# Shallow vs. Deep Brain Network Models for Disease Classification

Erica Choi[1], Sally Smith[2], Ethan Young[3]

[1]Columbia University, [2]Georgia Institute of Technology, [3]University of California, Los Angeles

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## Abstract

In this project, we analyze different approaches for modeling brain networks, ranging from traditional **shallow graph kernel models** to modern **deep graph neural networks**. Our goal is for these models to aid in the analysis of mental disorders and diseases such as bipolar disorder, HIV, PTSD, and depression. We adapt different graph mining techniques for brain networks, statistically and visually analyze the results, and quantitatively evaluate them in the standard graph classification setting. We found that deep models (GNNs) outperformed shallow models (kernel methods), and the most successful model was able to classify HIV patients with 81% accuracy.

## Problem Formulation

- The standard graph classification task considers the problem of classifying graphs into two or more categories; in this project, we perform binary classification on neuroimaging data to classify patients as either diseased or healthy.
- Our datasets consist of brain networks, represented as weighted, undirected adjacency matrices constructed from fMRI scans. For more details on network construction, we refer you to Section 3 of a paper by Cui et al. [2].
- Depending on the classification model, we further preprocess the datasets with various methods, such as threshold rounding.

## Graph Kernels & SVM

Our first classification method is a "shallow" model: computing graph kernels and plugging them into **support vector machines** (SVM). We employ three graph kernels: Weisfeiler-Lehman (WL), Weisfeiler-Lehman optimal assignment (WLOA), and propagation (Prop) kernels. Figure 1 shows a high-level visualization of SVM. For more details on graph kernels, we refer you to Section 2 of a recent paper proposing a "deep" graph kernel framework [6].

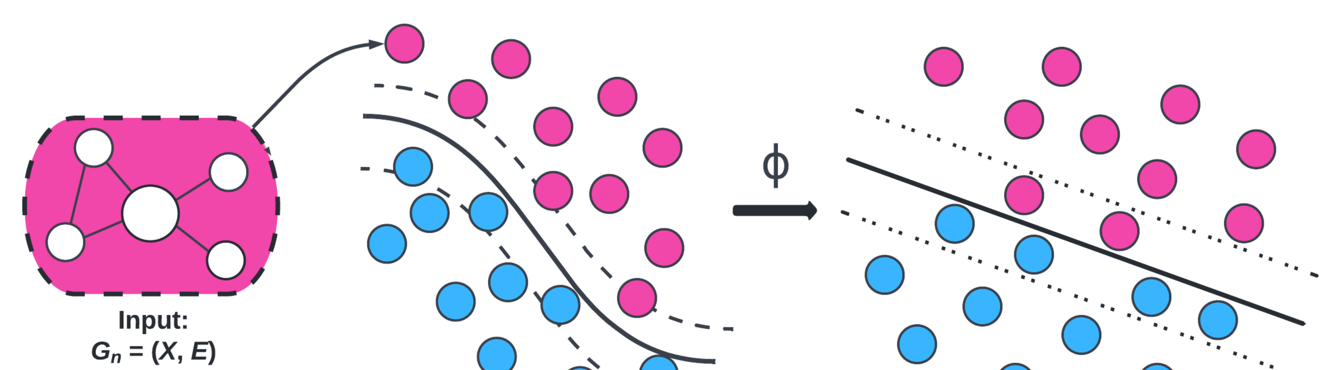


Fig. 1: Graph Kernel SVM.

## Results

| SVM Classification Accuracy | | |
|---|---|---|
| Dataset-Kernel | Threshold = 0.5 | Optimal Threshold* |
| HIV-WL (0.2*) | $0.59_{\pm 0.18}$ | $0.65_{\pm 0.17}$ |
| HIV-WLOA (0.2*) | $0.59_{\pm 0.18}$ | $0.64_{\pm 0.15}$ |
| HIV-Prop (0.2*) | $0.63_{\pm 0.18}$ | $0.66_{\pm 0.15}$ |
| BP-WL (0.4*) | $0.53_{\pm 0.14}$ | $0.63_{\pm 0.19}$ |
| BP-WLOA (0.4*) | $0.54_{\pm 0.15}$ | $0.63_{\pm 0.18}$ |
| BP-Prop (0.4*) | $0.54_{\pm 0.13}$ | $0.60_{\pm 0.17}$ |

The highest mean classification accuracy is highlighted (for ties, we highlight the accuracy with the lowest standard deviation).

## Graph Neural Networks

Our second classification method is a "deep" model: **graph neural networks** (GNNs). Specifically, we implement message passing GNNs (MPGNN) using the *BrainGB* Python package, which is built on the *Pytorch* and *Pytorch Geometric* libraries. Section 4 of the paper presenting the MPGNN framework by Cui et al. [2] gives further details on the MPGNN design choices. Figure 2 visualizes the MPGNN architecture.

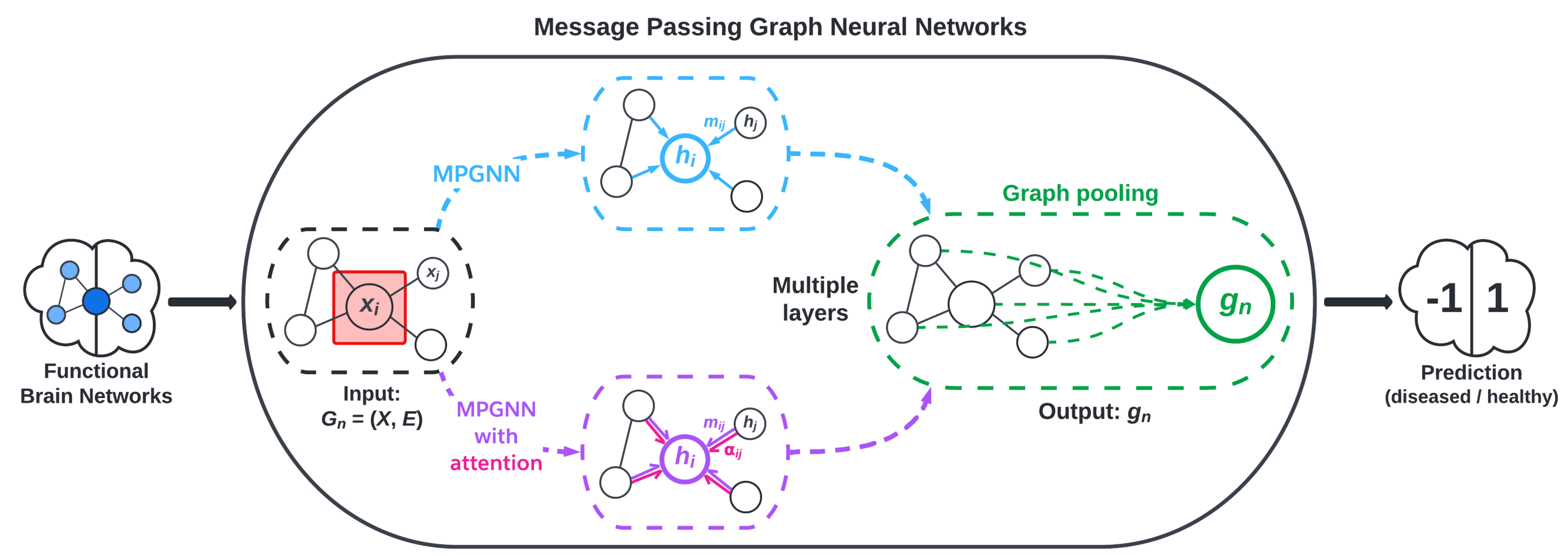


Fig. 2: BrainGB Framework. Adapted from p. 2 of [2]

Lastly, we seek to leverage any higher-order information given by graph kernels as well as local information given by GNNs. To this end, we intend to combine both approaches and benchmark the performance of graph neural networks that integrate graph kernels on our datasets. Of particular interest to us are:

- the **graph convolution layer** (GKC) proposed by Cosmo et al. [1] and
- the **kernel graph neural network** (KerGNN) proposed by Feng et al. [4].

Figure 3 is a simplified overview of the KerGNN framework.

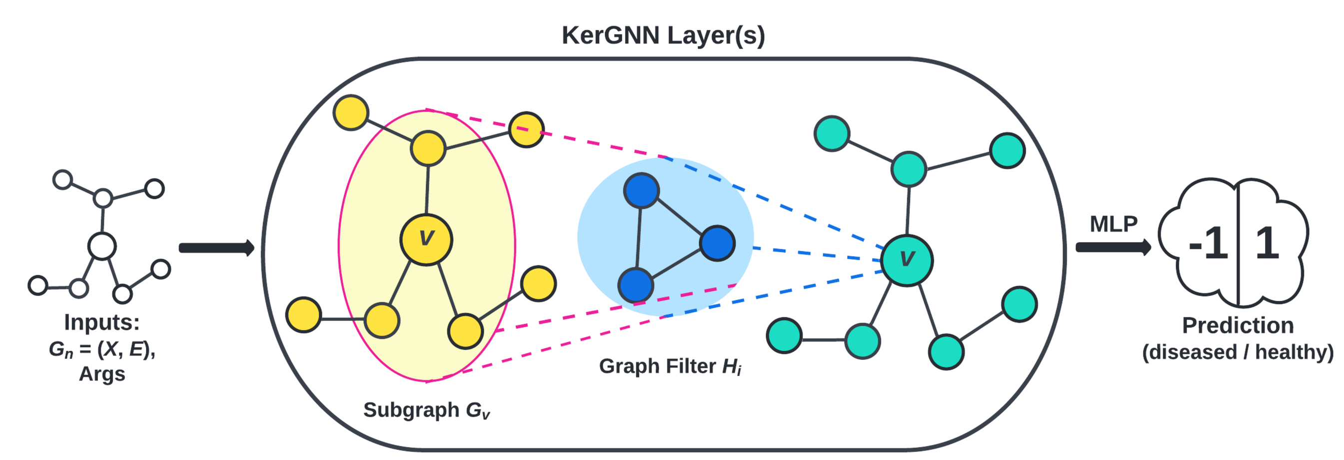


Fig. 3: KerGNN Framework. Adapted from p. 12 of [4]

## Results

| BrainGB Classification Performance | | | |
|---|---|---|---|
| Dataset-GNN | Accuracy | F1 | AUC |
| HIV-GCN (concat) | $0.64_{\pm 0.15}$ | $0.59_{\pm 0.20}$ | $0.77_{\pm 0.20}$ |
| HIV-GAT (concat) | $0.73_{\pm 0.16}$ | $0.71_{\pm 0.17}$ | $0.81_{\pm 0.19}$ |
| HIV-GCN (edge concat) | $0.71_{\pm 0.11}$ | $0.69_{\pm 0.12}$ | $0.77_{\pm 0.17}$ |
| HIV-GAT (edge concat) | $0.69_{\pm 0.18}$ | $0.67_{\pm 0.19}$ | $0.73_{\pm 0.24}$ |
| BP-GCN (concat) | $0.53_{\pm 0.13}$ | $0.51_{\pm 0.14}$ | $0.54_{\pm 0.16}$ |
| BP-GAT (concat) | $0.53_{\pm 0.13}$ | $0.50_{\pm 0.13}$ | $0.57_{\pm 0.19}$ |
| BP-GCN (edge concat) | $0.63_{\pm 0.12}$ | $0.61_{\pm 0.13}$ | $0.61_{\pm 0.17}$ |
| BP-GAT (edge concat) | $0.52_{\pm 0.17}$ | $0.51_{\pm 0.16}$ | $0.59_{\pm 0.19}$ |

The highest AUC is highlighted (this measure is not sensitive to changes in the class distribution). GCN (graph convolutional network) and GAT (graph attention network) indicate the GNN implemented in the experiments. Concat and edge concat are different message passing schemes.

## Findings and Discussion

- **Graph Kernels & SVM**
  - The mean classification accuracy of both BP and HIV datasets is relatively consistent for each kernel.
  - The WL, WLOA, and propagation kernels iteratively update node labels based on the node's local information (e.g., subtrees in the WL kernel).
  - From the generally poor performance, we are uncertain whether there is higher-order information in brain networks useful for classification with graph kernels.
- **Graph Neural Networks**
  - While GNN's capture local node information well, they are prone to overfitting and lack transparency in their predictions.
  - It is clear that GNN's are effective on the HIV data; however, its poor performance on the BP data indicates a lack of generalizability.
  - For a more thorough analysis on the performance of the BrainGB framework, please refer to [2].
- **Dataset Limitations**
  - Our datasets are prohibitively small for robust model training.
  - The BP data shows consistently worse performance than the HIV data. Cui et al. [3] observes that HIV significantly affects the connectivity within both the visual network (VN) and default mode network (DMN), while bipolar disorder mainly affects the bilateral limbic network (BLN).
  - Because HIV patients' data show less connectivity across two sub-networks and BP patients' data show less connectivity in only one sub-network, it is harder to classify BP patients.
  - Li et al. [5] found that using multimodal neuroimagery increased their SVM model's performance in classifying bipolar disorder, so only utilizing a single modality (fMRI) rather than both fMRI data and MRI data may also limit our model's classification accuracy on the BP dataset.

## Future Work

There are many ways to incorporate graph kernels with graph neural networks and make them more interpretable. For example, we seek to integrate the GKC layer from [1] into BrainGB's MPGNN framework. We also hope to test the performance of KerGNN architecture, illustrated by Figure 3, on our datasets to analyze the effectiveness of incorporating WL graph kernels into GNN's message passing process.

## Acknowledgements

- Thank you to Dr. Carl Yang, our mentor, for his guidance.
- Thank you to Hejie Cui and Dai Wei for their technical assistance.
- This work is supported in part by the US National Science Foundation awards DMS-2051019 and DMS-1751636.

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