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A comprehensive survey of complex brain network representation

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Abstract

Recent years have shown great merits in utilizing neuroimaging data to understand brain structural and functional changes, as well as its relationship to different neurodegenerative diseases and other clinical phenotypes. Brain networks, derived from different neuroimaging modalities, have attracted increasing attention due to their potential to gain system-level insights to characterize brain dynamics and abnormalities in neurological conditions. Traditional methods aim to pre-

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Declaration of interests

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define multiple topological features of brain networks and relate these features to different clinical measures or demographical variables. With the enormous successes in deep learning techniques, graph learning methods have played significant roles in brain network analysis. In this survey, we first provide a brief overview of neuroimaging-derived brain networks. Then, we focus on presenting a comprehensive overview of both traditional methods and state-of-the-art deep-learning methods for brain network mining. Major models, and objectives of these methods are reviewed within this paper. Finally, we discuss several promising research directions in this field.

Keywords

Brain structural network; Brain functional network; Brain network analysis; Network representation learning; Deep learning

1. Introduction

In recent decades, brain studies have gained more and more attention for understanding brain structures and functions, as well as their changes related to different clinical phenotypes or neurodegenerative diseases. The advancement of neuroimaging technologies has provided a broad research perspective and foundation for the studies of brain structure and function. These neuroimaging technologies, such as functional magnetic resonance imaging (fMRI), diffusion tensor imaging (DTI), and electroencephalography (EEG), provide insights into brain inner working patterns, allowing us to capture detailed snapshots of brain activities, organizations, and architectures. One of the valuable resources to promote the development of neuroimaging studies is the neuroimaging data samples. Credit to the advancement of medical informatics technologies (e.g., picture archiving and communication system, or PACS[1]) and the contributions provided by the amount of neuroimaging communities, the longitudinal collections of neuroimaging data serve as a strong foundation of current brain imaging studies, particularly for the big-data imaging studies (e.g., machine learning and deep learning on neuroimaging studies). Another factor that boosts the progress of this field is the development and spread of high-performance computing technologies, such as super-computing servers with advanced Central Processing Units (CPUs) and Graphics Processing Units (GPUs), which provide powerful computation resources for neuroimaging data computing. Moreover, a large number of studies have been proposed to establish many computational methods for neuroimaging data analysis from different perspectives, which is the third significant impetus in this research field. This paper reviews the current neuroimaging studies from one of the significant perspectives of brain imaging computational methods, i.e., brain network methods, to summarize a few current studies and provide some potential future research directions.

1.1. Introduction to brain networks

Current neuroimaging studies can be roughly categorized based on the structure of utilized data. Some studies focus on time sequences obtained by different neuroimaging modalities (e.g., EEG signal, fMRI Blood Oxygen Level-Dependent, or BOLD signal) with signal processing techniques.[2–5] Many other studies[6–10] focus on using imaging features From

voxels or regions-of-interest (ROIs). However, increasing evidence[11–14] indicates the brain is organized and functionalized based on the interactions among many brain regions, particularly in explaining various brain-related clinical phenotypes, resulting in more and more attention in using brain networks for these clinical phenotype predictions. Brain network[15–17] represents a 3D brain graph model, comprising the nodes and the edges among brain nodes. The nodes are brain ROIs and the edges can be defined using DTI-derived fiber tracking or fMRI-derived correlation. Brain network has great potential to gain system-level insights into the brain dynamics related to different clinical phenotypes. The details of brain network definitions and constructions will be discussed in Section 2.

1.2. Traditional methods

We state that the term "traditional methods" here refers to methods distinct from deep neural network methods. The traditional methods aim to design novel algorithms to extract discriminative network features from brain networks and investigate specific clinical tasks based on these network features. The network features are pre-defined by researchers with different research purposes, and we may leverage these purposes to roughly categorize these traditional methods. Many research works aim to explore the heterogeneity of topological structures of brain networks from different groups (e.g., disease group and healthy group), which propose various network topological measures such as the betweenness centrality to measure the node centralities in brain networks.[18] Some other studies[19,20] aim to distinguish brain networks from different groups based on network similarities, which defines many distance metrics or kernels to measure the network similarity features. A few other studies focus on the frequency domain, which yields methods for spectrum feature analysis.[21–24] Typical dimension reduction methods, such as Principal Component Analysis, are also utilized to extract informative brain network features for different clinical prediction tasks. The details of traditional methods of brain network analysis will be discussed in Section 3.

1.3. Deep learning methods

Though great progress has been achieved, there are several limitations existing in the traditional methods for brain network analysis. Traditional methods may be sub-optimal since the pre-defined brain network features contain less information than the original whole networks, which may also ignore important brain network attributes. Meanwhile, a few traditional methods, due to the algorithm complexity, may not be utilized for large-scale brain network studies. To analyze the large-scale complex network data (e.g., brain networks), deep graph learning techniques[25–31] have gained significant attention. A few outstanding review papers[32,33] have summarized recent deep learning methods on brain network analysis, where the reviewed studies are categorized based on the methodologies proposed in their works. However, our survey paper reviews the current studies from another perspective, where we categorize current deep learning methods in brain network studies based on their research objectives. We conducted a comprehensive review of a series of papers published in top-tier journals and conferences about deep learning on brain networks over the past three years. Particularly, we collected 126 papers in this direction mainly from *Medical Image Computing and Computer Assisted Interventions (MICCAI), Information Processing In Medical Imaging (IPMI), Knowledge Discovery and Data Mining (KDD), IEEE Transactions on Medical Imaging (TMI), IEEE Transactions on Neural Networks and*

Learning Systems (TNNLS), Medical Image Analysis, and Nature Neuroscience published in the year of 2020, 2021 and 2022. Based on their research objectives, these papers can be broadly summarized into 4 categories including multimodal brain network representation learning, multiscale brain network representation learning, dynamic brain network modeling, and interpretable brain network learning models. The details of deep learning methods on brain network studies will be discussed in Section 4.

The following sections of this review paper are organized as follows. We provide an overview of the brain network data, including the data constructions and publicly available datasets in Section 2. In Section 3 and Section 4, we provide a taxonomy for the traditional methods and deep neural networks on brain network studies, respectively. In Section 5, we propose a few potential challenges and future research directions for brain network studies. And we conclude our paper in the Section 6.

2. Brain network overview

In this section, we first introduce some preliminaries of graph-structured data which is a standard mathematical model utilized to represent the brain network. We then introduce different types of typical brain networks as well as their construction methods. Finally, we summarize several public brain network datasets that are widely utilized in current brain network studies.

2.1. Preliminaries of graph structured data

We denote an attributed graph with N nodes as $G = \{V, E\} = (A, X)$, where V is the set of graph vertices (or nodes) and E is the set of the graph edges. Let $v_i \in V$ denote a graph node (i.e., $i-th$ node) in the graph and $e_{ij} \in E$ denote a graph edge pointing from the node v_i to v_j. Particularly, e_{ij} equals e_{ji} in an undirected graph, while this may not true in the directed graph. Given a node v_i, its neighbor nodes can be defined as $N(v) = \{u \in V \mid (u, v) \in E\}$. $A \in \mathscr{R}^{N \times N}$ is the adjacency matrix of G, where the element a_{ij} of A is the weight of the edge e_{ij}. Particularly, A is a symmetric matrix for an undirected graph, while is an asymmetric matrix for a directed graph. $X \in \mathscr{R}^{N \times c}$ is the node feature matrix of G, where $x_i \in \mathscr{R}^{1 \times c}$ of X is a c-dimensional feature vector of v_i.

2.2. Construction of brain networks

Due to the vast number of neurons, synapses, and fibers existing in the human brain that will cause a computationally expensive task, it may be intractable to construct the brain network based on each signal brain neuron. Generally, a node in brain networks represents a brain region-of-interest (ROI) that consists of a group of brain neurons, while an edge in brain networks represents anatomical or functional connections among these ROIs.[34] Different types of brain networks (e.g., functional networks, structural networks, morphological networks) can be derived from the corresponding neuroimaging modalities (e.g., functional magnetic resonance imaging, diffusion tensor imaging, T1-weighted MRI). Here, we mainly introduce 4 different types of brain networks including structural networks, functional networks, morphological networks, and effective networks.

2.2.1. Structural networks—A structural network is formulated through the abstraction of a graph originating from diffusion tensor imaging (DTI)[35] or diffusion spectrum imaging (DSI).[36–38] These neuroimaging techniques gauge the diffusion patterns of water molecules to create contrast in MRI scans, facilitating the differentiation between gray matter and the underlying white matter. With the preprocessed DTI data, 5 key steps are involved in constructing a structural network:

- Estimate the diffusion tensor based on the preprocessed DTI data at each voxel. The diffusion tensor provides information on the local orientation and anisotropy of white matter tracts.
- Perform fiber tracking or tractography (e.g., deterministic algorithms or probabilistic algorithms[39–43]) to identify white matter pathways based on the estimated diffusion tensor information.[44]
- Define regions of interest (ROIs) within the brain, where the defined ROIs correspond to different anatomical regions or functional regions.
- Identify fibers between pairs of ROIs. A fiber is considered to connect two ROIs if it passes through both regions. The presence of a fiber between two ROIs indicates a potential structural connection between them.
- Count the number of fibers connecting each pair of ROIs or compute the average fractional anisotropy along the fibers connecting the ROIs as the edge weights within structural networks.

2.2.2. Functional networks—Traditionally, the construction of a functional network entails the utilization of functional Magnetic Resonance Imaging (fMRI), specifically focusing on the blood-oxygen-level-dependent (BOLD) signal indicating changes in blood oxygenation linked to neural activity in a brain region.[45] With the preprocessed fMRI data, 4 key steps are involved in constructing a functional network:

- Extract the BOLD time series for each voxel or brain ROI. Brain ROIs can be defined anatomically, functionally, or through parcellation techniques.
- Process and filter the BOLD time series data to remove low-frequency drifts and high-frequency noise.
- Estimate the edge weights in functional networks by computing the correlation between the time series of different brain regions.
- Threshold the correlation matrix to maintain meaningful connections and denoise.

2.2.3. Morphological networks—Morphological networks utilize cortical metrics, such as sulcal depth and cortical thickness, to quantify morphological differences between brain regions.[46–48] Extracted from T1-weighted MRI via Freesurfer preprocessing,[49] the steps include skull stripping, motion correction, normalization, topology correction, and hemisphere delineation.[50] Hemispheres are segmented into regions using atlases (e.g., Desikan-Killiany). For each region, average cortical attribute values are computed. The

absolute difference in these values between pairs of regions establishes edge weights in the networks. With the preprocessed T1-weighted data, 6 key steps are involved in constructing a morphological network:

- Extract the brain regions by demarcating the boundary between brain and non-brain tissues with specialized techniques, such as FSL-BET.[51,52]
- Segment the brain to discern the distinct tissues in T1-weighted images, such as gray matter, white matter, and cerebrospinal fluid.
- Partition the brain into discrete ROIs using parcellation strategies rooted in anatomical landmarks and/or functional considerations.
- Extract a comprehensive array of pertinent morphological attributes from each ROI, including volumetric measures, surface area, thickness, and geometrical descriptors.
- Quantify the inter-ROI morphological resemblances through the computation of a similarity matrix, delineating the degree of structural convergence between pairs of ROIs.
- Present the emergent morphological relationships as graph structured data, where the nodes correspond to the designated ROIs and edges encapsulate the ascertained morphological interconnections among the identified regions.

2.2.4. Effective networks—Effective networks aim to capture the causal relationships and directional influences among different brain regions, which is essential to understanding the brain functional activities under specific tasks and different.[53–55] Several techniques, such as Dynamic Causal Modeling (DCM)[56–59] and Granger Causality Analysis,[60–64] are used in inferring and modeling the effective connections between brain regions by analyzing the temporal dynamics of neural activities. The construction of effective networks can be summarized in the following steps:

- Obtain the signals from different modalities (e.g., fMRI, EEG, MEG) to record brain activities of subjects engaged in specific cognitive tasks or at a resting-state.
- Define regions of interest (ROIs) within the brain. These ROIs can correspond to specific anatomical regions or functional areas that are relevant to the study. ROIs can be defined based on anatomical atlases or functional parcellation schemes.
- Extract time series data from the selected ROIs that represent the neural activities of each brain region over time.
- Apply different methods, such as DCM and Granger Causality, to estimate the effective connectivity within effective brain networks. The parameter estimation in for the applied will determine the strength and directionality of these effective connections.

- Conduct statistical tests to assess the significance of the effective connections, and correct the reconstructed brain effective networks.

2.3. Datasets and implementation tools

We overview widely used publicly available brain network datasets and algorithm implementation toolboxes (or libraries) in brain network analysis.

2.3.1. Public brain network datasets—In recent years, the efforts invested in collecting and organizing large-scale neuroimaging datasets have empowered researchers to design and implement innovative computational intelligent approaches, including deep learning models, for different brain studies. Based on this, multiple brain connectomic projects were proposed to initiate and provide a series of brain network datasets for brain connectome studies. We briefly summarize several representative brain network datasets here.

- Human Connectome Project (HCP[a]). The HCP is one of the most comprehensive brain mapping initiatives, providing high-quality data on functional and structural connectivity in the human brain. It includes data from multiple modalities, such as resting-state fMRI, task-based fMRI, DTI, and behavioral assessments.[65,66]
- Open Access Series of Imaging Studies (OASIS[b]). The OASIS (Open Access Series of Imaging Studies) dataset is a well-known and publicly available collection of neuroimaging data that primarily focuses on structural MRI (Magnetic Resonance Imaging) scans of the brain. It has been a valuable resource for researchers studying various aspects of brain structure, aging, and neurodegenerative diseases.[67,68]
- Alzheimer's Disease Neuroimaging Initiative (ADNI[c]). The ADNI dataset is a well-known and publicly available collection of neuroimaging and clinical data primarily focused on Alzheimer's disease (AD) research. ADNI is a landmark project that aims to accelerate the understanding of AD by providing valuable resources for researchers studying various aspects of the disease, including its diagnosis, progression, and treatment.[69,70]
- Autism Brain Imaging Data Exchange (ABIDE[d]): The ABIDE offers a collection of resting-state fMRI data from individuals with autism and typically developing controls. It is a valuable resource for studying brain connectivity in the context of autism spectrum disorders.[71,72]
- Center for Biomedical Research Excellence (COBRE[e]). The COBRE provides resting-state fMRI and structural MRI data from individuals with

[a] https://www.humanconnectome.org
[b] https://www.oasis-brains.org
[c] https://adni.loni.usc.edu
[d] http://fcon_1000.projects.nitrc.org/indi/abide/
[e] http://fcon_1000.projects.nitrc.org/indi/retro/cobre.html

schizophrenia and healthy controls. It supports research into the neural basis of schizophrenia.[73–76]

- NKI-Rockland Sample (NKI[f]). This dataset includes resting-state fMRI and other neuroimaging data from the Nathan Kline Institute (NKI) Rockland Sample, offering insights into various aspects of brain connectivity.[77]
- BNU1[g] and BNU3[h] Dataset. These datasets provide resting-state fMRI data from the Beijing Normal University (BNU), which can be used to study brain connectivity and its variations across different populations.[78]
- ADHD-200 Dataset.[i] The ADHD-200 offers neuroimaging data, including resting-state fMRI, from individuals with attention-deficit/hyperactivity disorder (ADHD) and controls. It supports research into the neural basis of ADHD.[79,80]
- The Human Brainnetome Atlas[j]. This atlas provides comprehensive connectivity data, including resting-state fMRI and diffusion MRI, to map and understand the human brain's functional and structural connectivity.[81,82]

2.3.2. Programming toolboxes and libraries—We summarize a few important programming toolboxes and libraries in this section to facilitate researchers to implement their algorithms on brain network studies.

2.3.2.1. Neuroimaging DATA Preprocessing.: The widely used toolboxes for neuroimaging data preprocessing include but are not limited to: SPM[k] (Statistical Parametric Mapping),[83] FSL[l] (FMRIB Software Library),[84] FreeSurfer,[m],49 AFNI[n] (Analysis of Functional NeuroImages),[85] ANTs[o] (Advanced Normalization Tools),[86] MRtrix3[p],87 and CONN[q](Functional Connectivity Toolbox).[88]

The key services, benefits, and drawbacks of these toolboxes are summarized in Table 1.

2.3.2.2. Graph analysis.: The broadly utilized graph analysis libraries for brain network studies include but are not limited to: NetworkX[r],89 Graph-tool,[s],90 brainGraph[t],91 BCT (Brain Connectivity Toolbox),[u],18 GRETNA (Graph Theoretical Network Analysis),[v],92

[f] https://fcon_1000.projects.nitrc.org/indi/enhanced/
[g] http://fcon_1000.projects.nitrc.org/indi/CoRR/html/bnu_1.html
[h] https://fcon_1000.projects.nitrc.org/indi/CoRR/html/bnu_3.html
[i] http://fcon_1000.projects.nitrc.org/indi/adhd200/
[j] http://atlas.brainnetome.org
[k] https://www.fil.ion.ucl.ac.uk/spm/
[l] https://fsl.fmrib.ox.ac.uk/fsl/fslwiki
[m] https://surfer.nmr.mgh.harvard.edu
[n] https://afni.nimh.nih.gov
[o] http://stnava.github.io/ANTs/
[p] https://www.mrtrix.org
[q] https://web.conn-toolbox.org
[r] https://networkx.org
[s] https://graph-tool.skewed.de
[t] https://github.com/cwatson/brainGraph
[u] https://sites.google.com/site/bctnet/
[v] https://www.nitrc.org/projects/gretna/

scikit-network,[w],93 PyG (Pytorch-Geometric),[x],94 DGL (Deep Graph Library),[y],95 and BGL (Boost Graph Library).[z],96

The primary services, advantages, and disadvantages of these libraries are outlined in Table 2.

3. Traditional brain network mining methods

Generally, traditional pipelines for brain network analyses include two stages. The first stage refers to feature extraction, where the effective network features are extracted by different pre-defined methods. After the feature extraction stage, statistical analysis will be conducted based on the extracted features in the second stage. We summarize a few traditional and widely-used methods for brain network analyses in both stages in this section.

3.1. Network feature extraction

Four different types of network feature extraction methods are summarized here including (1) network topological measure, (2) graph kernel, (3) spectral graph analysis, and (4) dimension reduction.

3.1.1. Network topological measure—In network science, network measures refer to various quantitative metrics or characteristics used to describe and quantify the topological structures and/or functional properties of brain networks. These measures assist in gaining biological insights into the organization and properties of brain networks. The network measures, proposed to investigate brain networks from a different perspective, can be categorized as follows:

- Degree and Similarity such as brain node degree and node strength.
- Density and Rentian Scaling such as brain node density and Rentian scaling.
- Clustering and community structure such as clustering coefficient, mularity, and transitivity.
- Assortativity and core structure such as Rich club coefficient and core/periphery structure.
- Paths and distances such as characteristic path length and cycle probability.
- Efficiency and Diffusion such as global and local efficiency, as well as diffusion efficiency.
- Centrality such as betweenness centrality and within-module degree z-score.
- Motifs and self-similarity such structural motifs and functional motifs.

[w] https://github.com/sknetwork-team/scikit-network
[x] https://pytorch-geometric.readthedocs.io
[y] https://www.dgl.ai
[z] https://www.boost.org/doc/libs/1_82_0/libs/graph/doc/index.html

The full list of network measures categories is summarized in Table 3. The definition of each network measure is summarized in Rubinov and Sporns [18]; and the implementation of these measures can be found in the Brain Connectivity Toolbox (BCT-Toolbox).

3.1.2. Graph kernel—Graph kernel-based methods are a set of techniques employed in the field of network analysis to extract valuable features from graph structured data. The primary objective of graph kernel methods is to capture the inherent structural information and patterns within these graphs, thereby to simplify the high-dimensional complex network data which facilitates the following statistical analysis. These methods rely on mathematical functions known as graph kernels to compute similarity measures between pairs of graphs, effectively quantifying their structural similarities or differences. By applying these kernel functions to pairs of brain networks, similarity scores are generated, serving as high-dimensional features that depict the likeness between two brains. The advantages and disadvantages of different graph kernel methods, including Graph Edit Distance Kernel,[97,98] Graphlet Kernel,[99,100] Weisfeiler-Lehman Kernel,[101,102] Subgraph Matching Kernel,[103,104] Graph Path Kernel,[105,106] and Graph Alignment Kernel,[107,108] are summarized in Table 4.

3.1.3. Spectral graph analysis—Spectral analysis methods focus on analyzing different frequency components for the connectivity patterns of brain networks (particularly for functional brain networks derived from fMRI, EEG, and MEG). These methods are specially considered to understand the oscillatory dynamics of brain activity, and the role of different frequency bands in information processing and communication among different brain regions. Numerous studies for special analysis methods on brain networks have been proposed, yielding various analysis methods such as frequency decomposition,[22–24,109,110] power spectrum analysis,[21,111–113] and time-frequency analysis.[114–116]

3.1.4. Dimension reduction—Since the brain networks are high-dimensional complex graph structural data, it will result in information redundancy and dimension explosion if we directly apply machine learning algorithms to original brain network data, particularly for small-size datasets. Hence, a dimension reduction or feature engineering (e.g., feature extraction and selection) should be performed to remove redundancy information and maintain discriminative features of brain networks before we apply machine learning algorithms for specific tasks. General dimension reduction methods include Principal Component Analysis (PCA),[117] Independent Component Analysis(ICA),[118] Isometric Mapping (Isomap),[119] t-Distributed Stochastic Neighbor Embedding (t-SNE),[120] Linear Discriminant Analysis (LDA),[121] and Laplacian Eigenmaps.[122]

3.2. Statistical analysis

After extracting features from brain networks, various statistical analyses can be employed to unveil patterns of brain changes across different groups, such as control versus disease or male versus female. Diverse statistical tests, including t-tests, ANOVA tests, and network permutation tests, can be applied to investigate the presence of significant group differences among various brain network groups. Currently, machine learning techniques, such as linear regression, logistic regression, support vector machines, and k-means clustering, serve as powerful tools for classifying and performing regressions on brain networks. Additionally,

network visualization techniques (e.g., BrainNet visualization as demonstrated in Ref. 123) are sometimes employed to visually represent distinctions within brain networks.

4. Deep brain network representation learning

With the development of artificial intelligence (AI) techniques, learning-based methods (e.g., machine learning, deep learning) are broadly investigated and applied to brain network data for different research purposes. Most of these learning methods are based on the graph neural networks (GNN), a class of deep neural networks for graph-structured data representations.[27–29,124–128] Many research objectives on brain network learning have been proposed in recent years. For example, a few studies focus on developing deep learning methods to model the multiview representations across different modalities-derived brain network data. Some other studies focus on investigating the interpretability of the deep learning models to yield biological insights (e.g., finding new biomarkers that closely relate brain networks to different neurological disorders) for the model outcomes. As shown in Fig. 1, we summarize these studies based on these research objectives.

4.1. Multimodal brain network learning

Brain networks can be generated from different neuroimaging modalities to depict and record the human brain from diverse perspectives. Two main perspectives are generally considered, including brain anatomical structures and brain functionalities, in multimodal brain network studies. The target of the multimodal brain network learning is to aggregate effective information from multiple data modalities to yield comprehensive brain network representations for different clinical tasks.[129–154] For example, Li et al.[141] proposed a joint graph convolution network (joint-GCN) to combine the functional and structural networks by introducing inter-network edges between the corresponding brain regions within these two brain networks. The weights of these inter-network edges are trainable parameters that reflect the non-uniform structure-function coupling strength across the brain. This structure-function joint graph is embedded by a single GCN, which allows for the integration of both functional and structural information in the brain network learning stage. Another strategy to combine multimodal networks is to model the network communications by constructing a map between different network modals, where networks of different modals constrain each other. For example, Zhang et al.[150] and Tang et al.[145] proposed generative graph neural networks to construct mappings from functional brain network to the structural counterpart, while Zhang et al.[155] construct the mapping inversely. Ye et al.[156] propose a bidirectional mapping framework to model the communication between functional and structural networks from both sides and an ROI-level contrastive learning method is utilized to yield a unified multimodal network representation. Besides combining the networks of different modals in the latent space, Zhang et al.[149] performed the network fusion directly original graph space by creating a fused adjacency matrix based on both structural networks and the corresponding functional network profiles. In Table 5, we compare several multimodal brain network learning approaches on HCP and OASIS datasets for two classification tasks: gender classification and disease classification.

4.2. Multiscale brain network learning

The complex human brain networks are organized hierarchically, where different brain regions collaborate to maintain brain functionalities. Multiscale brain network learning refers to the process of modeling high-order patterns in brain networks at multiple levels or scales of organization, aiming to capture and understand the interactions within and between these different levels of the organization.[148,157–178] One of the strategies for multiscale brain network learning is based on multigraph investigation. For example, Tang et al.[171–173] proposed a series of hierarchical graph representation learning models to extract hierarchical structures (e.g., network communities) within brain networks, and perform the graph pooling for brain network downscale based on the captured the structures. The multiscale network representations yielded from different pooling layers are fused for downstream task predictions (e.g., neurodegenerative disease classifications). The generative graphic model is also a promising method to capture the hierarchical high-order information from brain networks for multiscale learning. For example, Pang et al.[169,179] proposed different deep belief networks (e.g., a prior knowledge guided deep belief network (PKG-DBN)) which fully leverage prior knowledge to capture the hierarchical structures in functional brain networks. Moreover, the diffusion kernel-based graph learning models may also be considered for multiscale brain network learning. For example, Zhang et al.[178] proposed a Diffusion Kernel Attention Network that uses the Transformer model to incorporate high-order information from interactions among much broader brain regions. Similarly, we compare several multiscale brain network learning methods on HCP and OASIS datasets in Table 5.

4.3. Dynamic brain network learning

Dynamic brain network learning refers to the process of modeling and analyzing the time-varying or dynamic aspects of brain networks, which are representations of the functional or structural connections between different regions of the brain over time. Static brain network analysis treats connectivity as constant, instead, dynamic brain network learning considers that brain connectivity patterns change over time and can capture fluctuations in brain activity or organization. The common neuroimaging data sources for dynamic brain network learning include fMRI, EEG, MEG, and DTI-derived brain networks. Dynamic brain network learning can be used to study cognitive processes, investigate brain changes resulting from neurological and psychiatric disorders, and understand brain development.[152,153,166,180–206] The recurrent neural network (RNN) based architecture is one of the methods to model temporal dynamics in brain networks. For example, Demirbilek and Rekik[183] proposed a recurrent multigraph integrator network (ReMI-Net) to predict the longitudinal evolution of population-driven brain connectivity templates over time, which enables the identification of brain biomarkers in dementia prediction. Dynamic Bayesian Networks (DBNs) are another class of powerful modeling frameworks for capturing temporal dependencies and dynamics in dynamic brain networks. For example, Moguilner et al.[207] introduced a Bayesian machine learning pipeline based on dynamic connectivity fluctuation analysis (DCFA) on resting-state fMRI data for neurodegenerative condition predictions. Moreover, the transformer plays an undoubted role in modeling the brain dynamics over time sequences. For example, Zhao et al.[153] proposed a continuous multi-

head attention-based graph transformer for Brain Dynamics modeling, where heterogeneous network representations can be extracted from both spatial and temporal domains.

4.4. Interpretable brain network learning

Many deep graph learning models have been proposed for brain network analysis, yet most current models lack interpretability, which makes it hard to gain any heuristic biological insights into the results, and to identify novel biomarkers indicating brain pattern heterogeneity among different clinical phenotypes. A few recent studies make contributions to proposing interpretable graph learning models which, from different perspectives, yield biological insights and explanations on their model outputs.[145,152,171–173,208–216] For example, Cui et al.[210] proposed an explainable mask to identify the most important brain nodes and edges as closely related biomarkers to different disease prediction tasks.[172,173] designed an interpretable hierarchical graph pooling module to identify the important brain regions as biomarkers related to multiple clinical phenotypes and brain disorders. Liu et al.[215] proposed a framework, DeepHoloBrain, that represents a region-adaptive interference pattern between neural activities and a collection of reference harmonic wavelets as a symmetric and positive-definite (SPD) matrix, allowing for interpretability and analysis of brain states and disease connectomes. D'Souza and Venkataraman[211] proposed an mSPD neural network with bilinear fully connected layers with tied weights, which achieves interpretability by leveraging the underlying geometric structure of connectomes in fMRI brain networks to discover stable biomarkers associated with attention deficit hyperactivity disorder (ADHD).

4.5. Other research topics

The scope of brain network studies is so broad that many additional topics are also worthy of attention, such as causality exploration,[189,192,206,217] powerful reconstruction tools,[168,218–221] and multisite brain network learning.[143,222] Causal inference in brain networks refers to the study of causal relationships between different brain regions that involves identifying and understanding how one brain region's activity or state causally affects the activity or state of another brain region. For example, Zhuang et al.[206] proposed a Bayesian framework, named Multiple-Shooting Adjoint (MSA), to perform dynamic causal modeling to estimate the directed causality among different brain regions in the functional brain networks. Neuroimaging dataset is typically in small size, therefore, data obtained from different sites as well as different scanners may be jointly trained for deep learning models. However, domain gaps obviously exist across different scanners introduced by the heterogeneity of imaging modalities, radiologists, and imaging protocols, which makes multisite learning exceptionally important.

5. Discussions and challenges

Although recent studies have made significant strides in the domain of brain network analysis, numerous open questions persist, providing ample opportunities for researchers to explore. In this section, we delineate several noteworthy challenges that could serve as potential future directions.

Initially, this review consolidates the construction procedures of several frequently employed brain networks, along with publicly accessible datasets for brain network analysis. Most existing studies focus more on structural brain networks and functional brain networks, where both brain networks are undirected attributed graphs with undirected edge e_{jj} between v_i and v_j (i.e., $e_{ij} = e_{jj}$). The difference between structural networks and functional networks is that the $e \in E$ in structural networks are positive values, while they can be negative in functional networks. Since the functional networks are constructed based on the BOLD signal correlation among different brain nodes, the positive and negative edges represent synchronous activation and asynchronous activation among brain regions, respectively. However, the directed brain graph (e.g., effective brain networks) is rarely studied, which may be a potential direction to explore the functional influence among brain regions (e.g., causality influence between brain nodes). To this end, preliminary studies should be conducted first to build up several effective directed brain network datasets. Another challenge of the current brain network dataset is data insufficiency, which will further limit the progress of big data mining on brain network studies. For example, the current brain network datasets may not be easy to utilize for the group difference studies based on the deep learning model since the number of networks in a few subgroups may not be enough to train the neural networks. Instead of enlarging the current dataset, technical methods in addressing data quantity issues should also be strictly considered. These methods include but are not limited to data augmentation techniques, fast algorithms for brain network constructions from neuroimaging data, multisite learning for dataset combinations, and pre-trained model development.[223]

We also discussed the model interpretability for current brain network learning methods in this review, which is a very important direction in the future that is closely related to clinical translations. Most of the current studies provide biological explanations of their model outcomes based on identified biomarkers related to different clinical phenotypes, such as the most important brain regions corresponding to Alzheimer's Disease. However, the pattern changes of the pathway of information flow among brain regions, resulting from neurodegenerative diseases, gain more attention in clinical translation studies. Also, the generalization ability of current interpretable models is always challenged across diverse populations and brain network datasets. The proposed model may yield different explanations (e.g., identify different biomarkers) for the same prediction task when utilizing different brain network datasets, which may be due to the diversity of different population groups, heterogeneity of brain network data, and the model's robustness. Another more profound challenge is that the current model yielded explanations (e.g., discovered biomarkers) are only evaluated by the previous clinical references, while real clinical validations are required for these biomarkers before the clinical translation stage in the future.

Another future direction is distributed computing and resource-decentralized techniques in medical big-data studies, which will boost the development efficiency of AI communities. The collaborations across multiple institutions and research centers will be closer in the future, where the machine learning algorithms may be collaboratively trained without sharing raw medical data. Therefore, distributed algorithms such as federated learning,

aiming to address privacy, security, and data ownership sensitivities, will be a promising future direction undoubtedly. Moreover, Large Language Models (LLMs) such as GPT (Generative Pre-trained Transformer) are also likely to have a substantial impact on brain network studies in the future, opening up new possibilities and enhancing various aspects of research in this field. The large language pre-trained model can serve as a powerful feature extractor for brain network representation learning. It also has great potential to tackle the brain network annotation issues, model interpretability issues, and data augmentation issues by generating more synthetic brain networks.[224]

6. Conclusion

This survey paper commences with an overview of brain network constructions and publicly available brain network datasets. Then the research objectives of recent studies, encompassing both traditional and deep learning methods for brain network analysis, are comprehensively discussed. Finally, we propose several pertinent future directions, aiming to serve as a catalyst for additional contributions to this evolving field.

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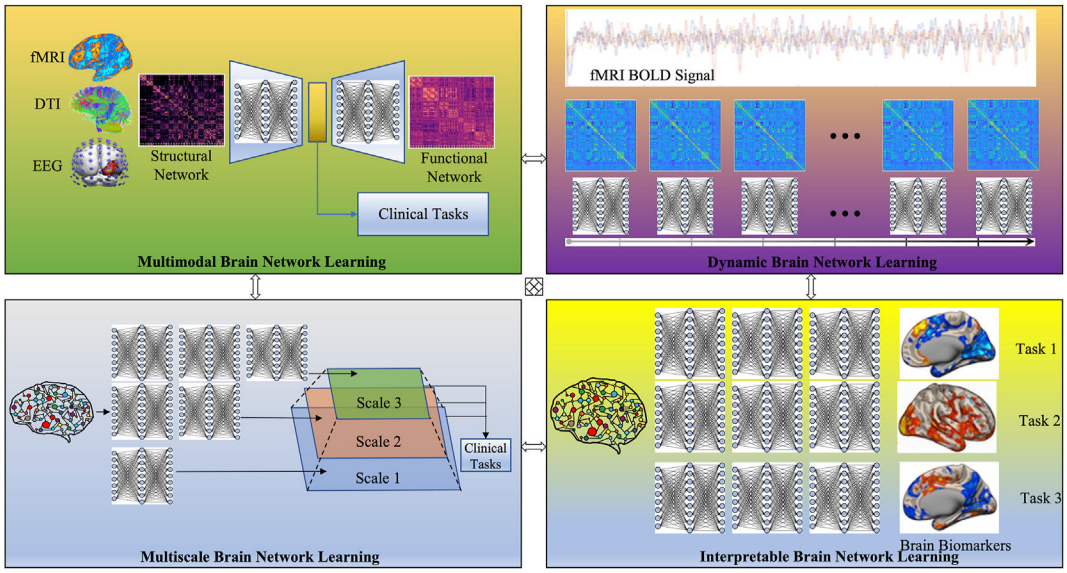

Fig. 1.

Key research objectives of deep learning models on brain network studies.

Table 1

Toolboxes for neuroimaging data preprocessing.

Toolboxes	Main Service	Advantages	Disadvantages
SPM	Functional and structural MRI analysis	Widely used and comprehensive tools	MATLAB dependency, steep learning curve
FSL	fMRI and DTI data analysis	User-friendly with GUI, extensive functionality	Some tasks are memory-intensive
FreeSurfer	Structural MRI analysis	Specialized for brain morphometry, quality segmentation	Limited for fMRI data, resource-intensive
AFNI	fMRI and neuroimaging data analysis	Broad analysis techniques, active user community	Command-line interface, learning curve
ANTs	Image registration and normalization	Powerful image registration, multi-modal support	Command-line usage, learning curve
MRtrix3	DTI data processing	Specialized for diffusion MRI, advanced tractography	Limited to diffusion MRI, learning curve
CONN	fMRI connectivity analysis	Specialized for connectivity, user-friendly	Focus on functional connectivity, MATLAB-based

Table 2

Libraries for brain network analysis.

Libraries	Main Service	Advantages	Disadvantages
NetworkX	Graph analysis and manipulation	Python-based, extensive documentation	Slower for large graphs, not optimized for performance
Graph-tool	Graph analysis and modeling	Efficient C++ library, supports large graphs	Steeper learning curve
BrainGraph	Brain network analysis	Specialized for neuroimaging data, user-friendly	Limited scope outside neuroimaging, fewer features
BCT	Brain network analysis	Comprehensive toolset for neuroimaging data	MATLAB-based, may require additional toolboxes
GRETN	Brain network analysis	User-friendly GUI, supports multiple imaging modalities	Limited flexibility for custom analysis
scikit-network	Graph analysis and machine learning	Integration with scikit-learn, Pythonic API	Smaller user community, fewer specialized tools
PyG	Graph analysis and deep learning	Deep learning integration, GPU support	Requires familiarity with PyTorch or TensorFlow
DGLD	Dynamic graph analysis	Specialized for temporal and dynamic graphs	Less support for static graph analysis
BGL	General-purpose graph analysis	High-performance C++ library, extensive features	Steeper learning curve for non-C++ users

Table 3

Network measures on brain network analysis.

Network Measure	Examples
Degree and similarity	Node degree and strength, joint degree, topological overlap, neighborhood overlap, matching index
Density and rentian scaling	Density, rentian scaling
Clustering and community structure	Clustering coefficient, transitivity, local efficiency, connected components, community structure and modularity, modularity degeneracy and consensus partitioning
Assortativity and core structure	Assortativity, rich club coefficient, core/periphery structure, K-core, S-core
Paths and distances	Paths and walks, distance and characteristic path length, cycle probability, Characteristic path length, global efficiency, eccentricity, radius, diameter
Efficiency and diffusion	Global and local efficiency, mean first passage time, diffusion efficiency, resource efficiency, path transitivity, search information, navigation
Centrality	Betweenness centrality, edge betweenness centrality, within-module degree z-score, participation and related coefficients, eigenvector centrality, PageRank centrality, subgraph centrality, k-coreness centrality, flow coefficient, shortcuts
Motifs and self-similarity	Structural motifs, functional motifs, quasi-idempotence

Table 4

Advantages and disadvantages of different graph kernel methods. GEDK = Graph Edit Distance Kernel, GLK = GraphLet Kernel, WLK = Weisfeiler-Lehman Kernel, SGMK = Subgraph Matching Kernel, GPK = Graph Path kernel, and GAK = Graph Alignment Kernel.

Methods	Advantages	Disadvantages
GEDK	Captures structural differences effectively Can incorporate domain-specific knowledge	Computationally expensive for large graphs Sensitivity to edit operation costs
GLK	Efficient and quick for large graphs Captures local structural patterns	May not capture global structural properties Limited in handling variations in graph size and structure
WLK	Captures both local and global structure Computationally efficient, especially with hashing	May not perform well on highly irregular graphs Limited in capturing fine-grained structural differences
SGMK	Captures local and global structural patterns Measures similarity based on common subgraphs	Computationally expensive for large graphs Sensitive to subgraph size and similarity definition
GPK	Captures structural info through shortest paths Can handle weighted graphs effectively	Computationally expensive for large graphs May not capture fine-grained structural variations
GAK	Handle labeled and attributed graphs effectively Capture both structural and semantic information	Computationally expensive for large graphs

Table 5

Accuracy (%) for gender classification on HCP data and Alzheimer Disease classification on OASIS dataset by applying different deep learning models.

Multimodal Methods	Gender	Disease	Multiscale Methods	Gender	Disease
Joint-GCN[141]	83.45 ± 1.61	78.26 ± 0.71	MMTGCN[148]	81.97 ± 0.71	78.47 ± 1.13
DSBGM[145]	82.19 ± 2.01	78.92 ± 1.38	HSGPL[173]	81.51 ± 1.14	77.51 ± 1.84
EC-GNN[152]	85.20 ± 0.05	–	Dual-HINet[160]	82.20 ± 0.25	76.42 ± 0.77