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Introduction

The human brain consists of complex networks of interconnected neurons. Understanding how these brain networks are organized is key to studying brain function. Advances in neuroimaging techniques, combined with modern network research, have enabled detailed analysis of brain functional connectivity. Recently, deep learning methods have been applied to brain network analysis for tasks such as image segmentation, brain disorder prediction, and network modeling. In this chapter, we discuss the opportunities and challenges in brain network analysis, outline the thesis objectives and research questions, present our contributions, and provide an overview of the thesis structure.

1.1 BRAIN NETWORK ANALYSIS

The human brain has an exceptionally intricate structure. The human brain consists of roughly 100 billion neurons Herculano-Houzel [2009]. Neurons are the fundamental functional components of the human brain, mainly responsible for transmitting information to specific cells. Examining the human brain is crucial for comprehending the operations of the mind. Functional magnetic resonance imaging (fMRI) offers new prospects for understanding the brain's functioning. fMRI is a technique to measure changes in blood flow to identify and analyze brain activity. This approach can produce time-series data from multiple sources, resulting in millions of pairwise relationships gathered via various experimental designs. The advancement of this approach and its widespread use pose a significant difficulty in analyzing fMRI data for cognitive neuroscience research. A complex network refers to several real-world systems, such as social networks, gene networks, or neurobiological networks. Examining the dynamic process of complex networks is crucial for exploring the functionalities of complex systems. For instance, the configuration of brain networks influences the transmission of information inside the brain and the spread of diseases. Due to the advancement of approach and the extensive accumulation of data, it is imperative to create novel computational models that can effectively learn valuable data representations for various purposes, including node/link categorization, anomaly detection, and dynamic analysis. Node/link categorization in brain network analysis refers to classifying brain regions (nodes) and their interconnections (links) based on functional or structural connectivity. This categorization helps in understanding how different brain regions communicate and contribute to cognitive functions. Deep learning has several benefits in acquiring valuable data representations, including reducing errors caused by manually selected features and using multi-layered non-linear graph representations. Brain imaging deep learning is an ongoing research field that faces challenges related to the large volumes, complex architectures, and dynamic nature of the data. Several outstanding research studies have shown the effectiveness of classifying brain functional connectivity networks. Functional connectivity refers to characterizing the brain's functional network structure, which may be easily retrieved from fMRI data for classification purposes. Connectivity-based approaches are widely used for classifying brain disorders; however, they come with specific challenges. One major issue is the overlapping nature of functional networks, where multiple brain regions may be involved in different cognitive processes, making it difficult to isolate disorder-specific biomarkers.

Additionally, inter-individual variability in functional connectivity can introduce noise, reducing the generalizability of models. Interpretability remains a concern, as traditional machine learning and deep learning models often function as black boxes, making it challenging to explain why certain connectivity patterns lead to specific predictions. Finally, overfitting can arise due to the high dimensionality of fMRI data combined with limited sample sizes, which may lead to models that perform well on training data but fail to generalize to new subjects. A significant amount of research has focused on using functional connectivity as a feature to train classifiers. A functional network consists of regions of interest (ROIs), also known as nodes. The connectedness between nodes is determined by analyzing the time-series data of pairwise areas of interest (ROIs). An efficient and direct method is to use functional connectivity measures extracted from the connectivity matrix as features and input them directly into a deep learning model. This allows for fMRI image categorization based purely on brain functional activation patterns.

1.2 DEEP LEARNING FRAMEWORKS TO STUDY BRAIN FUNCTIONAL CONNECTIVITY PATTERNS

1.2.1 Functional and Structural Connectivity

Neuroscience is moving toward a "big data" era due to the development of neuroimaging methods. Massive datasets provide information on structural and functional synaptic connection patterns. Structural connectivity describes a comprehensive map of the connections inside the brain Dennis *et al.* [2013], whereas Functional connectivity is the correlation of the time course of activation across brain regions Zeng *et al.* [2012].

Brain network analysis examines neurobiological patterns that help in understanding how the brain performs high-level functions through different measures. One approach that uses magnetic resonance imaging (MRI) to map the human brain at a large scale is the Human Connectome Project (HCP) Frégnac and Laurent [2014]. Specific laboratories construct three-dimensional neural maps of brain tissues at the microscale, while others meticulously track each neuron and synapse at the nanoscale Paus *et al.* [1999]; Wedeen *et al.* [2005].

Brain networks have an irregular architecture and dynamic properties, unlike regular-gridded medical imaging. They illustrate how the brain regulates information flow among neuronal components to support cognition and behavior. The topological properties of brain networks show neurobiological fingerprints that serve as biomarkers for identifying numerous neurological disorders, including Alzheimer's disease (AD) and autism spectrum disorder (ASD) Wang *et al.* [2007]; Wass [2011]. Furthermore, dynamic variations in brain activity are associated with information regulation and cognitive state Li *et al.* [2016].

1.2.2 Resting-State Functional Connectivity

Resting-state functional connectivity (rs-FC) provides insights into spontaneous brain activity and network organization in the absence of task-related stimuli. It plays a crucial role in understanding both typical and atypical neural processes Smith *et al.* [2009]. Studies have shown that functional connectivity patterns observed during rest correspond to intrinsic large-scale networks, such as the default mode network (DMN), central executive network (CEN), and salience network (SN) Greicius *et al.* [2003]. Alterations in rs-FC have been linked to various neuropsychiatric conditions, including schizophrenia, depression, and ASD.

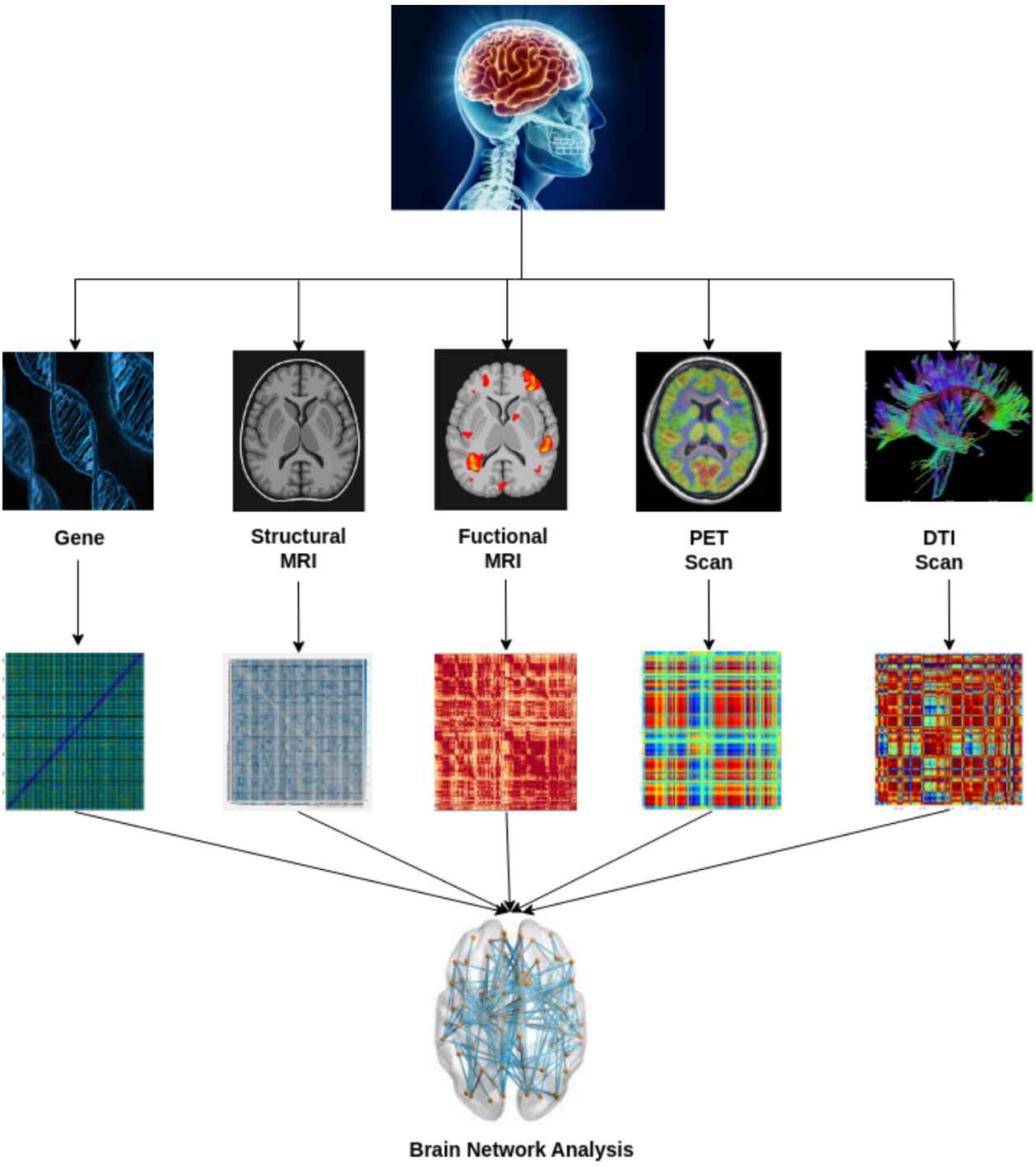

Figure 1.1: Different types of neuroimaging approaches, such as gene imaging, structural MRI, functional MRI, PET scan, and DTI scan, used to study brain dynamics.

1.2.3 Brain Development and Connectivity

Brain development is constrained by its structure, and researchers commonly study changes in brain dynamics by analyzing correlation patterns in spontaneous fluctuations of functional MRI (fMRI) signals. The maturation of functional connectivity follows a trajectory from local, short-range connections in early childhood to long-range network integration in adulthood Fair *et al.* [2009]. Developmental changes in connectivity influence cognitive abilities such as memory, attention, and executive function.

Accurately modeling the temporal dynamics of brain activity remains a challenge in neuroscience due to the complexity of estimating dynamic functional connections. Advanced neuroimaging techniques, such as dynamic functional connectivity (DFC) analysis, allow for the examination of temporal fluctuations in connectivity and their relationship to cognitive and behavioral outcomes Hutchison *et al.* [2013a].

1.2.4 Clinical Conditions and Functional Connectivity

Abnormal functional connectivity has been implicated in various neurological and psychiatric disorders. For instance, ASD is characterized by disrupted connectivity in key networks associated with social cognition and executive function Rudie *et al.* [2013]. Similarly, Alzheimer's disease exhibits connectivity alterations that correlate with cognitive decline, particularly in the DMN Greicius *et al.* [2004].

Multimodal neuroimaging approaches, integrating structural and functional data, have been proposed to enhance disease diagnosis and prognosis Calhoun and Sui [2016]. Recent research suggests that machine learning techniques can improve classification accuracy in clinical populations by identifying disease-specific connectivity biomarkers Dosenbach *et al.* [2010].

1.2.5 Image Analysis in the Context of Brain-Activated Regions

The study of brain-activated regions relies on neuroimaging techniques that capture structural and functional aspects of neural activity. Functional Magnetic Resonance Imaging (fMRI) has been widely utilized to measure blood-oxygen-level-dependent (BOLD) signals, providing insights into spontaneous and task-evoked brain activity Ogawa *et al.* [1990]. Unlike electroencephalography (EEG) and magnetoencephalography (MEG), which offer high temporal resolution, fMRI provides superior spatial resolution, making it well-suited for mapping large-scale brain networks.

Analyzing functional connectivity (FC) from fMRI data requires robust image processing techniques. Traditional methods, such as Independent Component Analysis (ICA) Beckmann and Smith [2004] and seed-based correlation analysis Biswal *et al.* [1995], have been extensively used to extract patterns of synchronized brain activity. These approaches segment the brain into functionally connected regions based on statistical dependencies in BOLD signal fluctuations. However, they often require predefined assumptions about network structure, which may limit their applicability in studying complex neural interactions.

With advancements in artificial intelligence, deep learning models have emerged as powerful tools for neuroimaging analysis. Convolutional Neural Networks (CNNs) have been particularly effective in extracting spatial patterns from fMRI data, enabling the identification of functional brain networks with minimal manual feature selection Litjens *et al.* [2017]. Moreover, Graph

Neural Networks (GNNs) provide a structured representation of brain connectivity, capturing the topological organization of neural circuits Bronstein *et al.* [2017]. These methods enhance the ability to characterize individual differences in brain function, offering a novel approach to studying typical and atypical neurodevelopment.

1.2.6 Deep Learning for Analyzing Functional Connectivity

Artificial neural networks (ANNs) were initially inspired by neuroscience to mimic the brain's information-processing mechanisms McCulloch and Pitts [1943]; Rumelhart *et al.* [1994]. Convolutional neural networks (CNNs), a type of ANN, are particularly suited for image processing and have been adapted for neuroimaging analysis. With the increasing availability of data and computational power, deep learning has emerged as a leading artificial intelligence approach. These techniques utilize multilayer neural networks to extract intricate features and hierarchical representations from input data, improving predictive accuracy in medical and neuroimaging applications Esteva *et al.* [2017]; Gulshan *et al.* [2016].

Deep learning has demonstrated its potential in medical imaging, offering benefits such as increased efficiency in diagnostic processes, cost reduction in healthcare, early disease detection before symptom onset, and improved treatment personalization in precision medicine. Despite these advantages, the application of deep learning in neuroscience remains challenging due to the complexity of the human brain. Traditional neuroscience focuses on detailed mechanistic explanations of neuronal networks, whereas deep learning models emphasize computational efficiency and generalization.

In neuroimaging, various deep learning architectures are employed to analyze brain connectivity patterns. Artificial Neural Networks (ANNs) serve as foundational computational models that capture non-linear relationships in data. Convolutional Neural Networks (CNNs), designed for spatial data, are particularly effective in processing neuroimaging data by extracting hierarchical features. Meanwhile, Deep Neural Networks (DNNs), with their multilayer structures, enhance classification tasks in cognitive neuroscience, enabling better understanding of brain function. Recent studies have leveraged DNNs to predict cortical representations of the human brain, demonstrating their utility in decoding complex neural patterns Wen *et al.* [2018].

However, the integration of deep learning into cognitive neuroscience is not without challenges. One significant hurdle is the variability in brain networks, as differences in functional connectivity across individuals can lead to biased results. Additionally, the temporal dynamics of brain activity—fluctuations influenced by development, external stimuli, and neurobiological disorders—pose difficulties in modeling and interpretation. Another challenge lies in algorithm validation, where ensuring the robustness and generalizability of deep learning models remains a critical concern. Furthermore, there is a pressing issue of trust and interpretability in AI-driven healthcare applications. While deep learning models can distinguish between healthy and pathological conditions, their decision-making processes are often opaque, raising concerns among healthcare professionals and patients about their reliability and transparency.

Despite these challenges, the application of deep learning in functional brain connectivity analysis holds immense promise. By addressing these limitations through improved model interpretability, robust validation techniques, and interdisciplinary collaborations, deep learning can significantly enhance our understanding of brain function and its association with neurological disorders.

1.3 MOTIVATION FOR THE PROJECT

1.3.1 Characterizing Development of Brain Networks From Early Childhood

The first two decades of life encompass remarkable developmental transformations in sensory, motor, and cognitive abilities Fair *et al.* [2009]. Developmental cognitive neuroscience aims to establish a connection between extensive behavioral milestones and the corresponding functional and structural alterations in the neural substrate. Understanding these changes not only provides insight into typical development but also helps in comprehending the neural basis of developmental disorders.

Key developmental milestones include the maturation of language networks, the theory of mind (ToM) network, and the prefrontal cortex (PFC), which play crucial roles in cognitive and social development. The ToM network is responsible for understanding others' thoughts and intentions, while the PFC supports executive functions, such as decision-making, impulse control, and working memory. These regions undergo significant structural and functional changes from early childhood through adolescence, influencing cognitive flexibility and social behavior.

Magnetic Resonance Imaging (MRI) is a widely used neuroimaging technique that allows the study of brain structure and function. Functional MRI (fMRI), in particular, measures blood-oxygen-level-dependent (BOLD) signals to infer neural activity. Compared to electroencephalography (EEG) and magnetoencephalography (MEG), which offer high temporal resolution but low spatial resolution, fMRI provides superior spatial resolution, making it ideal for mapping brain networks at a macroscopic level. However, fMRI has limitations, such as low temporal resolution due to the sluggish nature of hemodynamic responses and its susceptibility to motion artifacts, particularly in developmental studies Power *et al.* [2012]. Despite these constraints, resting-state and task-based fMRI have been extensively used to study functional connectivity (FC) in both typically developing and clinical populations.

While fMRI is a powerful tool for studying brain maturation, its use in young children poses challenges. MRI scanning requires individuals to remain still for extended periods, which can be difficult for young participants. Additionally, the potential risks associated with MRI imaging, such as exposure to loud scanner noise and the need for sedation in certain cases, raise ethical concerns. These factors contribute to limited MRI data availability for normal healthy children, emphasizing the need for innovative computational methods that maximize insights from available datasets.

1.3.2 Identifying Brain Connectivity-Based Features as Individual Fingerprints

Functional connectivity analysis has revealed significant interindividual variability in brain network organization Finn *et al.* [2015]. This variability extends across developmental stages, and deep learning approaches can help uncover the underlying patterns that distinguish different age groups. The application of deep learning to neuroimaging data has gained traction due to its ability to capture complex, nonlinear relationships between brain regions Heinsfeld *et al.* [2018]. Traditional methods, such as independent component analysis (ICA) and graph-theoretic approaches, have contributed to our understanding of functional brain networks but often require extensive manual feature engineering and may not generalize well across datasets.

Recent studies have demonstrated that deep learning models can learn subject-specific neurobiological features, effectively treating functional connectivity patterns as a form of "brain fingerprint" that allows for the prediction of age, cognitive abilities, and susceptibility to disorders Kawahara *et al.* [2017]. The ability to extract meaningful, data-driven representations from

high-dimensional fMRI data is a significant advancement in developmental neuroscience, allowing for the identification of neurobiological markers with high precision. However, treating brain activity as an individual fingerprint raises several questions. Unlike traditional fingerprints, which are static and unique to each person, functional brain connectivity is dynamic and influenced by internal and external factors, including cognitive states, environmental stimuli, and developmental trajectories. Addressing these nuances is essential for ensuring the robustness and reliability of connectivity-based biometrics in neuroscience research.

1.3.3 Design of Explainable and Generalized AI Framework to Study Atypical Brain Network Development

A major goal in neuroimaging research is to identify biomarkers for early diagnosis of neurodevelopmental disorders, such as Autism Spectrum Disorder (ASD) and Attention Deficit Hyperactivity Disorder (ADHD). Deep learning techniques provide an opportunity to analyze neurobiological disorders in an automated and scalable manner, without relying on predefined feature sets. Methods such as static functional connectivity (SFC) and dynamic functional connectivity (DFC) have been employed to characterize brain network alterations in clinical populations Calhoun *et al.* [2014].

Despite these advancements, the use of deep learning in neuroimaging faces critical challenges. Many existing models operate on Euclidean data, whereas brain networks are inherently graph-structured, requiring specialized architectures such as graph neural networks (GNNs). Furthermore, deep learning models often lack interpretability, making it difficult to pinpoint the neural mechanisms underlying their predictions. Developing an explainable and generalized AI framework is crucial to bridge this gap, allowing for both accurate classification of neurodevelopmental disorders and mechanistic insights into atypical brain development. Incorporating attention mechanisms, feature attribution methods, and hybrid modeling approaches can enhance the interpretability and clinical applicability of deep learning models in cognitive neuroscience. Additionally, collaborations between neuroscientists, clinicians, and AI researchers will be essential for translating computational findings into meaningful clinical insights.

1.4 RESEARCH GAP

There are a few major gaps that are listed below:

1.4.1 Identification of Brain Features

Identifying reliable neurobiological fingerprints across individuals remains a challenge due to the inherent heterogeneity of brain structure and function. The human brain is a dynamic system, and its functional organization evolves over time, influenced by both genetic and environmental factors. Capturing these temporal dynamics requires robust computational models capable of disentangling developmental trajectories from interindividual differences. Additionally, structural connectivity (determined via diffusion tensor imaging, DTI) places constraints on functional interactions, which should be considered in comprehensive analyses of brain networks Hagmann *et al.* [2008].

1.4.2 Deep Learning in Predicting Brain Disorder

The emergence of large-scale neuroimaging datasets has enabled the application of deep learning models to classify and predict brain disorders Heinsfeld *et al.* [2018]. However, applying deep learning to fMRI data presents unique challenges, including high-dimensionality, limited sample sizes, and the irregular structure of brain networks. Standard convolutional neural networks (CNNs) struggle to capture the complex relationships within brain connectivity data, necessitating the development of specialized frameworks such as graph-based neural networks (GNNs).

Moreover, most existing deep learning frameworks for neuroimaging focus on classification accuracy without addressing generalization across diverse populations. Differences in scanning protocols, preprocessing pipelines, and demographic variables can impact model performance, highlighting the need for more robust and generalizable AI solutions.

1.4.3 Interpretation of Deep Learning Results

A major limitation of deep learning in neuroimaging is its interpretability. Artificial neural networks (ANNs) rely on distributed representations, making it challenging to trace the decision-making process from input to output. Unlike decision trees, which provide explicit decision paths, deep learning models function as "black boxes," limiting their clinical utility Samek *et al.* [2017].

To address this, researchers have explored techniques such as saliency maps, layer-wise relevance propagation, and attention mechanisms to enhance interpretability Montavon *et al.* [2018]. However, these methods are still in their infancy and require further validation. An explainable AI framework is needed to provide neuroscientists and clinicians with meaningful insights into the neural correlates of developmental disorders.

1.5 CONTRIBUTIONS

1.5.1 Cognitive Development of Brain Networks

Cognitive development pertains to the progression and refinement of cognitive processes, including social cognition (like reasoning, cognitive flexibility, recall, linguistic abilities, sensory interpretation, and other cognitive functions) and operations associated with obtaining, processing, retaining, and using knowledge. This development process takes place continuously over an individual's whole lifetime. Theory of Mind (ToM) refers to the cognitive ability to attribute mental states—such as beliefs, intentions, and emotions—to oneself and others Bhavna *et al.* [2024]. This ability is essential for social interactions, allowing individuals to predict and interpret others' behaviors. The neural basis of ToM primarily involves the temporoparietal junction (TPJ), medial prefrontal cortex (mPFC), precuneus, and posterior superior temporal sulcus (pSTS) Bhavna *et al.* [2024]. Research indicates that while the basic ToM ability emerges around the age of three, its neural representations continue to mature throughout childhood and adolescence, becoming more refined and functionally segregated from other networks. However, the development of the ToM network throughout early life, as young as a 3-year-old kid, and its segregation from other networks are still unresolved questions Bhavna *et al.* [2024]. Traditional ToM studies have used controlled, structured experimental tasks (e.g., false belief tasks, animated scenarios), which may not fully capture real-world social cognition. In contrast, naturalistic task-based fMRI involves stimuli that closely

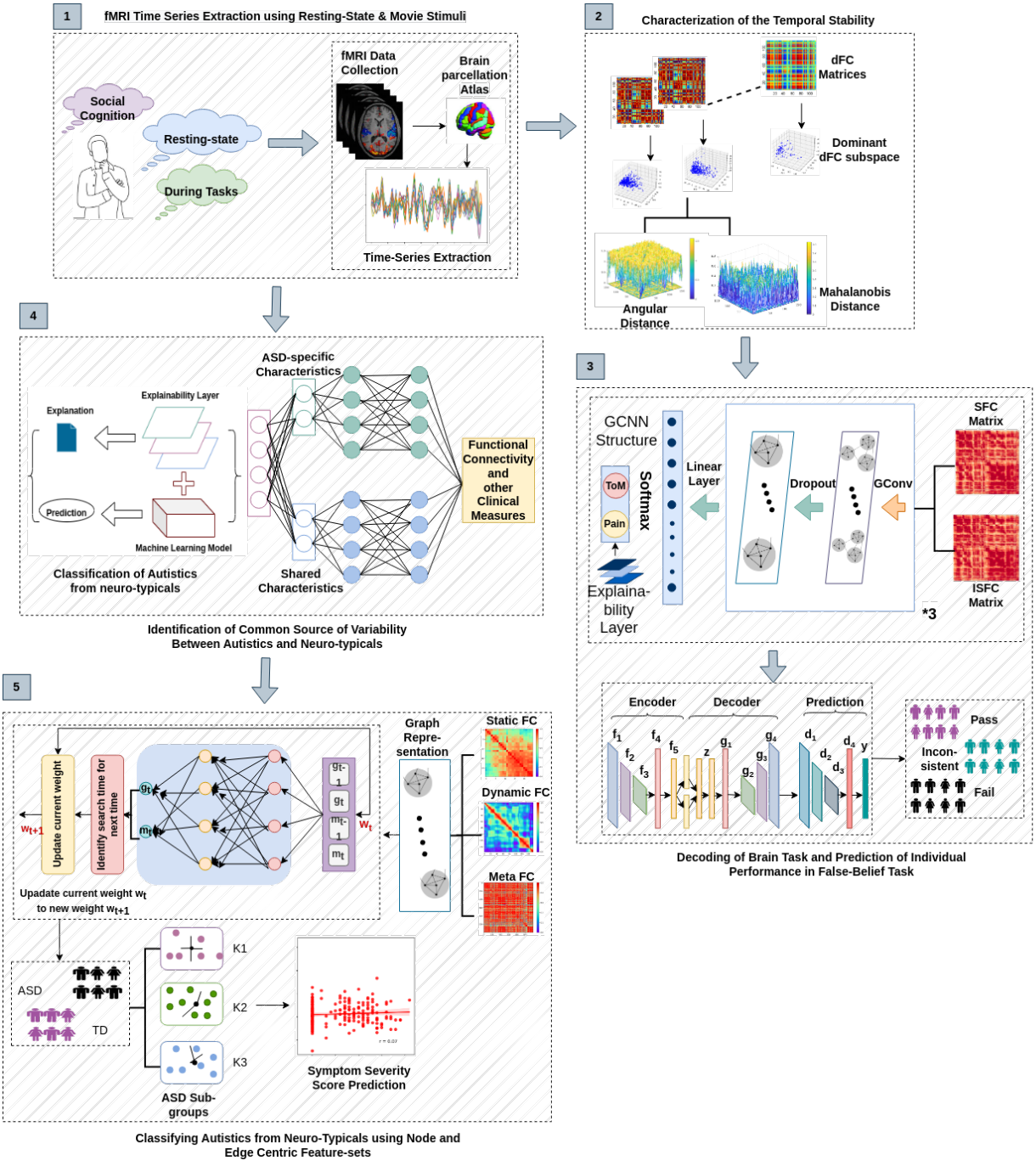

Figure 1.2: Figure shows the overall pipeline of the thesis, in which, 2 illustrates characterization of temporal stability, Whereas, 3 is representing decoding of brain brain states and prediction of individual performance in false-belief tasks. Finally 4 and 5 represent deep learning model to classify autistics and neurotypicals, as well as identifying sub-groups within ASD-samples and their symptom-severity scores.

resemble real-life social interactions, such as watching movies or listening to stories with complex character interaction. Such tasks engage the ToM network dynamically, allowing researchers to examine functional connectivity in ecologically valid settings. To overcome this limitation, Firstly, we used naturalistic stimuli that included significant ToM and pain network activations during movie watching task to track temporal characterization of brain dynamics during early development (From 3-yrs to 12-yrs). Our study utilized a naturalistic viewing paradigm to assess how ToM-related brain activity unfolds over time, providing novel insights into its temporal stability and developmental patterns. We have selected the stimuli validated to activate ToM and pain networks because pain processing and social cognition are closely linked, as both networks involve overlapping neural structures such as the anterior cingulate cortex (ACC) and insula. Our study demonstrated that, unlike the ToM network, which undergoes prolonged developmental changes, the pain network exhibits relatively stable activation patterns, providing a comparative framework for understanding developmental trajectories Bhavna *et al.* [2024]. Additionally, to identify at what age reasonable temporal stability was obtained and how the development of ToM ability could be predicted over time. Temporal stability' refers to the consistency of network activations across different time points during scanning sessions rather than developmental stability over years Bhavna *et al.* [2024]. This stability metric helps differentiate functionally specialized networks from those still undergoing developmental reorganization. We identified the change in temporal stability using an unsupervised characterization of ToM and Pain networks dFC patterns using Angular and Mahalanobis distance between dominant dynamic functional connectivity subspaces. We also analyzed how temporal stability could be associated with performance on ToM-related false-belief tasks.

1.5.2 Decoding of Brain Task using Graph Convolutional Neural Networks

We performed decoding of brain tasks to identify how the brain processes social cognition tasks from early childhood to adulthood. It aims to identify brain states using neural activity, further helping understand behavior crucial for cognitive neuroscience and neural engineering. However, despite recent neuroscience research emphasizing the network patterns of brain dynamics, existing machine-learning approaches for fMRI-based brain decoding need to improve classification performance and better explainability. We aimed to identify how early childhood participants are processing cognitive states. We performed brain decoding on a naturalistic movie-watching task activating ToM and pain networks in the developmental dataset. We proposed a novel, explainable spatiotemporal connectivity-based graph convolutional neural network (Ex-stGCNN) model for decoding time courses where a participant was experiencing a particular cognitive task (either ToM or pain). We identified brain regions that contributed most to the prediction as brain fingerprints. We also implemented the unsupervised Explainable Convolutional Variational Autoencoder model (Ex-Convolutional VAE) to predict individual performance in false-belief tasks.

1.5.3 Identification of Source of Variability Between Autistic and Neuro-typicals using Contrastive Varaitional Auto-Encoder Model

Social cognition is an evolving ability that significantly impacts human learning and cognition. The ToM brain network is mainly responsible for social cognition. Early development of ToM ability allows one to comprehend other people's aims and ambitions, as well as thinking that differs from one's own. Autism Spectrum Disorder (ASD) is the prevalent pervasive neurodevelopmental disorder in which participants' brains appeared to be marked by diffuse variations throughout large-scale brain systems made up of functionally connected but physically separated brain areas that got abnormalities in willed action, self-monitoring and monitoring the intents of others, often

known as the deficit in social cognition, interaction, and communication. Although functional neuroimaging techniques have been widely used to establish the neural correlates implicated in ToM, the specific mechanisms still need to be clarified. The availability of current Big data and Artificial Intelligence (AI) frameworks is still facing issues in classifying autistics from neuro-typicals due to a lack of feature extraction techniques and model architecture. In this work, we develop an Explainable deep learning framework that quantifies the common sources of variability in ToM brain regions between typically developing and ASD individuals. Our results identify a feature set on which the classification model can be trained to learn characteristics differences and classify ASD and TD ToM development more distinctly.

1.5.4 Explainable and Generalized AI Framework for Classification of Autistics from Neuro-typicals

The current era, marked by the availability of big data and Artificial Intelligence (AI) frameworks, provides an unprecedented opportunity to leverage connectome-based features associated with ASD. However, despite recent neuroscience research emphasizing machine learning (ML) and deep neural network (DNN) frameworks to classify ASD from neuro-typicals (TD), the specific mechanisms still need to be clarified for non-Euclidean space. We proposed a lightweight, explainable, generalized Deep neural network framework, in which we considered Theory-of-Mind, Default-mode Network, Central executive, and Salience networks from which calculated meta-connectivity as an edge-centric feature set that measured the correlation between edges associated with the mentioned brain networks. Then, to classify ASD samples from TD samples, we trained an Explainable and Generalized node-edge connectivity-based graph attention neural network (Ex-NEGAT). We also identified three sub-groups that were present within ASD samples using meta-connectivity as a feature set and their association with each other using the Rough Fuzzy c-means algorithm. Finally, we identified symptom severity scores for each individual using meta-connectivity using Connectome-based Prediction Modelling (CPMM) and identified brain networks that contributed positively and negatively to the prediction. Our approach accurately predicted ADOS-Total, ADOS-Social, ADOS-Communication, ADOS-Module, ADOS-STEREO, and FIQ scores.

1.6 ORGANIZATION OF THESIS

The thesis is organized as follows: 1) Chapter 2 is literature review and current status related to study of brain networks, network dynamics during typical and atypical brain network development. 2) Chapter 3 represents characterization of the temporal stability of ToM and pain functional brain networks from early childhood (as early as 3-yrs) to adulthood during naturalistic viewing. 3) Chapter 4 represents explainable deep learning framework: decoding brain task and prediction of individual performance in false-belief task at early childhood stage. 4) Chapter 5 shows identifying functional variations in theory of mind brain networks between autism and typically developing individuals using contrastive machine learning and explainable DNN model. 5) Chapter 6 a lightweight, end-to-end explainable, and generalized graph neural network framework to classify autistics from neuro-typicals 6) Chapter 7 shows identifying heterogeneity within autistics samples using Rough Fuzzy c-means approach.