exemplar blocks from the Random Seed MMSB applied to the 30000 node network (K = 68); the first row shows three views of a block spanning both hemispheres. The second row shows medial and lateral views of one hemisphere for a different block with high connectivity in one contiguous region. Here, p is the probability that a surface point is included in the given block.

DIC suggested networks perform well, though they are not the most accurate observed.

In recent literature, several excellent papers have made use of similar models for automated segmentation. While they do not perform a classification task, nor do they use exactly the same model, their work is nevertheless highly relevant to our own.

Anwander et al. [22] produced one of the first automated connectivity based parcellation methods, using k-means clustering on Broca's Area to produce a parcellation; their method restricted the clusters to be spatially contiguous. Jbabdi et al. [13] introduced a non-parametric Bayes approach to connectivity based parcellation, leveraging a Dirichlet process to learn the posterior distribution of the number of clusters. While this is very important, due to the inherent variability in the number of clusters (by design) comparisons between model fits between subjects and between data sets become quite difficult.

More recently two papers have used the same non-parametric Bayes style of model, notably Hinne et al. [10] and Baldassano et al. [23], the latter of which considers a more general problem of spatially coherent network clustering. Both define Chinese Restaurant Process based models in order to produce posterior estimates of the number of clusters. Relevant to our paper, Hinne et al. use a relative of the SBM, the infinite relational model [12]. This paper particularly highlights the "rich club" theory of brain organization in their choice of models, defining a measure of uncertainty for cluster membership.

Outside of human connectomes, Palovic et al. [9] fit a SBM variant to the C. elegans connectome. Their particular domain has data with cellular resolution (the C. elegans neural system is only 300 cells total), but they make use of very similar techniques, using Akaike's Information Criterion (AIC) for model selection.

Finally, the importance of the work of Sporns et al. [1, 24, 3, 25] cannot be understated; though their methods are mostly based on graph measures and discriminative modularity based models (opposed to the Bayesian generative paradigm), they have provided a strong mathematical foundation for work on human brain connectivity.

6 Conclusion

In this work, we have applied a Mixed Membership Stochastic Blockmodel to the structural connectivity networks of the human brain. After fitting the model for a range of parameters we apply two different selection criteria in order to select the optimal number of blocks. We validate these results by a classification task (independent of model selection or fitting).

For small, coarse resolution connectomes our results show that MMSB models accurately summarize these networks, providing comparable classification accuracy using a much smaller network. For large connectomes these models show a large improvement over anatomic parcellations for classification accuracy.

Though we use the accuracy as a measure of validation, it should be stressed that these parcellations hold interpretable meaning independent of the classification task. While as it stands the use of generative random network models in this work and in the literature has been restricted to preliminary results and explorations, we hope that the further development of these methods might allow for novel exploration and analysis of the brain as a complex biological network. Towards this end we hope to expand this model to incorporate real valued edge weights, data from multiple subjects, and more complex priors.

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