Ph.D. DISSERTATION DEFENSE

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Degree:	Doctor of Philosophy
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Date:	08/10/2026
Time/Location:	10:00 AM – 12:00 PM (EDT) Babbio 503
Title:	Deep Graph Theory and Mixture-of-Experts Framework for Multimodal Neurological Disorder Diagnosis
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ABSTRACT

Traditional graph theory has been widely adopted to address a broad range of graph-structured data problems. Recent advances in artificial intelligence have successfully integrated neural network techniques into network analysis. In particular, Graph Neural Networks (GNNs) have demonstrated remarkable effectiveness in learning node representations and identifying clustering patterns in graph-structured data. These advances can be further extended to the investigation of functional connectivity in brain networks. Nevertheless, neurological, neurodegenerative and mental disorders are increasingly characterized by heterogeneous multimodal data, including functional magnetic resonance imaging (fMRI), diffusion tensor imaging (DTI), single photon emission computed tomography (SPECT), and electroencephalography (EEG), together with demographic and clinical information, which present new challenges for modeling complex brain networks. Integrating heterogeneous data sources has become increasingly important for identifying abnormal functional connectivity associated with neurodegenerative diseases and, ultimately, improving diagnostic accuracy.

This dissertation proposes deep graph learning and mixture-of-experts frameworks for the multimodal diagnosis of neurological, neurodegenerative and neuropsychiatric disorders. The overarching goal is to

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move beyond black-box classification by developing interpretable and dynamically adaptive graph-based architectures that jointly model spatial brain topology, temporal dynamics in fMRI, cross-modal feature interactions, and disease heterogeneity across diverse neuroimaging and physiological modalities. The proposed framework is systematically evaluated across a broad range of neurological and psychiatric conditions, including marijuana dependence, schizophrenia, Parkinson's disease subtypes, Alzheimer's disease, frontotemporal dementia, and post-traumatic epilepsy following traumatic brain injury.

First, a High-Order Graph Attention Neural Network (HOGANN) is developed to analyze spatiotemporal craving-related connectivity patterns in long-term marijuana users from fMRI-derived multigraph representations. By integrating high-order neighbor mixing with sequential graph attention learning via a GAT-LSTM submodel, HOGANN captures both inter-regional dependencies and temporal evolution, improving the classification of substance use disorder while identifying craving-related subnetworks. Analysis across two datasets and the Yeo seven-network atlas consistently implicates the frontoparietal, default mode, and dorsal attention networks, and further links demographic factors such as age to distinct connectivity alterations.

Second, NeuroTree is introduced as a hierarchical functional brain pathway decoding framework that represents fMRI networks as tree-structured pathways. Coupling a k-hop ODE-based AGE-GCN with hierarchical tree construction and contrastive masking optimization, NeuroTree models both static and dynamic connectivity, incorporates demographic information into message passing, and decodes disease-specific hierarchical subnetworks. This approach achieves state-of-the-art graph classification performance while interpreting how addiction and schizophrenia alter functional connectivity in relation to brain age.

Third, a Cross-Graph Modal Contrastive Learning (CGMCL) framework extends the methodology to multimodal medical imaging by modeling heterogeneous modalities, such as imaging data and quantitative clinical metadata, as distinct graph structures. Using graph attention encoders, an inter-modality feature enhancement and scaling (IMFES) module to mitigate modality imbalance, and cross-graph contrastive alignment within a unified embedding space, CGMCL improves robustness, interpretability, and subtype discrimination in Parkinson's disease.

Fourth, a Variational Mixture of Graph Experts (VMoGE) framework is presented for the recognition of Alzheimer's disease and frontotemporal dementia in EEG brain networks. VMoGE combines multi-granularity transformer-based node feature extraction, a Gaussian Markov random field prior, and variational graph-structured inference with adaptive expert routing, enabling the model to characterize heterogeneous frequency-band-specific patterns and identify clinically meaningful EEG signatures with improved explainability and computational efficiency.

Finally, this dissertation investigates the fusion of functional and structural multimodal connectivity information within brain connectome representations to distinguish post-traumatic epilepsy (PTE) from traumatic brain injury (TBI) using machine learning methods. However, static fusion of fMRI and diffusion MRI (dMRI) may limit the model's ability to capture dynamic, time-dependent features in fMRI data. To address this limitation, we further propose the Dynamic Functional–Structural Mixture-of-Experts (DynFS-MoE) framework, which extends the mixture-of-experts paradigm to time-aware multimodal modeling of brain disorders. By integrating fMRI and structural MRI through dynamic functional–structural expert routing and class-conditioned multimodal expert allocation, the proposed framework aims to characterize the network mechanisms underlying epileptogenesis and facilitate early, individualized diagnosis.

Collectively, these contributions demonstrate a coherent progression from high-order graph modeling to hierarchical decoding, multimodal alignment, and adaptive expert-based architectures. By integrating deep graph theory with dynamic expert routing, this dissertation establishes an interpretable, robust, and scalable computational paradigm that advances biomarker discovery and clinical decision support for precision computational neuroscience.