Bayes Optimal Shuffled Graph Classification: Applications in Statistical Connectomics

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Abstract—Graph classification algorithms often do not incorporate vertex label information in their classifiers. In this work, we investigate the extent to which discarding vertex labels can hinder classification performance, and for which random graph models it would be expected to matter. Via theory we demonstrate a collection of results. Specifically, if one "shuffles" the graphs prior to classification, the vertex label information is irretrievably lost, which can degrade misclassification performance (and does whenever the vertex labels have class-conditional signal). Thus, while one cannot hope to recover the labels, trying to recover the labels actually results in a consistent estimate of the optimal graph invariant. This approach therefore solves the question of "which invariant to use" for any graph classification problem, at least asymptotically. Via simulation we demonstrate that a finite (and small) number of training samples can be sufficient to achieve this bound. Finally, we apply this approach to a "connectome" classification problem (a connectome is the complete set of connections within a brain). Unshuffling the graphs indeed improves performance, although not over the best performance achievable composing a number of graph invariant and machine learning tools. Thus, given any unlabeled graph classification problem, the relative performance of an unshuffling approach might be difficult to predict with small sample sizes.

Index Terms—statistical inference, graph theory, network theory, structural pattern recognition, connectome.

1 Introduction

This work addresses graph classification in the presence of vertex label shuffling. A (labeled) graph $G = (\mathcal{V}, \mathcal{E})$ consists of a vertex set, $\mathcal{V} = [n]$, where $n < \infty$ is number of vertices and $[n] = \{1, \dots, n\}$, and an edge set $\mathcal{E} \subseteq [\binom{n}{2}]$. Vertex labels may or may not be observed. In the latter case, vertex v in one graph cannot be assumed to correspond to vertex v in another graph.

MOTIVATION

2 Graph Classification Models

2.1 A labeled graph classification model

Let $\mathbb{G} : \Omega \mapsto \mathcal{G}_n$ be a graph-valued random variable taking values $G \in \mathcal{G}_n$, where $\mathcal{G}_n$ is the set of graphs on n vertices, and $|\mathcal{G}_n| = 2^{\binom{n}{2}} = d_n$. Let Y be a categorical random variable, $Y : \Omega \mapsto \mathcal{Y} = \{y_1, \dots, y_c\}$, where $c < \infty$. Assume the existence of a joint distribution, $\mathbb{P}_{\mathbb{G},Y}$ which can be decomposed into the product of a class-conditional distribution (likelihood) $\mathbb{P}_{\mathbb{G}|Y}$ and a prior π_Y. Because n is finite, the class-conditional distribution distributions $\mathbb{P}_{\mathbb{G}|Y=y} = \mathbb{P}_{\mathbb{G}|y}$ can be considered discrete distributions $\text{Discrete}(G; \boldsymbol{\theta}_y)$, where $\boldsymbol{\theta}_y \in \boldsymbol{\Theta}_{d_n}$ are d_n-dimensional vectors with entries satisfying $\theta_{G|y} \geq 0$ $\forall G \in \mathcal{G}_n$ and $\sum_{G \in \mathcal{G}_n} \theta_{G|y} = 1$.

2.2 A shuffled graph classification model

In the above, it was implicitly assumed that the vertex labels were observed. However, in certain situations (such as the motivating connectomics example presented in Section 1), this assumption is unwarranted. To proceed, we define two graphs $G, G' \in \mathcal{G}_n$ to be isomorphic if and only if there exists a vertex permutation (shuffle) function $Q : \mathcal{G}_n \mapsto \mathcal{G}_n$ such that $Q(G) = G'$. Let $\mathbb{Q}$ be a permutation-valued random variable, $\mathbb{Q} : \Omega \mapsto \mathcal{Q}_n$, where $\mathcal{Q}_n$ is the space of vertex permutation functions on n vertices so that $|\mathcal{Q}_n| = n!$. Extending the model to include this vertex shuffling distribution yields $\mathbb{P}_{\mathbb{Q},\mathbb{G},Y}$. We assume throughout this work (with loss of generality) that the shuffling distribution is both *class independent* and *graph independent*; therefore, this joint model can be decomposed as

$$\mathbb{P}_{\mathbb{Q},\mathbb{G},Y} = \mathbb{P}_{\mathbb{Q}}\mathbb{P}_{\mathbb{G},Y} = \mathbb{P}_{\mathbb{Q}}\mathbb{P}_{\mathbb{G}|Y}\pi_Y. \quad (1)$$

As in the labeled case, the shuffled graph class-conditional distributions $\mathbb{P}_{\mathbb{Q}(\mathbb{G})|y}$ can be represented by discrete distributions $\text{Discrete}(G; \boldsymbol{\theta}'_y)$, where again $\boldsymbol{\theta}'_y \in \boldsymbol{\Theta}_{d_n}$. When $\mathbb{P}_{\mathbb{Q}}$ is uniform on $\mathcal{Q}_n$, all shuffled graphs within the same isomorphism set are equally likely; that is $\{\theta'_{G_i|y} = \theta'_{G_j|y} \, \forall G_i, G_j : Q(G_i) = G_j \text{ for some } Q \in \mathcal{Q}_n\}$.

2.3 An unlabeled graph classification model

Let $\widetilde{\mathcal{G}}_n$ be the collection of isomorphism sets. An *unlabeled graph* $\widetilde{G}$ is an element of $\widetilde{\mathcal{G}}_n$. The number of unlabeled graphs on n vertices is $|\widetilde{\mathcal{G}}_n| = \widetilde{d}_n \approx d/n!$ (see **[?]** and references therein). A *unlabeling function* $U : \mathcal{G}_n \mapsto \widetilde{\mathcal{G}}_n$ is a function that takes as input a graph and outputs the corresponding unlabeled graph. Let $\widetilde{\mathbb{G}} : \Omega \mapsto \widetilde{\mathcal{G}}_n$ be a unlabeled graph-valued random variable taking values $\widetilde{G} \in \widetilde{\mathcal{G}}_n$. The joint distribution over unlabeled graphs and classes is therefore $\mathbb{P}_{\widetilde{\mathbb{G}},Y} = \mathbb{P}_{U(\mathbb{G}),Y} = \mathbb{P}_{U(\mathbb{Q}(\mathbb{G})),Y}$, which decomposes as $\mathbb{P}_{\widetilde{\mathbb{G}}|Y}\pi_Y$. The

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class-conditional distributions $\mathbb{P}_{\widetilde{\mathbb{G}}|y}$ over isomorphism sets (unlabeled graphs) can also be thought of as discrete distributions Discrete$(\widetilde{G};\widetilde{\boldsymbol{\theta}}_y)$ where $\widetilde{\boldsymbol{\theta}}_y \in \boldsymbol{\Theta}_{\widetilde{d}_n}$ are $\widetilde{d}_n$-dimensional vectors. For the shuffle channel associated with the independent and uniform $\mathbb{P}_{\mathbb{Q}}$, we have $\{\theta'_{G|y} = \widetilde{\theta}_{\widetilde{G}|y}/|\widetilde{G}| \,\forall : G \in \widetilde{G}\}$.

3 Bayes Optimal Graph Classifiers

We consider classification in the above three scenarios. To proceed, in each scenario we define three mathematical object: (i) a classifier, (ii) the Bayes optimal classifier, and (iii) the Bayes risk.

3.1 Bayes Optimal Labeled Graph Classifiers

A *labeled graph classifier* $h : \mathcal{G}_n \mapsto \mathcal{Y}$ is any function that maps from graph space to class space. The risk of a labeled graph classifier under $0-1$ loss is the expected misclassification rate $L(h) = \mathbb{E}[h(\mathbb{G}) \neq Y]$, where the expectation is taken against $\mathbb{P}_{\mathbb{G},Y}$.

The *labeled graph Bayes optimal classifier* is given by

$$h_* = \operatorname*{argmin}_{h\in\mathcal{H}} L(h), \tag{2}$$

where $\mathcal{H}$ is the set of possible graph classifiers.

The *labeled graph Bayes risk* is given by

$$L_* = \min_{h\in\mathcal{H}} L(h), \tag{3}$$

where L_* implicitly depends on $\mathbb{P}_{\mathbb{G},Y}$.

3.2 Bayes Optimal Shuffled Graph Classifiers

A *shuffled graph classifier* is also any function $h : \mathcal{G}_n \mapsto \mathcal{Y}$. However, by virtue of the input being a shuffled graph as opposed to a labeled graph, the shuffled risk under $0-1$ loss is given by $L'(h) = \mathbb{E}[h(\mathbb{Q}(\mathbb{G})) \neq Y]$, where the expectation is taken against $\mathbb{P}_{\mathbb{Q}(\mathbb{G}),Y}$.

The *shuffled graph Bayes optimal graph classifier* is given by

$$h'_* = \operatorname*{argmin}_{h\in\mathcal{H}} L'(h) \tag{4}$$

The *shuffled Bayes risk* is given by

$$L'_* = \min_{h\in\mathcal{H}} L'(h), \tag{5}$$

where L'_* implicitly depends on $\mathbb{P}_{\mathbb{Q}(\mathbb{G}),Y}$.

3.3 Bayes Optimal Unlabeled Graph Classifiers

An *unlabeled* graph classifier $\widetilde{h} : \widetilde{\mathcal{G}}_n \mapsto \mathcal{Y}$ is any function that maps from unlabeled graph space to class space. The risk under $0-1$ loss is given by $\widetilde{L}(\widetilde{h}) = \mathbb{E}[\widetilde{h}(\widetilde{\mathbb{G}}) \neq Y]$, where the expectation is taken against $\mathbb{P}_{\widetilde{\mathbb{G}},Y}$.

The *unlabeled graph Bayes optimal classifier* is given by

$$\widetilde{h}_* = \operatorname*{argmin}_{\widetilde{h}\in\widetilde{\mathcal{H}}} L(\widetilde{h}), \tag{6}$$

The *unlabeled Bayes risk* is given by

$$\widetilde{L}_* = \min_{\widetilde{h}\in\widetilde{\mathcal{H}}} L(\widetilde{h}), \tag{7}$$

where $\widetilde{\mathcal{H}}$ is the set of possible unlabeled graph classifiers and $\widetilde{L}_*$ implicitly depends on $\mathbb{P}_{\widetilde{\mathbb{G}},Y}$.

3.4 Parametric Classifiers

The three Bayes graph classifiers can be written explicitly in terms of their model parameters:

$$h_*(G) = \operatorname*{argmax}_{y\in\mathcal{Y}} \theta_{G|y}\pi_y, \tag{8}$$

$$h'_*(G) = \operatorname*{argmax}_{y\in\mathcal{Y}} \theta'_{G|y}\pi_y, \tag{9}$$

$$\widetilde{h}_*(\widetilde{G}) = \operatorname*{argmax}_{y\in\mathcal{Y}} \widetilde{\theta}_{\widetilde{G}|y}\pi_y. \tag{10}$$

4 Shuffling Can Degrade Optimal Performance

The result of passing a graph through a shuffle channel can only degrade, but not improve Bayes risk. This is a restatement of the data processing lemma for this scenario. Specifically, [2] shows that the data processing lemma indicates that in the classification domain, $L^*_X \leq L^*_{T(X)}$, for any statistic T and data X. In our setting, this becomes:

Theorem 1. $L_* \leq \widetilde{L}_* = L'_*$.

Proof: Assume $|\mathcal{Y}| = 2$ and $\pi_0 = \pi_1 = 1/2$.

$$\begin{aligned}\widetilde{L}_* &= \sum_{\widetilde{G}\in\widetilde{\mathcal{G}}_n} \min_y \widetilde{\mathbb{P}}_y(\widetilde{G}) = \sum_{\widetilde{G}\in\widetilde{\mathcal{G}}_n} \min_y \sum_{G'\in\widetilde{G}} \mathbb{P}_y(G') \\ &\geq \sum_{\widetilde{G}\in\widetilde{\mathcal{G}}_n} \sum_{G'\in\widetilde{G}} \min_y \mathbb{P}_y(G') = L_*. \end{aligned} \tag{11}$$

It is trivially true that $\widetilde{L}_* = L'_*$. □

An immediate consequence of the above proof is that the inequality in Theorem 1 is a *strict inequality* whenever the inequality in Eq. 11 is strict:

Theorem 2. $L_* < \widetilde{L}_*$ *if and only if*

$$\min_y \widetilde{\mathbb{P}}_y(\widetilde{G}) > \sum_{G'\in\widetilde{G}} \min_y \mathbb{P}_y(G').$$

The above result demonstrates that even when the labels *do* carry some class-conditional signal, it may be the case that a shuffle channel does not degrade performance. In other words, to state that labels contain information is equivalent to stating that some graphs within an isomorphism set are class-conditionally more likely than others: $\exists\, \theta_{i|y} \neq \theta_{j|y}$ and $Q(G_i) = G_j$ for some $G_i, G_j \in \mathcal{G}_n$ and $Q \in \mathcal{Q}_n$, and that $\theta_{i|y} \neq \theta_{i|y'}$ or $\theta_{j|y} \neq \theta_{j|y'}$. Shuffling has the effect of "flattening" likelihoods within isomorphism sets, from $\boldsymbol{\theta}_y$ to $\boldsymbol{\theta}'_y$, where $\boldsymbol{\theta}'_y$ satisfies $\{\theta'_{i|y} = \widetilde{\theta}_{j|y}/|\widetilde{G}_j| \,\forall i : G_i \in \widetilde{G}_j\}$. But just because the shuffling changes class-conditional likelihoods does *not* mean that Bayes risk must also change. This result

follows immediately upon realizing that posteriors can change without classification performance changing. The above results hold in the absence of equal priors, and are easily generalized to c-class classification problems. To see that, ignoring ties, simply replace each minimum with a sum over all non-maxima:

$$\min_y \mathbb{P}_y(G) \mapsto \sum_{y \in \mathcal{Y}'} \mathbb{P}_y(G) \text{ where } \mathcal{Y}' = \{y : y \neq \operatorname*{argmax}_y \mathbb{P}_y\}.$$

5 Bayes Optimal Graph Invariant-Based Classification After Shuffling

A graph invariant is any function: $\psi : \mathcal{G}_n \mapsto \mathbb{R}^{d'}$ for some $d' < \infty$ such that $\psi(G) = \psi(Q(G))$ for all $G \in \mathcal{G}_n$ and $Q \in \mathcal{Q}_n$. A graph invariant based classifier is a composition of a vector-based classifier with an invariant function, $h^\psi = f^\psi \circ \psi$, where $f^\psi : \mathbb{R}^{d'} \mapsto \mathcal{Y}$. The Bayes optimal graph invariant classifier minimizes risk over all invariants:

$$h^\psi_* = \operatorname*{argmin}_{\psi \in \Psi, f^\psi \in \mathcal{F}^\psi} \mathbb{E}_{\mathbb{P}'}[f(\psi(\mathbb{G})) \neq Y], \tag{12}$$

where Ψ is the space of all possible invariants and $\mathcal{F}^\psi$ is the space of classifiers using invariant ψ. L^ψ_* is the Bayes invariant risk.

Theorem 3. $\widetilde{L}_* = L^\psi_*$.

Proof: Let ψ indicate in which equivalence set G resides; that is, $\psi(G) = j$ if and only if $G \in \widetilde{G}_j$. Then

$$h^\psi = \operatorname*{argmax}_{y \in \mathcal{Y}} \widetilde{\theta}_{\psi(G)|y} \pi_y. \tag{13}$$

Thus, this graph invariant based classifier is the unlabeled Bayes optimal classifier. □

6 A consistent and efficient unshuffling-based classifier

Section 4 shows that one cannot fruitfully "unshuffle" graphs: once they have been shuffled by a uniform shuffler, the label information is lost. Section 5 shows that if graphs have been uniformly shuffled, there is a relatively straightforward algorithm for optimally classifying. However, that classifier depends on knowing $\mathbb{P}' = \mathbb{P}_{\mathbb{Q},\mathbb{G},Y}$ a priori. Instead we consider $(\mathbb{Q}_i, \mathbb{G}_i, Y_i) \overset{iid}{\sim} \mathbb{P}'$. For shuffled graph classification we only observe the *training data* $\mathcal{T}_s = \{\mathbb{G}'_i, Y_i\}_{i \in [s]}$, where $\mathbb{G}'_i = \mathbb{Q}_i(\mathbb{G}_i)$, and are thusly unable to observe useful vertex labels. Moreover, $\mathbb{P}_\mathbb{Q}$ is uniform, such that all label information is both unavailable and irrecoverable. Our task is to utilize training data to induce a classifier, $\hat{h}_s : \mathcal{G}_n \times (\mathcal{G}_n \times \mathcal{Y})^s \mapsto \mathcal{Y}$ that approximates $\widetilde{h}_*$ as closely as possible.

A Bayes plugin unlabeled graph-classifier estimates the likelihood and prior terms and plugs them in to Eq. (10):

$$\hat{h}_s(G) = \operatorname*{argmax}_{y \in \mathcal{Y}} \hat{\widetilde{\theta}}_{j|y} \hat{\pi}_y, \text{ where } G \in \widetilde{G}_j \tag{14}$$

Theorem 4. $\hat{h}_s \to \widetilde{h}^*$ *as* $s \to \infty$

Proof: Given consistent estimators for $\widetilde{\boldsymbol{\theta}} = \{\widetilde{\boldsymbol{\theta}}_y\}_{y \in \mathcal{Y}}$ and $\boldsymbol{\pi} = \{\pi_y\}_{y \in \mathcal{Y}}$, the Bayes plugin classifier is also consistent [2]. Formally, if $\hat{\widetilde{\boldsymbol{\theta}}} \to \widetilde{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\pi}} \to \boldsymbol{\pi}$ as $s \to \infty$, then $\hat{h}_s \to \widetilde{h}_*$ as $s \to \infty$. Because $\mathcal{G}_n$ and $\mathcal{Y}$ are both finite, the empirical distributions are guaranteed to converge by law of large numbers. Thus, $\hat{h}_s \to \widetilde{h}^*$ as $s \to \infty$. □

7 A Practical Approach to Unlabeled Graph Classification

Although Eq. 14 yields consistency from Theorem 4, utilizing this is practically hopeless. In the unlabeled case, this requires solving an infinite number of NP-hard problems. Specifically, using Eq. **??** requires $\boldsymbol{f}$ from Section 5, which is a graph matching function. Graph matching is known to be NP-hard [**?**]. Although there is some hope because most graph matching problems can be solved in polynomial time [**?**], that hope is lost upon discovering that the constant is crazy large [**?**]. We therefore consider an approximate approach as follows.

We assume $(\mathbb{Q}, \mathbb{G}, Y), (\mathbb{Q}_1, \mathbb{G}_1, Y_1), \ldots, (\mathbb{Q}_s, \mathbb{G}_s, Y_s) \overset{iid}{\sim} \mathbb{P}'$, and we only observe $\mathbb{G}', \mathcal{T}_s$, where $\mathcal{T}_s = \{(\mathbb{G}'_i, Y_i)\}_{i \in [s]}$ and $\mathbb{G}'_i = \mathbb{Q}_i(\mathbb{G}_i)$. Given these training data $\mathcal{T}_s$, we proceed as follows.

For each class, $y \in \mathcal{Y}$, choose an exemplar (or prototype [**?**]) shuffled graph, $\mathbb{G}'_{y+} \in \{\mathbb{G}'_i\}_{i:y_i=y}$. Then, try to "unshuffle" each shuffled graph in each class to its corresponding prototype using an inexact graph matching algorithm, $\hat{f}_y = \hat{f}_{\mathbb{G}'_{y+}}$. Although many inexact graph matching algorithms are available, we select the quadratic assignment problem (QAP) based approach developed in [3], which is cubic in n and outperforms the previous state-of-the-art on all benchmarks tested. This yields $\{\hat{\mathbb{G}}_i\}$, which we can then use to estimate the *labeled* likelihoods, $\mathbb{P}_{\mathbb{G}|Y=y}$.

Now, although it may seem as we projected our graphs from a space of cardinality $\widetilde{d}$ to $\widetilde{d} \times n!$, given the labeled graphs, a variety of asymptotically optimal graph classification algorithms are available with much faster convergence rates (under much simpler models). Specifically, we choose to use the signal-subgraph classifier developed in [4]. Under the independent edge assumption, the likelihood of an edge is given by $\mathbb{P}[A_{uv}|Y = y] = \mathbb{P}_{uv|y}$, yielding a likelihood factorization: $\mathbb{P}_y = \prod_{uv} \mathbb{P}_{uv|y}$. Thus, the class-conditional distribution is given by a matrix, $P_y \in (0,1)^{n \times n}$. The labeled graphs, $\{\hat{\mathbb{G}}_i\}$ can be used to estimate these likelihood matrices, $\{P_y\}$, as described in [4] using L-estimators to bound the estimates from the boundaries. Now, we can use a Bayes plugin labeled graph classifier via the class-conditional posterior estimates:

$$\hat{y} = \operatorname*{argmax}_{y \in \mathcal{Y}} \hat{\rho}_y \text{ where } \hat{\rho}_y = \hat{\mathbb{P}}_{uv|y}(\hat{f}_y(G)) \hat{\pi}_y. \tag{15}$$

To gain some intuition with regard to why this approach would be successful, consider the following simple yet illustrative example. Let each $\widetilde{\mathbb{P}}_y$ puts all its mass

on a single but distinct isomorphism set, so $\widetilde{\theta}_{j|y_j} = 1$ and $\widetilde{\theta}_{j'|y_j} = 0 \, \forall j' \neq j$. Thus, if $\hat{f}_y$ worked, then every edge present in a class would have unity likelihood, and all other edges would have zero likelihood. Thus, a single class will have a posterior estimate equal to unity, which will therefore be the maximum a posteriori class. This simple example can be extended without modification to allow each class have a non-overlapping set of non-zero likelihoods. Moreover, reverting to the simple two-class and two non-zero likelihood scenario, consider a different generalization.

8 Simulated Experiment

To demonstrate the practically of an isomorphism-based unlabeled graph classifier, we conduct the following simulated experiment. Sample $s+1$ triplets identically and independently from the joint shuffler/graph/class model, $(\mathbb{Q}_i, \mathbb{G}_i, Y_i) \overset{iid}{=} \mathbb{P}' = \mathbb{P}_{\mathbb{Q}} \mathbb{P}_{\mathbb{G}|Y} \pi_Y$, where $\mathbb{P}_{\mathbb{Q}}$ is uniform, and π_Y is Bernoulli so $\pi_0 = \pi_1 = 1/2$. The edges are independent so the likelihood factorizes as above. Specifically, we let $\mathbb{P}_{uv|0}$ =Bernoulli($p_{uv|y}$), where $p_{uv|0} \overset{indep.}{\sim}$Uniform$(0, 0.7)$, and $p_{uv|0} = p_{uv|1} + 0.3$.

Figure 1 shows the performance of this Bayes plugin classifier as a function of the number of training samples. As we had hoped, performance monotonically increases towards optimal performance (gray dot), even though the graph matching algorithm we used was approximate, and only $\mathcal{O}(n^3)$ instead of exponential.

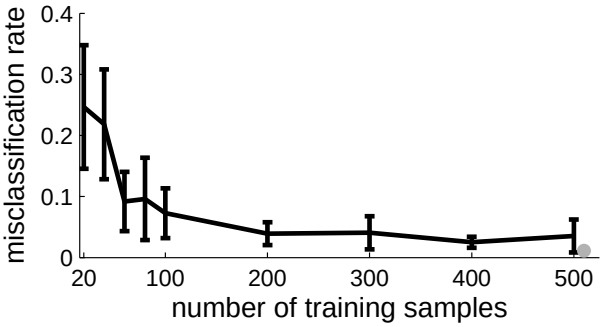

Fig. 1. Inexact graph matching can be used to approximate a consistent shuffled graph classifier. Data in this simulation was sampled from the independent edge model described above. For each number of training samples, we tested using 5000 test samples, and repeated 10 times. The gray dot indicates Bayes optimal performance. (NOTE TO CEP: actually, i forgot to QAP the test data to each training class in this example. i think it would converge much "faster" if i included that step. that is, faster in s, but now testing requires performing 2 QAPs, whereas before, it did not, so it might actually take longer. we will see soon, as i'm running that now.)

9 Unlabeled Connectome Classification

Inspired by the simulated performance of our unlabeled graph classifier, we decided to try it on a real-world application. A "connectome" is a graph in which vertices correspond to biological neural nodes, and edges correspond to connections between the nodes. Diffusion Magnetic Resonance (MR) Imaging and related technologies are making the acquisition of MR connectomes routine [5]. 49 subjects from the Baltimore Longitudinal Study on Aging comprise this data, with acquisition and connectome inference details as reported in [6]. Each connectome yields a 70×70 element binary adjacency matrix. Associated with each graph is class label based on the gender of the individual (24 males, 25 females). Because the vertices are labeled, we can compare the results of having the labels and not having the labels. A k_n nearest neighbor ($k$nn) classifier is universally consistent; that is, guaranteed to achieve optimal performance in the limit [7], and therefore seems more appropriate than an independent edge model. Performance is evaluated with leave-one-out misclassification rate and reported in Table 1. When using the vertex labels, a standard $k$nn achieves 20% misclassification rate. Chance performance (only using the estimated prior) on this data is 49%. These two numbers provide bounds on performance. When all graphs are passed through a shuffle channel, we first try to unshuffle the graphs using the above mentioned QAP algorithm. Given the unshuffled graphs, performance changes to 45%, not particularly impressive. The performance of the independent edge model based Bayes plugin classifier for unlabeled graphs is similarly unimpressive. We therefore develop a hybrid approach in which the independent edge model is assumed, and parameters are estimated using the vertex labels. Given these estimates, we can use the QAP algorithm to match each test graph to the two likelihood matrices, and then use the Bayes plugin classifier. This approach yields a 31% misclassification rate. In contrast, a "standard" graph invariant based approach, which computes the graph invariants from [8], and plugs them into various machine learning algorithms (including the winner [9]), yields misclassification rates as low as 25%.

TABLE 1
MR Connectome Leave-One-Out Misclassification Rates

N/A-QAP	1-QAP	48-QAP	1NN-GI
20%	31%	45%	25%

10 Discussion

In this work, we have address both the theoretical and practical limitations of classifying graphs with and without including labels. Specifically, we show that shuffling the vertex labels results in an irretrievable situation, with a possible degradation of classification performance, and

a necessary degradation if the vertex labels contained class-conditional signal. Moreover, although one cannot hope to recover the vertex labels, estimating them yields an asymptotically optimal classifier. This suggest that efforts to estimate the vertex labels may yield useful classification results, outperforming "standard" graph-invariant based classifiers. Via simulation we show that an approximate graph matching algorithm converges to the optimal performance with only about 500 training samples for a particular independent edge random graph model. Finally, we demonstrate with connectome data that estimating the vertex labels can be useful, but that there remains room to grow to exceed misclassification performance of a carefully chosen graph invariant ∘ machine learning based approach on this data. These connectome data, much like other collections of graphs, can also be equipped with both vertex and edge attributes. As such, we hope to extend the results herein to consider the more general cases.

ACKNOWLEDGMENTS

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Joshua T. Vogelstein is a spritely young man, engorphed in a novel post-buddhist metaphor.

Carey E. Priebe Buddha in training.