

Bayes Optimal 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 the 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 $\mathbb{G}: \Omega \rightarrow \mathcal{G}_n$ 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, $Y: \Omega \rightarrow \mathcal{Y} = \{y_1, \dots, y_c\}$, 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 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 $\text{Discrete}(G; \theta_y)$, where θ_y is an element of the d_n -dimensional unit simplex Δ_{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 $Q: \mathcal{G}_n \rightarrow \mathcal{G}_n$ such that $Q(G) = G'$. Let \mathbb{Q} be a permutation-valued random variable, $\mathbb{Q}: \Omega \rightarrow \mathcal{Q}_n$, 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 $\theta'_y \in \Delta_{d_n}$. 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 [1] and references therein). An *isomorphism function* $U: \mathcal{G}_n \rightarrow \tilde{\mathcal{G}}_n$ is a function that takes as input a graph and outputs the corresponding unlabeled graph. Let $\tilde{\mathbb{G}}: \Omega \rightarrow \tilde{\mathcal{G}}_n$ be an 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 $\tilde{\theta}_y \in \Delta_{\tilde{d}_n}$ are vectors in the \tilde{d}_n -dimensional unit simplex. Comparing shuffling and unlabeled for the independent and uniform shuffle distribution $\mathbb{P}_{\mathbb{Q}}$, we have $\{\theta'_{G|y} = \tilde{\theta}_{\tilde{G}|y}/|\tilde{G}| \text{ for all } G \in \tilde{G}\}$.

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* $h: \mathcal{G}_n \rightarrow \mathcal{Y}$ 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

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

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

The *labeled graph Bayes risk* is given by

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

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 $h: \mathcal{G}_n \rightarrow \mathcal{Y}$ XXX: (note that the set of shuffled graphs is the same as the set of labeled graphs):XXX. 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

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

XXX:where \mathcal{H} is again the set of possible labeled (or shuffled) graph classifiers.:XXX 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* $\tilde{h}: \tilde{\mathcal{G}}_n \rightarrow \mathcal{Y}$ 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

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

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 optimal graph classifiers can be written explicitly in terms of their model parameters:

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

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

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

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 transformation T and data X . In our setting, this becomes:

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

Proof: Assume for simplicity $|\mathcal{Y}| = 2$ 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 the statement of Theorem 1 is strict 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 shuffling or unlabeled 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 θ_y to θ'_y , so that θ'_y satisfies $\{\theta'_{G|y} = \tilde{\theta}_{\tilde{G}|y} | \forall G \in \tilde{G}\}$. 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 are easily extended to consider non-equal class priors and c -class classification problems. To see this, ignoring ties, simply replace each minimum likelihood with a sum over all non-maximum posteriors:

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

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:

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

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

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

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

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

□

6 A CONSISTENT AND EFFICIENT 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, $\tilde{\theta} = \{\tilde{\theta}_y\}_{y \in \mathcal{Y}}$ 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 observe only the *training data*

$\mathcal{T}_s = \{\mathbb{G}'_i, Y_i\}_{i \in [s]}$, where $\mathbb{G}'_i = Q_i(G_i)$, and are thusly unable to observe useful vertex labels. Moreover, \mathbb{P}_Q is uniform, so that all label information is both unavailable and irrecoverable. Our task is to utilize training data to induce a classifier $\hat{h}_s: \mathcal{G}_n \times (\mathcal{G}_n \times \mathcal{Y})^s \rightarrow \mathcal{Y}$ 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):

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

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. $\hat{L}_s \rightarrow \tilde{L}^*$ as $s \rightarrow \infty$.

Proof: Because $\tilde{\mathcal{G}}_n$ 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 \tilde{L}_* [2]. □

7 A PRACTICAL APPROACH TO SHUFFLED GRAPH CLASSIFICATION

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 $s \gg \tilde{d}_n$. Specifically, using Eq. (14) requires first enumerating all \tilde{d}_n isomorphism sets, then determining in which isomorphism set the to-be-classified graph and each of the training graphs resides. There are no known polynomial time solvers for graph isomorphism. This approach is therefore, in general, impractical on two levels: (i) the number of parameters to estimate, \tilde{d}_n , is too large, and (ii) exact graph isomorphism is too computationally taxing. We therefore consider a modified approach.

A k_s nearest-neighbor (k NN) classifier using Frobenius norm is universally consistent to L_* for labeled graph classification as long as $k_s \rightarrow \infty$ with $k_s/s \rightarrow 0$ as $s \rightarrow \infty$ [3]. This non-parametric approach circumvents the need to estimate \tilde{d}_n parameters. For shuffled graphs, we use a graph-matched Frobenius norm as the distance function,

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

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 [4], which is only cubic in n . Note that while the k NN approach with exact matching maintains universal consistency to L'_* , k NN with inexact graph matching approximation may not be consistent.

The k NN classifier for shuffled graphs proceeds as follows. First, compute the graph-matched Frobenius

norm distance between the test graph G and all training graphs, $\{\delta_i = \delta(G, G_i)\}_{i \in [s]}$. Second, order the graph/class pairs according to their distances, $\delta_{(1)} \leq \dots \leq \delta_{(s)}$. Finally, let the estimated class be the plurality class of the k_s closest graphs; that is, $\hat{y} = \operatorname{argmax}_{y \in \mathcal{Y}} \sum_{i \in [k_s]} \mathbb{I}\{y(i) = y\}$.

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, $(Q_i, G_i, Y_i) \stackrel{iid}{=} \mathbb{P}_Q \mathbb{P}_G | Y \pi_Y$, 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 $p_{uv|0} = p_{uv|1} + 0.3$.

We let $k_s = 1$ for $s < 10^6$ and then $k_s = 1/s$ thereafter.

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.

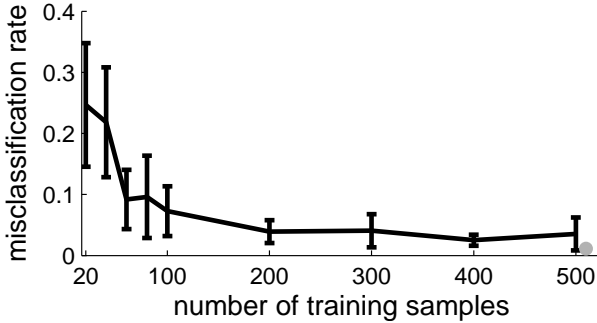


Fig. 1. Inexact graph matching can be used to approximate a consistent shuffled graph classifier. Data in this simulation was sampled from the independent edge model described above. For each number of training samples, we tested using 5000 test samples, and repeated 10 times. The gray dot indicates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

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Carey E. Priebe Buddha in training.

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