Shuffled Graph Classification: Theory and Connectome Applications

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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 shuffling vertex labels can hinder classification performance, and for which random graph models one might expect this invariance to be impactful. 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 often does). A specific graph-invariant classifier is shown to be Bayes optimal. Moreover, this classifier may be induced by training data in a consistent and efficient fashion. Unfortunately, both computational and sample size burdens make this "plugin" classifier impractical. A graph-matched Frobenius norm k_n nearest neighbor (GM-kNN) classifier, however, is also universally consistent, and expected to converge faster whenever "nearness" implies same class. Finally, we apply this approach to a connectome classification problem (a connectome is brain-graph where vertices correspond to (groups of) neurons and edges correspond to connections between them). An approximate GM-kNN classifier on the shuffled graphs performs better than a typical graph-invariant based kNN strategy, but not quite as well as the kNN on the labeled graphs. Thus, we demonstrate the practical utility of the theoretical derivations herein. Extending these results to weighted and (certain) attributed random graph models is straightforward.

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

1 Introduction

Representing data as graphs is becoming increasingly popular, as technological progress facilitates measuring "connectedness" in a variety of domains, including social networks, trade-alliance networks, and brain networks. While the theory of pattern recognition is deep [1], previous theoretical efforts regarding pattern recognition almost invariably assume data are collections of vectors. Here, we assume data are collections of graphs (where each graph is a set of vertices and a set of edges connecting the vertices). For some data sets, the vertices of the graphs are *labeled*, that is, one can identify the vertex of one graph with a vertex of the others. For others, the labels are either unobserved or assume to not exist. We investigate the theoretical and practical implications of the absence of vertex labels.

These implications are especially important in the emerging field of "connectomics", the study of connections of the brain [2], [3]. In connectomics, one represents the brain as a graph (a brain-graph), where vertices correspond to (groups of) neurons and edges correspond to connections between them. In the lower part of the evolutionary hierarchy (e.g., worms and flies), many neurons have been assigned labels [4]. However, for even the simplest vertebrates, vertex labels are mostly unavailable when vertices correspond to neurons. A common strategy for dealing with this "unmatchedness" is to operate in a quotient space of graphs. In the quotient space, a vertex represents a collection of neurons, and this collection is assigned a label. Edges become multi-edges, although they are commonly binarized to obtain simple graphs [5]. Operating in the quotient space of labeled vertices eases graph comparison, as the "graph-matching" sticky-wicket is avoided. Embedding the unlabeled graphs in this quotient space will likely be advantageous for some exploitation tasks, and disastrous for others (for instance, whenever the vertex labels contain all the signal for the specified task). We aim to understand under what circumstances one could expect a classification performance degradation, and to what extent we can recover from losing the vertex label information.

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2 Graph Classification Models

2.1 A labeled graph classification model

A (labeled) graph $G = (\mathcal{V}, \mathcal{E})$ consists of a vertex set, $\mathcal{V} = [n]$, where $n < \infty$ is the number of vertices and $[n] = \{1, \ldots, n\}$, and an edge set $\mathcal{E} \subseteq \binom{[n]}{2}$. Let $\mathbb{G}\colon \Omega \to \mathcal{G}_n$ 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, $Y\colon \Omega \to \mathcal{Y} = \{y_1, \ldots, y_c\}$, 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 class prior π_Y. Because n is finite, the class-conditional distributions $\mathbb{P}_{\mathbb{G}|Y=y} = \mathbb{P}_{\mathbb{G}|y}$ can be considered discrete distributions Discrete$(G; \boldsymbol{\theta}_y)$, where $\boldsymbol{\theta}_y$ is an element of

the d_n-dimensional unit simplex $\triangle_{d_n}$ (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 $Q\colon \mathcal{G}_n \to \mathcal{G}_n$ such that $Q(G) = G'$. Let $\mathbb{Q}$ be a permutation-valued random variable, $\mathbb{Q}\colon \Omega \to \mathcal{Q}_n$, 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

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

As in the labeled case, the shuffled graph class-conditional distributions $\mathbb{P}_{\mathbb{Q}(\mathbb{G})|y}$ can be represented by discrete distributions Discrete$(G; \boldsymbol{\theta}'_y)$, where again $\boldsymbol{\theta}'_y \in \triangle_{d_n}$. When $\mathbb{P}_{\mathbb{Q}}$ is uniform on $\mathcal{Q}_n$, all shuffled graphs within the same isomorphism set are equally likely; that is $\{\theta'_{G_i|y} = \theta'_{G_j|y}\ \forall G_i, G_j\colon Q(G_i) = G_j$ 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 [6] and references therein). An *isomorphism function* $U\colon \mathcal{G}_n \to \widetilde{\mathcal{G}}_n$ is a function that takes as input a graph and outputs the corresponding unlabeled graph. Let $\widetilde{\mathbb{G}}\colon \Omega \to \widetilde{\mathcal{G}}_n$ be an 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 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 $\widetilde{\boldsymbol{\theta}}_y \in \triangle_{\widetilde{d}_n}$ are vectors in the $\widetilde{d}_n$-dimensional unit simplex. Comparing shuffling and unlabeling for the independent and uniform shuffle distribution $\mathbb{P}_{\mathbb{Q}}$, we have $\{\theta'_{G|y} = \widetilde{\theta}_{\widetilde{G}|y}/|\widetilde{G}|$ for all $G \in \widetilde{G}\}$.

3 Bayes Optimal Graph Classifiers

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

3.1 Bayes Optimal Labeled Graph Classifiers

A *labeled graph classifier* $h\colon \mathcal{G}_n \to \mathcal{Y}$ is any function that maps from labeled 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 labeled 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 $h\colon \mathcal{G}_n \to \mathcal{Y}$ (note that the set of shuffled graphs is the same as the set of labeled graphs). 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 classifier* is given by

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

where $\mathcal{H}$ is again the set of possible labeled (or shuffled) graph classifiers. 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 $\widetilde{h}\colon \widetilde{\mathcal{G}}_n \to \mathcal{Y}$ 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 optimal 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 either shuffling or unlabeling a graph can only degrade, but not improve Bayes risk. This is a restatement of the data processing lemma for this scenario. Specifically, [7] shows that the data processing lemma indicates that in the classification domain $L^*_X \leq L^*_{T(X)}$ for any transformation T and data X. In our setting, this becomes:

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

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

$$\begin{aligned}\widetilde{L}_* &= \sum_{\widetilde{G}\in\widetilde{\mathcal{G}}_n} \min_y \widetilde{\theta}_{\widetilde{G}|y} = \sum_{\widetilde{G}\in\widetilde{\mathcal{G}}_n} \min_y \sum_{G\in\widetilde{G}} \theta'_{G|y} = L'_* \\ &= \sum_{\widetilde{G}\in\widetilde{\mathcal{G}}_n} \min_y \sum_{G\in\widetilde{G}} \theta_{G|y} \geq \sum_{\widetilde{G}\in\widetilde{\mathcal{G}}_n} \sum_{G\in\widetilde{G}} \min_y \theta_{G|y} = L_*. \quad (11)\end{aligned}$$

□

An immediate consequence of the above proof is that the inequality in the statement of Theorem 1 strict whenever the inequality in Eq. (11) is strict:

Theorem 2. *$L_* < \widetilde{L}_* = L'_*$ if and only if there exists $\widetilde{G}$ such that*

$$\min_y \widetilde{\theta}_{\widetilde{G}|y} > \sum_{G\in\widetilde{G}} \min_y \theta_{G|y}.$$

The above result demonstrates that even when the labels *do* carry some class-conditional signal, it may be the case that shuffling or unlabeling 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: $\exists\, \theta_{G_i|y} \neq \theta_{G_j|y}$ where $Q(G_i) = G_j$ for some $G_i, G_j \in \mathcal{G}_n$, $Q \in \mathcal{Q}_n$, and $y \in \mathcal{Y}$. Shuffling has the effect of "flattening" likelihoods within isomorphism sets, from $\boldsymbol{\theta}_y$ to $\boldsymbol{\theta}'_y$, so that $\boldsymbol{\theta}'_y$ satisfies $\{\theta'_{G|y} = \widetilde{\theta}_{\widetilde{G}|y}/|\widetilde{G}|\, \forall\colon G \in \widetilde{G}\}$. 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 are easily extended to consider non-equal class priors and c-class classification problems. To see this, ignoring ties, simply replace each minimum likelihod with a sum over all non-maximum posteriors:

$$\min_y \theta_{G|y}\pi_y \mapsto \sum_{y\in\mathcal{Y}'} \theta_{G|y}\pi_y \text{ where } \mathcal{Y}' = \{y\colon y \neq \operatorname*{argmax}_y \theta_{G|y}\}$$

5 Bayes Optimal Graph Invariant Classification After Shuffling

A graph invariant on $\mathcal{G}_n$ is any function ψ such that $\psi(G) = \psi(Q(G))$ for all $G \in \mathcal{G}_n$ and $Q \in \mathcal{Q}_n$. A graph invariant classifier is a composition of a classifier with an invariant function, $h^\psi = f^\psi \circ \psi$. The Bayes optimal graph invariant classifier minimizes risk over all invariants:

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

where Ψ is the space of all possible invariants and $\mathcal{F}^\psi$ is the space of classifiers composable with invariant ψ. The expectation in Eq. (12) is taken against $\mathbb{P}_{\mathbb{G},Y}$ or equivalently $\mathbb{P}_{\mathbb{Q}(\mathbb{G}),Y}$, since invariants are invariant. Let L^ψ_* denote the Bayes invariant risk.

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

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

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

□

6 A Universally Consistent Unshuffling 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 optimal classification. However, that classifier depends on knowing the parameters, $\widetilde{\boldsymbol{\theta}} = \{\widetilde{\boldsymbol{\theta}}_y\}_{y\in\mathcal{Y}}$ and $\boldsymbol{\pi} = \{\pi_y\}_{y\in\mathcal{Y}}$. Instead we consider the data are sampled identically and independently from some unknown joint distribution. $(\mathbb{Q}_i, \mathbb{G}_i, Y_i) \overset{iid}{\sim} \mathbb{P}_{\mathbb{Q},\mathbb{G},Y}$. For shuffled graph classification we observe only 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, so that all label information is both unavailable and irrecoverable. Our task is to utilize training data to induce a classifier $\hat{h}_s\colon \mathcal{G}_n \times (\mathcal{G}_n \times \mathcal{Y})^s \to \mathcal{Y}$ that approximates $\widetilde{h}_*$ as closely as possible.

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

$$\hat{h}_s(\widetilde{G}) = \operatorname*{argmax}_{y\in\mathcal{Y}} \hat{\widetilde{\theta}}_{\widetilde{G}|y}\hat{\pi}_y. \quad (14)$$

Let $\hat{L}_s = L(\hat{h}_s)$ be the risk of the induced classifier using maximum likelihood to obtain the plugin estimate for Eq. (14).

Theorem 4. $\hat{L}_s \to \widetilde{L}_*$ *as* $s \to \infty$.

Proof: Because $\widetilde{\mathcal{G}}_n$ and $\mathcal{Y}$ are both finite, their respective maximum likelihood estimates are guaranteed consistent by the law of large numbers. Hence, the unlabeled graph Bayes plugin classifier is also consistent to $\widetilde{L}_*$ [7]. Note that this classifier is universally consistent, meaning that it converges to $\widetilde{L}_*$ regardless of the true joint distribution, $\mathbb{P}_{\mathbb{Q}(\mathbb{G}),Y}$. □

7 k Nearest Neighbor Universally Consistent Shuffled Graph Classifiers

Although Eq. (14) yields consistency from Theorem 4, utilizing this is practically hopeless as it requires solving s computationally difficult graph isomorphism problems, and acceptable performance will typically require $s \gg \widetilde{d}_n$. Specifically, using Eq. (14) requires first enumerating all $\widetilde{d}_n$ isomorphism sets, then determining in which isomorphism set the to-be-classified graph and each of the training graphs reside. This approach is therefore, in general, impractical because the number of parameters to estimate, $\widetilde{d}_n$, is too large. We therefore consider modified approaches.

A k_s nearest-neighbor classifier using Euclidean norm distance is universally consistent to L_* for vector-valued data as long as $k_s \to \infty$ with $k_s/s \to 0$ as $s \to \infty$ [9]. This non-parametric approach circumvents the need to estimate many parameters in high-dimensional settings such as graph-classification. [10] extended this proof to the graph domain, which we include here for completeness. Specifically, to compare labeled graphs, they considered a Frobenius norm distance

$$\delta(G_i, G_j) = \|A_i - A_j\|_F^2 , \tag{15}$$

where A_i is the adjacency matrix representation of the labeled graph, G_i. Letting $\hat{L}_{kNN}$ indicate the misclassification rate for the Frobenius norm kNN classifier, [10] showed:

Theorem 5. *$\hat{L}_{kNN} \to L_*$ as $s \to \infty$.*

Proof: Because both $\mathcal{G}$ and $\mathcal{Y}$ having finite cardinality, the law of large numbers ensures that eventually as $s \to \infty$, the plurality of nearest neighbors to a test graph will be identical to the test graph. □

Let $\hat{L}'_{kNN}$ indicate the misclassification rate of the Frobenius-norm kNN on *shuffled* graphs. From the fact that the number of shuffled graphs is *equal to* the number of labeled graphs, $|\mathcal{G}'| = |\mathcal{G}|$, the following lemma holds immediately:

Corollary 1. *$\hat{L}'_{kNN} \to \widetilde{L}_*$ as $s \to \infty$.*

The number of unlabeled graphs is vastly less than the number of labeled or shuffled graphs, $|\mathcal{G}'| \approx \mathcal{G}/n!$. Therefore, given that we observed only labeled or shuffled graphs, but not unlabeled graphs, we consider the "graph-matched Frobenius norm" distance

$$\delta(G_i, G_j) = \underset{Q \in \mathcal{Q}_n}{\operatorname{argmin}} \|Q(G_i) - G_j\|_F^2 . \tag{16}$$

Let $\hat{L}'_{GM-kNN}$ indicate the misclassification rate of the kNN classifier using the above graph-matched norm. Given an exact graph matching function—a function that actually solves Eq. (16)—we have the following result

Corollary 2. *$\hat{L}'_{GM-kNN} \to \widetilde{L}_*$ as $s \to \infty$.*

Because $|\widetilde{\mathcal{G}}| \ll |\mathcal{G}|$, it must be that the rate of convergence for the graph-matched norm kNN is faster than the pure Frobenius norm kNN. We prove an even stronger result: the expected misclassification rate for any *finite* number of samples is lower upon using the graph-matched norm than using the pure Frobenius norm:

Theorem 6. $\mathbb{E}[L'_{GM-kNN}] < \mathbb{E}[L'_{kNN}]$

Proof: The expected number of shuffled graphs that are identical to a test shuffled graph G' in each class is equal to $\theta_{G'|y} s_y$, where s_y is the number of graphs in class y. Thus, the expected number of mistakes is simply

$$\mathbb{E}\Big[\sum_{i \in [s]} y \neq \hat{y}\Big] = \min_y \widetilde{\theta}_{G|y} s_y. \tag{17}$$

Let the unlabeled graph corresponding to $\widetilde{G}$ be G'. The number of mistaken unlabeled graphs is $\approx \mathbb{E}\Big[\sum_{i \in [s]} y \neq \hat{y}\Big]/n!$. □

7.1 Practical Shuffled Graph Classification

The discussion in the beginning of the previous section and Theorem 6 together motivate the use of GM-kNN for shuffled graph classification. Unfortunately, Eq. (16) requires solving a graph matching problem, which is NP-hard [8]. Therefore, we instead use an inexact graph matching approach based on the quadratic assignment formulation described in [11], which is only cubic in n. Note that universal consistency is lost upon using an approximate graph-matching function.

8 Unlabeled Connectome Classification

A "connectome" is a brain-graph in which vertices correspond to (groups of) neurons, and edges correspond to connections between them. 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 [12]. Each connectome yields a 70 vertex simple graph (binary, symmetric, and hollow 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. The performance of a 1NN algorithm is reported in Table 1. When using the vertex labels, a "labeled-1NN" achieves 37% misclassification rate. Chance performance (only using the estimated prior) on this data is 49%. These two numbers provide bounds on performance. We then pass all the graphs through a shuffle channel, and implement GM-1NN using the approximately graph-matched Frobenius norm. This approach yields 41% misclassification rate, slightly worse than the labeled graph case. Finally, we compare the performance of our graph-matched 1NN algorithm with

a more "standard" graph-invariant based algorithm, referred to as $\phi(G)$-1NN. In particular, we compute the following 4 graph invariants for each graph: size, max-degree, a greedy approximation to maximum-average-degree, and scan-statistic (see [13] for details). Thus, we obtain a 4×49 element matrix. We linearly squash each row such that all the elements are in $(0, 1)$. Then, we implement a 1NN classifier on this representation of the data, using the Euclidean norm as the distance. This results in 43% misclassification rate, slightly worse than the performance of our graph-matched 1NN.

TABLE 1: MR Connectome Leave-One-Out Misclassification Rates. Labeled-1NN refers to the 1NN classifier using Frobenius norm distance on the labeled graph adjacency matrices. GM-kNN refers to the approximately graph-matched Frobenius norm kNN on the shuffled graphs. $\phi(G)$-1NN refers to using the Euclidean norm distance kNN on the four graph-invariants described in the main text. Chance is the Bayes plugin classifier using only the prior probabilities.

Labeled-1NN	GM-1NN	$\phi(G)$-1NN	Chance
37%	41%	43%	49%

9 Discussion

In this work, we address both the theoretical and practical limitations of classifying shuffled graphs, relative to labeled and unlabeled graphs. Specifically, we show that shuffling the vertex labels results in an irretrievable situation, with a possible degradation of classification performance (Theorem 1). Even if the vertex labels contained class-conditional signal, Bayes performance may remain unchanged (Theorem 2). Moreover, although one cannot hope to recover the vertex labels, one can obtain a Bayes optimal classifier by solving a large number of graph isomorphism problems (Theorem 3). When the generative distribution is unavailable, one can induce a consistent and efficient "unshuffling" classifier by using a graph-matching strategy (Theorem 4). Unfortunately, this is intractable in practice due to the difficulty of graph matching and the large number of isomorphism sets. Instead, Frobenius norm kNN classifier applied to the adjacency matrices may be used, which is also universally consistent (Theorem 5). Convergence rates may be considerably sped up by using a graph-matching Frobenius norm (Theorem 6). Because graph-matching is NP-hard, we instead use an approximate graph-matching algorithm in practice (see **??** for details). Applying these kNN classifiers to a problem of considerable scientific interest—classifying human MR connectomes—we find that even with a relatively small sample ($s = 49$), the approximately graph-matched kNN algorithm performs nearly as well as the kNN algorithm *using* vertex labels, and slightly better than a kNN algorithm applied to a set of graph invariants proposed previously [13]. Thus, this theoretical insight has led us to improved practical classification performance. Extensions to weighted or (certain) attributed graphs are trivial.

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.