

Supplementary material

1 Demographics of the ADNI Dataset

Table 1: Demographics of the ADNI Dataset. There are a total of 2020 subjects, each with varying presence of specific node features.

| Biomarker | Category | CN | SMC | EMCI | LMCI | AD |
|--------------------|----------------------|----------------|----------------|----------------|----------------|----------------|
| Cortical Thickness | # of subjects | 843 | 197 | 490 | 250 | 240 |
| | Gender (Male/Female) | - | - | - | - | - |
| | Age (Mean \pm Std) | - | - | - | - | - |
| β -Amyloid | # of subjects | 434 | 173 | 423 | 145 | 167 |
| | Gender (Male/Female) | 195/239 | 62/111 | 248/175 | 96/49 | 108/59 |
| | Age (Mean \pm Std) | 72.4 \pm 6.0 | 72.0 \pm 5.2 | 70.5 \pm 7.6 | 71.2 \pm 5.5 | 74.9 \pm 8.6 |
| FDG | # of subjects | 363 | 182 | 442 | 180 | 167 |
| | Gender (Male/Female) | 178/185 | 69/113 | 253/189 | 119/61 | 105/62 |
| | Age (Mean \pm Std) | 72.8 \pm 6.1 | 72.0 \pm 5.3 | 71.0 \pm 7.8 | 70.9 \pm 6.1 | 74.7 \pm 8.7 |
| All Features | # of subjects | 337 | 173 | 418 | 145 | 161 |
| | Gender (Male/Female) | 156/181 | 62/111 | 243/175 | 96/49 | 104/57 |
| | Age (Mean \pm Std) | 72.4 \pm 5.8 | 72.0 \pm 5.2 | 70.4 \pm 7.6 | 71.2 \pm 5.5 | 75.0 \pm 8.7 |

2 Comparison in the Number of Edges and Performance

Table 2: Comparison regarding the effects of variations in the threshold ($=\sigma$) during edge preprocessing on the number of edges and model performance. The model performance is evaluated for our 1-hop model utilizing all features. We used $\sigma = 10,000$ for our main experiments.

| σ | # of Edges | | | | Performance using All Features | | | |
|----------|--------------------|------------------|-------|--------------|----------------------------------|----------------------------------|----------------------------------|----------------------------------|
| | Cortical Thickness | β -Amyloid | FDG | All Features | Accuracy | Precision | Recall | F1-score |
| 1,000 | 1,202 | 1,205 | 1,190 | 1,190 | 92.87 \pm 0.85 | 94.17\pm0.92 | 92.75 \pm 1.18 | 93.32 \pm 1.06 |
| 5,000 | 763 | 763 | 757 | 759 | 92.46 \pm 0.97 | 93.09 \pm 1.17 | 92.70 \pm 1.18 | 92.77 \pm 1.13 |
| 10,000 | 620 | 619 | 617 | 618 | 93.03\pm1.06 | 93.90 \pm 1.17 | 93.35\pm1.02 | 93.53\pm0.93 |
| 20,000 | 433 | 429 | 422 | 422 | 93.03\pm0.75 | 93.56 \pm 0.56 | 93.31 \pm 0.64 | 93.37 \pm 0.60 |

3 Additional Visualization on Grad-CAM Results

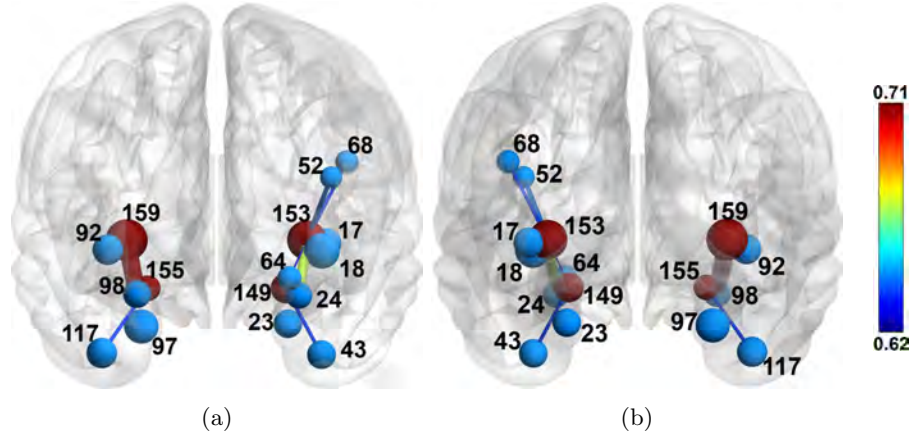


Fig. 1: Visualization of the top-10 ROIs and connectomes with the highest activation for classifying AD. (a)/(b): Front/rear view of the brain. Blue nodes belong to the cortical region, and red nodes belong to the subcortical region. Node size and edge color/thickness represent the activation. The indices on nodes correspond to the Destrieux atlas index values.