

**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 to use these models to aid in the analysis of mental disorders and diseases such as bipolar disorder, HIV, PTSD, and depression. We adopt 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 social networks.
- 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 graph kernels.

**Results**

<table>
<thead>
<tr>
<th>Dataset-Kernel</th>
<th>Accuracy</th>
<th>F1 Score</th>
<th>AUC</th>
</tr>
</thead>
<tbody>
<tr>
<td>HIV-GCN (concat)</td>
<td>0.64±0.15</td>
<td>0.59±0.20</td>
<td>0.84±0.05</td>
</tr>
<tr>
<td>HIV-R(GCN (concat))</td>
<td>0.73±0.16</td>
<td>0.74±0.17</td>
<td>0.84±0.18</td>
</tr>
<tr>
<td>HIV-GCN (edge concat)</td>
<td>0.71±0.14</td>
<td>0.69±0.12</td>
<td>0.71±0.17</td>
</tr>
<tr>
<td>HIV-R(GCN (edge concat))</td>
<td>0.69±0.10</td>
<td>0.67±0.19</td>
<td>0.73±0.21</td>
</tr>
<tr>
<td>BP-GCN (concat)</td>
<td>0.71±0.15</td>
<td>0.70±0.14</td>
<td>0.54±0.16</td>
</tr>
<tr>
<td>BP-R(GCN (concat))</td>
<td>0.53±0.11</td>
<td>0.58±0.13</td>
<td>0.57±0.20</td>
</tr>
<tr>
<td>BP-GCN (edge concat)</td>
<td>0.63±0.12</td>
<td>0.64±0.13</td>
<td>0.64±0.15</td>
</tr>
<tr>
<td>BP-R(GCN (edge concat))</td>
<td>0.52±0.17</td>
<td>0.54±0.16</td>
<td>0.59±0.17</td>
</tr>
</tbody>
</table>

The highest AUC is highlighted (this measure is not sensitive to changes in the class distribution). GNN (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., substructure 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 over-fitting 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.
- **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. [5] observes that HIV significantly affects the connectivity within both the visual network (VN) and default mode network (DMN), while bipolar disorder mainly affects the default limbic network (BLN).
  - Because HIV patients' data show less connectivity across subsets and BP patients' data show less connectivity in only one subset, it is harder to classify BP patients.
- **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 into BrainGB's MPGN 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**

- Thanks to Dr. Carl Yang, our mentor, for his guidance.
- Thanks to Hejie Cui and Dai Wei for their technical assistance.
- This work is supported in part by the US National Science Foundation awards CNS-2011019 and CNS-1735636.

**References**