

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

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

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

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

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

The *labeled graph Bayes risk* is given by

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

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

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

The *shuffled Bayes risk* is given by

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

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

3.3 Bayes Optimal Unlabeled Graph Classifiers

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

The *unlabeled graph Bayes optimal classifier* is given by

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

The *unlabeled Bayes risk* is given by

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

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

3.4 Parametric Classifiers

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

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

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

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

4 SHUFFLING CAN DEGRADE OPTIMAL PERFORMANCE

The result of either shuffling or unlabeled a graph 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. $L_* \leq \tilde{L}_* = L'_*$.

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

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

□

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. $L_* < \tilde{L}_*, L'_*$ if and only if there exists \tilde{G} such that

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

The above result demonstrates that even when the labels *do* carry some class-conditional signal, it may be the case that 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: $\exists \theta_{G_i|y} \neq \theta_{G_j|y}$ where $Q(G_i) = G_j$ for some $G_i, G_j \in \mathcal{G}_n$ and $Q \in \mathcal{Q}_n$, and that $\theta_{G_i|y} \neq \theta_{G_i|y'}$ or $\theta_{G_j|y} \neq \theta_{G_j|y'}$. Shuffling has the effect of “flattening” likelihoods within isomorphism sets, from θ_y to θ'_y , so that θ'_y satisfies $\{\theta'_{G|y} = \tilde{\theta}_{\tilde{G}|y}/|\tilde{G}| \forall : G \in \tilde{G}\}$. 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 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:

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

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:

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

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

Theorem 3. $\tilde{L}_* = L_*^\psi$.

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

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

□

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 the parameters, $\tilde{\theta} = \{\tilde{\theta}_y\}_{y \in \mathcal{Y}}$ and $\pi = \{\pi_y\}_{y \in \mathcal{Y}}$. Instead we consider $(Q_i, G_i, Y_i) \stackrel{iid}{\sim} \mathbb{P}_{Q,G,Y}$. For shuffled graph classification we only observe the *training data* $\mathcal{T}_s = \{G'_i, Y_i\}_{i \in [s]}$, where $G'_i = Q_i(G_i)$, and are thusly unable to observe useful vertex labels. Moreover, \mathbb{P}_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 \tilde{h}_* as closely as possible.

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

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

Theorem 4. $\hat{h}_s \rightarrow \tilde{h}^*$ as $s \rightarrow \infty$

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

7 A PRACTICAL APPROACH TO UNLABELED GRAPH CLASSIFICATION

Although Eq. 14 yields consistency from Theorem 4, utilizing this is practically hopeless as it requires solving an infinite number of NP-hard problems. Specifically, using Eq. 14 requires first enumerating all all \tilde{d}_n isomorphism sets, then determining in which isomorphism class each of the infinite training graphs resides. Each graph isomorphism problem is NP-incomplete (meaning that it is not known to belong in either P or NP). After solving an infinite number of NP-incomplete problems, to classify, we again solve graph isomorphism for the to-be-classified graph. This approach is therefore impractical on two levels: (i) the number of parameters to estimate, \tilde{d} , is too large and (ii) exact graph isomorphism is too computationally taxing. We therefore consider a modified approach.

Recall from [?] that a k_s nearest-neighbor (k NN) classifier is universally consistent for labeled graph classification problems. If k NN converges faster than the empirical CDF approach, it “must” be because the distance function used effectively smoothes over “nearby” parameters in $\tilde{\theta}_y$, where nearby is defined by the chosen distance. [?] chose squared-Frobenius norm as the distance, $d(G_i, G_j) = \|G_i - G_j\|_F^2$. Therefore, to deal with the excessively large number of parameters problem mentioned above, we use a graph-matched Frobenius norm as the distance function,

$$d(G_i, G_j) = \operatorname{argmin}_{Q \in \mathcal{Q}_n} \|Q(G_i) - G_j\|_F^2. \quad (15)$$

Eq. (15) requires solving a graph matching problem, which is NP-hard. Therefore, we instead use an inexact graph matching approach, based on the quadratic assignment formulation described in [3]. This strategy is only cubic instead of super-exponential in n , and therefore yields a further significant enhancement of convergence rate. Note that while the k NN approach maintains universal consistency [?], the inexact graph matching approximation may not be optimal under certain distributions.

The k NN classifier for shuffled graphs therefore proceeds as follows. First, compute the graph-matched Frobenius norm distance between the test graph and all training graphs, $\{d_i = d(G, G_i)\}_{i \in [s]}$. Second, order the graph/class pairs according to their distances, $d_{(1)} \leq \dots \leq d_{(s)}$. Finally, let the estimated class be the plurality class of the k_s closest graphs; that is, $\hat{y} =$

$\operatorname{argmax}_{y \in \mathcal{Y}} \sum_{i \in [k_s]} \mathbb{I}\{y(i) = y\}$. This algorithm depends on a rule for k_s that satisfies $k_s \rightarrow \infty$ but $k_s/s \rightarrow 0$ as $s \rightarrow \infty$. We let $k_s = 1$ for $s < 10^6$ and then $k_s = 1/s$ thereafter.

8 SIMULATED EXPERIMENT

To demonstrate the practicality 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, $(Q_i, G_i, Y_i) \stackrel{iid}{=} \mathbb{P}' = \mathbb{P}_Q \mathbb{P}_{G|Y} \pi_Y$, where \mathbb{P}_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 $\mathbb{P}_{uv|0} = \text{Bernoulli}(p_{uv|y})$, where $p_{uv|0} \stackrel{\text{indep.}}{\sim} \text{Uniform}(0, 0.7)$, 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.

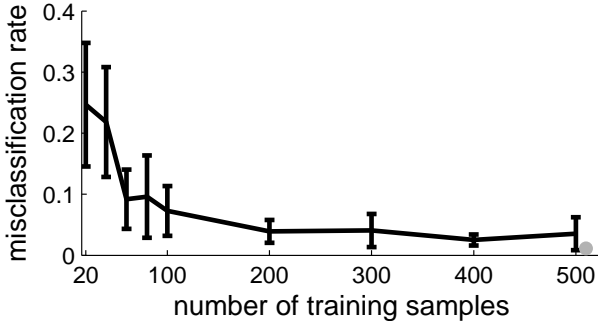


Fig. 1. Inexact graph matching can be used to approximate a consistent shuffled graph classifier. Data in this simulation was sampled from the independent edge model described above. For each number of training samples, we tested using 5000 test samples, and repeated 10 times. The gray dot indicates 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 (knn) 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 knn 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.

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PHOTO
HERE

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

PLACE
PHOTO
HERE

Carey E. Priebe Buddha in training.