Finding Butterfly Species Pattern: a Case Study on Butterfly Similarity Networks

Qiwen Wang

I. Introduction

OBJECT detection has recently been more and more thoroughly studied. The human visual system can distinguish objects with fast speed and great accuracy. A lot of object detection algorithms have also been developed to use machine learning to achieve real-time, multiple object detection. Although these algorithm can detect hundreds of object, but only top-level category of the objects can be specified (car, cat, person, etc), without any fine-grained detail information about the object. On the other hand, biology taxonomy plays an important role in distinguishing fine-grained features. Biological classification in the field of botany, mycology, zoology and entomology, classifies organisms using a set of rules. The goal of fine-grained image classification is to distinguish objects with subtle difference. The general deep learning algorithm is not suitable for classify organisms in a fine-grained level. The objects in different classes may share the similar shape and color, but have different scale and pattern, which makes it difficult to distinguish the subtlety in a general machine learning tasks. Thus the urge to have techniques to classify the domain-specific species is strong.

In this project, we want to use butterfly species network as a case study, to classify butterflies by studying the feature similarities between different categories of butterfly. In the following sections, we will try to answer the following questions by conducting different methods in network analysis. 1) What are the general features of the entomology similarity network? 2) what category of butterfly is easy to be classified/not easy to be classified? Does the result meet with the human visual classification? 3) Given an image of butterfly or its similarity information, can we tell which butterfly category does it related to? By answering these questions, we can better understand the characteristics of the fine-grained butterfly network, and are be able to classify the butterfly into the right species.

In Section III, we will introduce the butterfly species dataset and how the relationship between butterfly is represented. We will then analyze the characteristics of the network, and try to make prediction on the difficulty of classifying the species in Section IV. We further apply community detection to predict the number of species class there is from the dataset, and it's relationship between the actual species class in Section V. Lastly, we will perform Graph Convolutional Network on the dataset to classify butterfly label in Section VI.

Project Github Link: https://github.com/qwang70/cs224w

II. Related Work

In the past people have conducted many researches that study the biological network. Bo, Wang et al[1]. proposed a framework to denoise the biological networks using network enhancement. The algorithm uses a doubly stochastic matrix to diffuse the network. It reassigns weight to each of the edge, in that loosely interacted edges get lower weights, while edges with high similarity get higher weights. With Network Enhancement, weekly connected noisy edges can be removed, and it leads to better performance. This paper proposed an algorithm that pertains the original network information, and makes the network more sparse, thus increases the network analysis efficiency. However this pre-process step doesn't provide any structure information that closely related to the network. It still remains unknown whether the network enhancement can help us better classify the species. In this work, we will extract network features, and discover if these features can help improving classifying node labels

Deep learning algorithms to classify different objects have been widely studied in different areas. Krizhevsky et al.[2] suggested to use convolutional neural network to classify image categories; Liang and Hu[3] purposed to use recurrent convolutional neural network for object detection; real-time multiple object detection can be achieved by Redmon et al[5]. These algorithms can be applied directly on butterfly images, but we loss the information on how each butterfly species associated with each other, which is considered important in taxonomy. The problem can be addressed by the graph convolutional networks by Kipf and Welling[4]. The neural network model is constructed by utilizing the property of spectral graph convolution, and can capture the desired network structure. Although this algorithm is relatively efficient, for large scale graph such as the gene interaction graph, the worst space complexity is linear to the number of edges in the graph. Thus large graph might not be fitted into GPU, and have to run in CPU. In this work, we will discuss using different features as input to the graph convolutional network with Node2Vec embedding, and how different features perform.

III. Dataset and Representation

We will use the cleaned data provided by BioSNAP. Specifically, we will analyze the data from the enhanced butterfly similarity networks. The fine-grained BioSNAP butterfly species network is constructed by The dataset contains 832 nodes that represent the butterfly, and 86528 edges after the network enhancement representing the similarity between two butterfly. The original dataset that BioSNAP dataset is based on, is the Leeds butterfly species image dataset [7].

The original dataset consists of 832 butterfly images and the labeled class representing a butterfly species. There are 10 classes in total, and each butterfly image only has one unique class label. Each label corresponds to a relative balanced number of butterfly, ranging from 55 to 100 images per species. The class description is also included in the dataset.

The edge similarity between two butterflies in BioSNAP butterfly similarity networks is calculated by 1) computing the embedding of the corresponding images, 2) get the weight for the adjacent matrix and 3) enhance the network by adjusting the edge weight[1]. Two embedding method is applied to the butterfly images: Fisher Vector[8] and Vector of Linearly Aggregated Descriptors with dense SIFT[9]. Let x_i be the resulting feature vector for node i, the weighted adjacency matrix W for the similarity graph is then constructed by

$$W(i,j) = \exp\left(-\frac{||x_i - x_j||^2}{\sigma^2(\epsilon_i + \epsilon_j)^2}\right),$$

where ϵ adjusts the local scales of the distance, and is defined as

$$\epsilon = \frac{\sum_{j \in \text{neighbor}(i)} ||x_i - x_j||}{\#\text{ neighbor of } i}.$$

However, the result of such construction gives a fully connected network with a lot of weak edges. It significantly increases the input size and the amount of unimportant data. The network is enhanced by removing weak edges and enhancing the weight for the strong edges using the information flow from the random walks of length less than or equal to 3. The network after the network enhancement step is the fine-grained BioSNAP butterfly sprcies network we are using.

We read the dataset into Python using SNAP and Networkx library construct the network. The network is weighted and undirected. There exists an edge between two nodes if and only if the butterfly corresponding to two nodes are similar. Each edge has two attributes: similarity score and label. Label is a number from 1 to 10, and has a corresponding species name and description from Leeds Butterfly dataset.

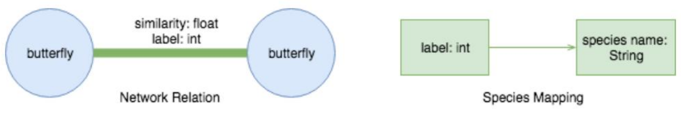


Fig. 1. The Butterfly Similarity Network Structure.

IV. Extracting Network Features

In order to measure the characteristics of the butterfly similarity network, we focus on several network analysis. They include: 1) Relationships between butterfly with common features 2) Similarity between different species in general 3) Species from the community detection

A. *Assortativity*

Correlation between nodes with similar degree is often find in networks. Assortativity describes the correlation between two nodes. A positive assortativity coefficient means that nodes with large degree tend to connect with nodes with large degree; nodes with few degree tend to connect with nodes with few degree. On the other hand, a negative assortativity coefficient represents the tendency that high degree nodes connect with low degree nodes. Social network is usually assortative mixing (has positive assortativity coefficient), and biology network is usually disassortative (has negative assortativity coefficient)[7].

Although our network is weighted, were expecting to see the assortativity coefficient on weighted and unweighted network to have the same sign, since we are confident on the similarity if theres an edge between two nodes.

We use Newmans metric to measure the assortativity for the unweighted network. The assortativity for unweighted network is defined as

$$r_{unweighted} = \frac{\frac{1}{M}\sum_{e(i,j)\in E} d_i d_j - [\frac{1}{2M}\sum_{e(i,j)\in E}(d_i + d_j)]^2}{\frac{1}{2M}\sum_{e(i,j)\in E}(d_i^2 + d_j^2) - [\frac{1}{2M}\sum_{e(i,j)\in E}(d_i + d_j)]^2}$$

where M is the total number of links/edges in the network. Edge $e(i,j)$ represents an edge connected by node i and node j. Degree di represents the degree of node i. This metrics considers the average edges and the variance of edge number, and is then normalized for the purpose of comparing different networks. The weighted assortativity metrics is similar to the unweighted metrics, but multiply the weight of edges:

$$r_{weighted} = \frac{\frac{1}{H}\sum_{e(i,j)\in E} w_e d_i d_j - [\frac{1}{2H}\sum_{e(i,j)\in E} w_e(d_i + d_j)]^2}{\frac{1}{2H}\sum_{e(i,j)\in E} w_e(d_i^2 + d_j^2) - [\frac{1}{2H}\sum_{e(i,j)\in E} w_e(d_i + d_j)]^2}$$

where His the total weight of links/edges in the network, and we is the weight of edge e.

From our network, $r_{unweighted} = 0.2238$ and $r_{weighted} = 0.5215$. We verify that both unweighted and weighted assortativity coefficient has the same sign. Since the assortativity coefficient is positive, nodes with high degree is more likely to connect with other nodes with high degree.

However, Newman suggested that biological networks tend to be disassortative[7], why is the assortativity coefficient positive? The biological networks that Newman used to generalize the network property are protein interaction network and neural network that contains low-level organic features. The butterfly similarity network, on the other hand, is more like a social network, in that it connects butterflies that are relative, despite it is also a biological network. Intuitively, butterfly with same labels are similar to each other. If there are more nodes in a cluster, the higher degree a node would have, and the node tends to connect with nodes in the same clustering. The assortativity coefficient implies that the butterfly similarity network can be clustered.

B. Species with Distinguishable Characters

We are also interested in finding out whether a species can be more easily classified than the others. To answer this question, we check the number of different species that the node is similar to. The less the other species the node is similar to, the easier the butterfly can be correctly classified. For butterflies in each category, we count the percentage of nodes that are related to the other categories. The higher the percentage is when the number of similar species is small, the species is easier to be classified or distinguished.

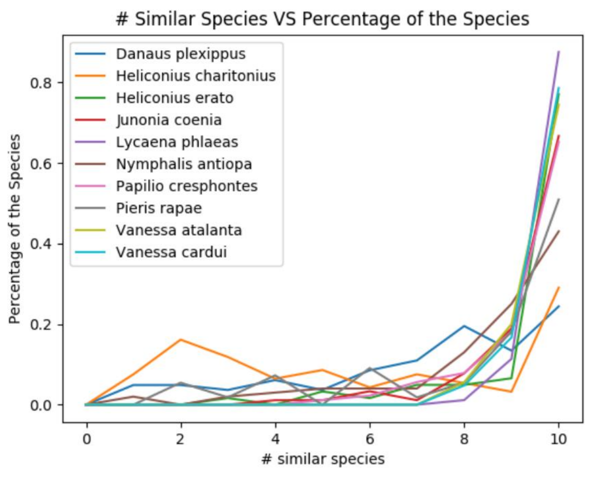


Fig. 2. Number of similar species related to each node in 10 species.

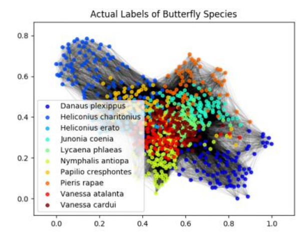
It is obvious from Figure 2 that a big portion of Heliconius Charitonius butterflies only connect to small number of species. But for species like Lycaena phlaeas and Vanessa cardui, almost every butterfly in these species is similar to all the other species. It makes distinguishing them from other species difficult. This observation also motivates us to use community detection based and machine learning based method.

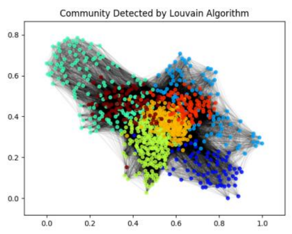
V. Community Detection

To further understand the network structure, we use community detection to achieve two goals: 1) find the similar species that are similar, 2) classify the butterfly purely based on the community detection. Communities S is a set of tightly connected nodes in a network. Modularity Q measures how well a network is partitioned into communities. We can identify the communities by maximizing the modularity

$$Q \propto \sum_{s\in S}[\text{ edges in group}s - E(\text{ edges in group}s)].$$

We use the efficient greedy Louvain algorithm to detect the community. Louvain algorithm is consists of two steps: 1) Optimize modularity by local changes of the communities, 2) aggregate the identified community. Iterate over these two steps until step 1 cant make any gain. Using Louvain algorithm, we achieved 7 groups in Figure 2. Compare to the actual groups plotted by Figure V, several communities are





merged by the louvain algorithm. These merged communities may share the similarity, and may be harder to classified.

Comparing Figure 2 V, we find that Vanessa Cardui and Lycaena Phlaeas species are combined species from the community detection algorithm. In the section IV, we have also observe that these two species is similar to lots of species. We have verified that these two species are hard to distinguish from each other. Species like Heliconius Charitonius and Nymphalis Antiopa are classified correctly with the corresponding community. With the community detection, we can distinguish these two species.

VI. Graph Convolutional Networks

As we discussed above, from our preliminary network feature extraction, the butterfly similarity network exhibit both neighborhood connectivity and community structure patterns. The butterfly similarity network offers a valuable dataset for classifying and predicting fine-grained butterfly species. However, unlike the structured dataset, the high-order network structure is not expressed from the raw data. Instead, structural information are latent in the weighted adjacent matrix of the network. In order to classify the nodes efficiently, we need a model that could incorporate the latent graph structure information. The network node classification problem is assemble to the image classification problem where the input data of both problems have local and global structure that is not expressed by the raw adjacent matrix. Using convolutional neural network has grown in popularity and is a common approach for image recognition. Thus it is natural to use neural network to the network label prediction problem.

A. From Convolutional Neural Network to Graph Neural Network

Convolutional Neural Network(CNN) is one of the most influential innovations in computer vision and have proven to be successful in a lot of real world applications. The input of CNN is a multi-channeled image (with RGB channels). In the convolutional step, it takes a filter and slide over the complete image, and take the dot product between the filter and chunks of the input image at the same time. The result of each dot product is a scalar, and the convolution over the image is a matrix.

CNN has the properties of local connectivity and parameter sharing. Local connectivity is the property that each neural in the network only connects to a small number of the input. A pixel of a image only has the local connectivity with the data representing the pixel that is around. Parameter sharing is sharing the weights by all neurons in the network in a specific feature matrix. In a standard neural network, all the neurons are fully connected and doesn't share the weight parameters. Thus the convolutional neural network reduces the number of parameters in the network, and make the forward and backward computation more efficient.

However, it is problematic to apply CNN directly on graph. There are two main problems. Firstly, because of the local connectivity in CNN, the data in the model only dependent on the data that is spatially close to it. When applying CNN to graph networks, the learned model would only be able to reveal the patterns that is related to the specific node in the works, but will be failed to consider the higher-order network structures.

Secondly, considering using the weighted adjacent matrix as a naive approach to feed the input feature matrix to CNN. The size of the input feature matrix is $O(n^2)$. For a social network, the number of node size can easily reach billions. Since the input matrix size and trainable parameters grow rapidly, it would make the backpropagation intractable, and limit the range of possible applications. Thus we need a method to choose the feature vector smartly. We propose a solution by using node2vec embedding as features, to limit the number of trainable parameter in section VI-B.

B. Node2Vec

The goal of Node2Vec is to encode nodes so that similarity in the embedding space approximates similarity in the original network. Compared to the original weighted adjacent matrix, using Node2Vec embedding, we can take control of the size of the embedding vector, and achieve a reasonable embedding for the node that could possibly reveal more node structure than the weighted matrix.

The idea of Node2Vec from the work by Leskovec et al[10] is to use flexible, biased random walks that can trade off between local and global views of the network. It first characterizes the feature learning problem in graphs as a maximum likelihood problem. Let $G = (V, E)$ be the network graph and $f : V \to R^d$ be the mapping function from nodes to feature representations we aim to learn. Let $N_s(u) \subset U$ be the network neighborhood that is generated from a sampling strategy starting from node u. The objective function can then be described by

$$\max_f \sum_{u \in V} \log \Pr(N_s(u)|f(u)).$$

Two assumptions are made to make the optimization problem computable:

- Conditional independence: the probability of traversing to a neighborhood node is independent to that of traversing to any other node. That is:

$$\log \Pr(N_s(u)|f(u)) = \prod_{n \in N_s(u)} \Pr(n_i|f(u)).$$

- Symmetry in feature space: in the feature space, A source node and neighborhood node have a symmetric effect over each other. This assumption also limits the feature extraction to the undirected graph. Note that our butterfly species similarity graph is also undirected. In the paper, it uses the softmax over a pair of connected nodes.

$$\Pr(n_i|f(u)) = \frac{\exp(f(n_i) \cdot f(u))}{\sum_{v \in V} \exp(f(v) \cdot f(u)))}.$$

The embedding problem can than be re-formed as a minimization problem and use negative sampling to approximate $\sum_{v \in V} \exp(f(v)\dot{f}(u)))$, which significantly reduces the computational cost.

Then Node2Vec proposed a way to interpolate three standard sampling strategies: random walk, Breath-First-Search (BFS) and Depth-First-Search (DFS) by setting a search bias α. The search bias α controls the direction of walk. Two hyperparameter is needed for Node2Vec: return parameter p and in-out parameter q. Parameter p controls the probability of revisiting a node in the walk. Parameter q allows the search a further away node from the last visited node. Let v be the current node on the walk, t be the last visited node on the walk, and x be the neighbor of v. The unnormalized transition probability can de formalized as the following:

$$\pi_{vx} = \alpha(t, x) \cdot w_{vx}$$

where

$$\alpha(t, x) = \begin{cases} \frac{1}{p}, & \text{if } dist_{tx} = 0 \\ 1, & \text{if } dist_{tx} = 1 \\ \frac{1}{q}, & \text{if } dist_{tx} = 2 \end{cases}$$

Thus if the return parameter p is big, the random walk is less likely to revisit a revisited node in the next two step. If the in-out parameter $q > 1$, the random walk is more likely to move towards nodes close to the last visited node t, thus generates a local view of the network with respect to the starting node, and approximates the behavior of BFS. On the other hand, if the in-out parameter $q < 1$, the random walk is more inclined to visit the neighbor nodes that are farther away from the last visited node t. The walk would obtain a global view of the network, and performs DFS-like exploration. Note that these random walks are not strictly BFS and DFS, but have higher bias towards BFS and DFS within the frame of random walk.

In our model, we generate features from the embedding of Node2Vec with three different sampling method: strict random walk, BFS-like, and DFS-like. We set the fixed length of the walk to be 80, and the number of walk to be 10. The hyperparameter we choose is in the following table I.

TABLE I
NODE2VEC PARAMETERS

Method	Return Parameter p	In-Out Parameter q
Random Walk	1	1
BFS	1	2
DFS	1	0.5

C. GCN Model

In this section, we introduce the architecture for the Graph Convolutional Model that was proposed by Kipf and Welling[4]. The overall structure of GCN model is similar to that of a Convolutional Neural Network, but will have different propagation model. We will first introduce the general structure of the network, and then derive the forward propagation model.

1) Architecture: For a graph $G = (V, E)$, the input layer of GCN is a a feature matrix $X = H^{[0]} = R^{N\times F}$ where $N = |V|$ and F is the number of features for each node i. $X[i, f]$ represents the f-th feature of node i. Our model will only contain 1 hidden layer $h^{[1]}$, since from the work of Kipf and Welling[4], increasing the number of layer can decreases the accuracy of the model, which is counter-intuitive. This is because increasing the layer is equivalent to increasing the size of k-th order neighborhood, and leads to the issue of overfitting. The best result obtained is with a 2- or 3-layer model. In the iteration of the hidden layer, we will apply the non-linear activation function ReLU. The non-linearity is required to ensure the neural network is not just a linear regression model. The activation function ReLU is the most popular activation function for the deep neural network, and is defined as $f(x) = max(0, x)$. We also drop off 50% of edges between the layer to avoid overfitting.

In the output layer, we will use softmax to map the vector to range 0 and 1. All the entries is added to 1 over F dimensions. Since our problem is a single label prediction problem, the label of the input data is decided by the max value among all the entries. The softmax function is defined as below:

$$\sigma(\mathbf{x})_i = \frac{\exp(x_i)}{\sum_{f=1}^{F}\exp(x_i)}.$$

The overall Graph Convolutional Network Model has the architecture shown in Figure 3.

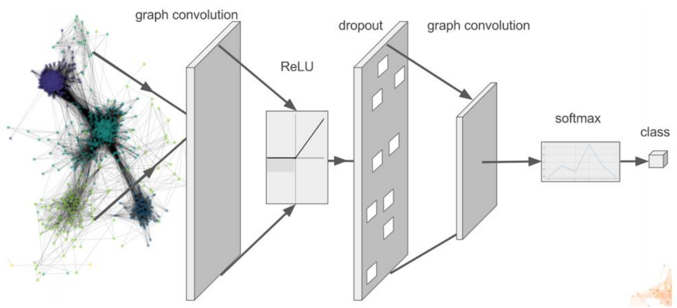


Fig. 3. GCN Model Architecture

2) Propagation Model: Now we will derive the propagation model that we will be using in our GCN Architecture. Firstly, we generalize the propagation rule for a multi-layer neural network. It can be written as a non-linear function

$$H^{(l+1)} = f(H^{(l)}, A),$$

where f is a non-linear function, and A is an adjacent matrix. One naive implementation of f is to incorporate the graph filtering at each hidden layer as following:

$$f(H^{(l)}, A) = \sigma(AH^{(l)}W^{(l)}),$$

where σ is some non-linear activation function, and $W^{(l)}$ is the weight matrix at level l.

There are two limitations of the function:

1) The aggregated representation of the node f doesn't include its own feature. Because the adjacent matrix A only consider the neighbors' features, the resulting matrix is also a sum of the neighbors' features without considering its own feature. This problem can be solved by adding a self loop to every node. Equivalently, we can add an identity matrix to the adjacent matrix. Let's define the new matrix as $\tilde{A}$. Thus,
$$\tilde{A} = A + I.$$
2) Nodes with large degrees will have large values in the adjacent matrix, and large values in the feature representation f. Similarly, node with small degrees will have small values in f. This would cause exploding or vanishing gradients, and would cause the stochastic gradient descent algorithms that used to update the parameters sensitive to the scale of the input features. Kipf and Welling[4] proposed the following pre-processing method to normalize the adjacent matrix. With the adjacent matrix with self loop $\tilde{A}$, they define $\tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$. Then they normalize the adjacent matrix with self loop by replacing $\tilde{A}$ with
$$\hat{A} = \tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2}.$$

Therefore, combining both improvement described above, the final forward propagation model we will use is

$$H^{(l+1)} = \sigma(\tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2}H^{(l)}W^{(l)}).$$

Since we will train a two-layer GCN model for the node classification problem on the network, we only have one hidden layer. Thus the forward model can then take the form as

$$Z = f(X, A) = \text{softmax}\left(\hat{A}\text{ReLU}\left(\hat{A}XW^{(0)}\right)W^{(1)}\right),$$

where the weight parameters $W^{(0)}, W^{(1)}$ are the trainable parameters.

D. Baseline: Multi-layer Perceptron

We compare the GCN model with the baseline model Multi-layer Perceptron(MLP) as in Sathyanarayana[11]. The architecture of MLP is similar to the GCN model proposed except the propagation function. Our baseline model is a 2-layer neural network with ReLU as the activation function and dropout random edges between layers. The MLP doesn't use the graph convolutional sum, but uses the standard matrix sum instead. Table II shows the difference of the propagation function between MLP model and GCN model.

TABLE II
COMPARISON OF PROPAGATION MODELS.

Description	Propagation Model
Baseline MLP	XW
Naive GCM	AXW
Normalized GCM	$\tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2}XW$

E. Experiment Set-Up

Using the same Butterfly Species Network dataset described in Section III, the network has 832 nodes and 10 labels. We will then describe how the network is set up.

1) Feature Selection: We first run Node2Vec algorithm implemented by Grover, Aditya and Leskovec[10] with different hyperparameter p, q values described in Table I. We configure the rest of the hyperparameters for Node2Vec for these three sampling methods based on Table III.

TABLE III
NODE2VEC HYPERPARAMETERS

Hyperparameters	Value
Weighted	True
Directed	False
Num. dimensions	128
Length of walk per source	80
Num. walks per source	10
Optimization context size	10
p, q	see Table VI-B

Besides using the embedding from Node2Vec as features, we will only explore the standard feature matrices with size $R^{N\times N}$: 1) Diagonal matrix and 2) weighetd matrix. It is more expensive to update the parameters with these two feature matrix. We want to see if the matrix with reduced size can outperform the traditional methods. We will also try the combination of traditional feature and node2vec embedding feature, by concatanating the weighted matrix and the node2vec feature matrix. We want to explore if a combination of different kind of features can outperform the model using only one of these features.

2) Graph Convolutional Network Hyperparameters: The GCN implementation we leveraged was from Kipf and WellingVI. Since our input data are sorted by labels, in order to ensure the training and testing is unbias, we first randomly shuffle the data. We then partition the data such that 70% of data are the training data, 20% of data are the evaluation data, and 10% of data are the testing data. Such partition can effectively avoid overfitting the training model.

The hyperparameters are shared between models with different input layer features. We don't limit the number of epoches for training. The optimization only terminates when the cost for the last iteration is greater than the average cost for the last s iterations, where s is the number of epoches for early stopping set in the hyperparameter. The stopping criterion is thus

$$cost[curr] > avg(cost[curr - s - 1 : curr - 1]),$$

where $curr$ is the current iteration. We configured the hyperparameters for GCN in Table III. In order to fairly compare the baseline model MLP and GCN model, we control variates of both model, so that MLP model also uses the hyperparameters in Table III.

TABLE IV
GCN AND MLP HYPERPARAMETERS

Hyperparameters	Value
Num. Hidden Layers	1
Num. Hidden Units	16
Initial learning rate	0.01
Dropout Rate	0.5
Weight for L2 loss	5e-4
# Epoches for Early Stopping	10

3) Performance Metrics: For each model we train, we compute the following metrics for the evaluation data and testing data.

Evaluation and Test Accuracy: This metric computes the fraction of butterflies that are correctly classified by the model.

Number of Training Epoches: This metric counts the number of epoches before the stopping criterion is met. The smaller number of epoches implies the GCN model converges faster.

Confusion Matrix of Testing Data: for the predicted label y_{pred} and the real label y_{real}, the confusion matrix computes the percentage of testing data with label y_{real} that has the predicted label y_{pred}.

F. Experiment Result

1) Baseline Model: MLP: With Node2Vec Embedding as features, our baseline model MLP underfits the dataset but converges fast.

TABLE V
MLP RESULTS ON NODE2VEC EMBEDDING

Node2Vec Embedding Method	Eval acc.	Test acc	Epoches
Random Walk	0.25904	0.29762	12
DFS	0.47590	0.60714	55
BFS	0.51807	0.42857	56

From the result table of MLP in Table V, the accuracy of the evaluating and testing scores are mostly lower than 0.5. A model that randomly guesses the label has the model accuracy 0.1, since there are 10 labels in total, and the dataset is roughly even. The MLP model outperforms the random guessing model.

Among the three embedding method, the random walk sampling performs the worst. This might be due to the fact that the network has low number of diameter; the random walk from the source walk becomes more random after the initial several steps. Thus it is likely that the embedding of the node is incline to be random and doesn't capture much information about the node structure. We also notice that the MLP model with random walk only takes 12 epoches to stop, where the number of early stopping is 10. This implies that the cost of the model is not improving significantly after 2 iterations, which is also due to the randomness of the embedding features.

The MLP models using BFS-like and DFS-like walk have similar performance in the evaluating and testing accuracy and the number of epoches. Note that the testing accuracy of the DFS-like MLP model is higher than the evaluating accuracy. This is counter-intuitive, but is still understandable due to the randomness of the training and evaluation data being selected. We should be able to get a lower testing accuracy by performing the experiment multiple times or applying cross-evaluation and take the average of the accuracy. The MLP models do not overfit the training data, since the gap between the accuracy for the evaluating data and testing data is small. Therefore, the hyperparameters we chose are reasonable.

2) Proposed Model: GCN: With Node2Vec Embedding as features, the GCN model we proposed significantly outperforms the baseline model MLP. Especially, the GCN model with BFS embedding outputs a higher accuracy than the other two models.

TABLE VI
MLP RESULTS ON NODE2VEC EMBEDDING

Node2Vec Embedding Method	**Eval acc.**	**Test acc**	**Epoches**
Random Walk	0.73024	0.70238	166
DFS	0.69244	0.702	62
BFS	0.77491	0.78571	134

From the result table of GCN in Table VI, the accuracy of model using three sampling methods increase significantly. The models are able to perform acceptable label predictions. Among these features with Node2Vec embedding, embedding with BFS-like random walk performs best. Recall that the embedding from BFS-like random walk reveals the local view of the network. It has similar embedding for the data point with similar structure role. For example, the dot product for the embedding of a pair of nodes with high degrees would be higher than the embedding of a pair of nodes whose degrees differ a lot. In the butterfly species network, butterflies within the same class are likely to connect to each other, thus would have similar degrees, and leads to good performance in label prediction.

The intuition behind BFS-like embedding optimize label prediction, but DFS-like embedding also performs decent classification. From Section V, we observed that the community detection can't predict the exact number of butterfly species class, and may merge multiple class into the same community. Because of the property of the butterfly similarity network that nodes in the same community are likely to have the same label, the GCN model with DFS-like embedding, that can be used to detect community, has a reasonable accuracy in predicting labels.

3) Confusion Matrix and Plot on Wronly Classified Labels: Next, we want to compare the confusion matrix of the GCN models with different embedding, and check whether the models has an inclination to predict a particular class wrong. From the confusion matrices for BFS embedding, Heliconius erato and Vanessa Altalanta are classified poorly.

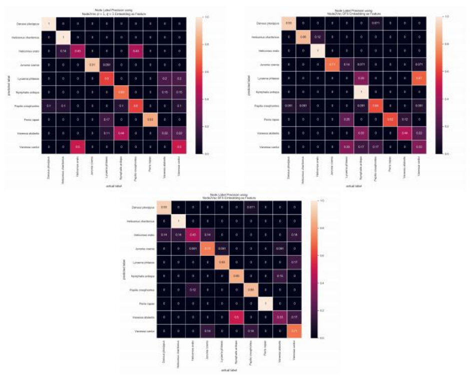


Fig. 4. Confusion Matrix for GCN model using Node2Vec Embedding

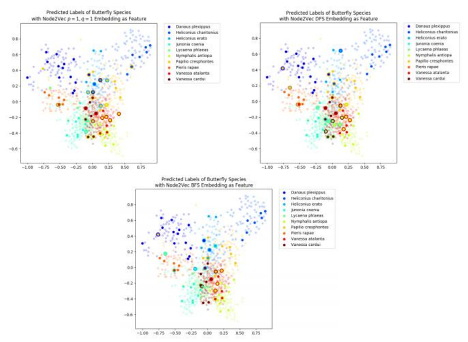


Fig. 5. Plot Nodes with Wrongly Classified Labels

Vanessa Altalanta is easily classified as Nymphalis Antiopa. In figure V, these two classes are actually really close to each other. Furthermore, in the community detection, these two classes are merged into one. Our testing classification result verifies the assumption we made previous that the Nymphalis Antiopa class is hard to distinguish from the Vanessa Altalanta class. From the confusion matrix for DFS embeding, it is interesting to see that none of the Lycaena Phlaeas is classified correctly. The Lycaena Phlaeas images are either classified as Nymphalis Antiopa or Vanessa Cardui. These three classes share the common characteristics that the neighbor of nodes in these class have high likelihood to also be in the same class, as shown in our previous data exploration part from Figure 2. Since the distance between these classes is only one hoop, when performing random DFS walk, the embedding for these three classes might look similar, and leads to the low classification accuracy.

To visually understand what are the nodes that are easily classified wrong, we plot Figure that consists all the training and testing data points. The nodes with low transparency are training and evaluating data, while the nodes with sold color are testing data. Furthermore, if the nodes with solid color have two different colors, then the nodes are wrongly classified. The outside color represent the predicted class label, and the inside color is the actual label of the node.

We observed from the plot that for the model from BFS embedding, the wrongly classified node may not be node that are close to each other in the spring layout in networkx (from the Fruchterman-Reingold force algorithm). But they share the similar structure roles; from the plot, we can see that these wrongly classified nodes all more likely to connect to other part of the network. However the wrongly classified nodes in DFS have small distance in the spring layout, and these nodes have similar community structure. These observations are inline with the BFS and DFS roles in the Node2Vec papers.

4) Further Discussion: The Node2Vec embedding with GCN generates models with good performance and is able to update the parameters efficiently due to the small number of features. Would these models outperform GCN using the a weighted adjacent matrix or a featureless matrix (Identity matrx) as features? It turns out that using a featureless matrix and a weighted adjacent matrix train could already train a nearly perfect model. Using the featureless matrix with MLP returns a 0.88 testing accuracy and using the weighted matrix with BML gets a 0.96 testing accuracy. The testing accuracies are higher than applying these features on GCN. If the computational resource is sufficient, directly using the featureless matrix or the weighted matrix can get a better result.

VII. Conclusion

In this paper, we first observe the network structure by extracting network features. We find that the network has high positive assortativity in the weighted network, which implies the higher correlation between nodes with similar degree. We further performs the community detection on the network. We observed that the number of network detected by the Louvain algorithm is less than the actual number of network, and find the communities that are merged by the network. We then make the assumption that these merged labels in the communities are more likely to be wrongly classified in the Label Classification. We then proposed our algorithm with Convolutional Neural Network. The model outperforms standard MLP model, with BFS-like node2vec embedding has the highest accuracy. We visualizes the wrongly labeled graph with the spring layout and find the differences between the wrongly labeled nodes between DFS-like and BFS-like random walk.

References

[1] Wang, Bo, et al. ”Network Enhancement: a general method to denoise weighted biological networks.” arXiv preprint arXiv:1805.03327 (2018).

[2] Krizhevsky, Alex, Ilya Sutskever, and Geoffrey E. Hinton. ”Imagenet classification with deep convolutional neural networks.” *Advances in neural information processing systems*. 2012.

[3] Liang, Ming, and Xiaolin Hu. ”Recurrent convolutional neural network for object recognition.” *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*. 2015.

[4] Kipf, Thomas N., and Max Welling. ”Semi-supervised classification with graph convolutional networks.” arXiv preprint arXiv:1609.02907 (2016).

[5] Redmon, Joseph, et al. ”You only look once: Unified, real-time object detection.” *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.

[6] M.E.J. Newman. Assortative mixing in networks. *Phys. Rev. Lett.* 89, 208701 (2002).

[7] Wang, Josiah, Katja Markert, and Mark Everingham. ”Learning models for object recognition from natural language descriptions.” (2009).

[8] Jorge Sanchez, F. P. Akata, Z. Fisher vectors for fine-grained visual categorization. In *CVPR* (2011).

[9] 16. Bosch, A., Zisserman, A. Muoz, X. Image classification using random forests and ferns. In *ICCV*, 18 (2007).

[10] Grover, Aditya, and Jure Leskovec. ”node2vec: Scalable feature learning for networks.” Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining. ACM, 2016.

[11] Sathyanarayana, Shashi. ”A gentle introduction to backpropagation.” URL: http://numericinsight. com/uploads/A$_Gentle_Introduction_to_Backpropagation.pdf[As of : 14.01.2017](2014).$