Topological Signatures of Altered Brain Network Centrality in ADHD: A TDA Mapper Study

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Abstract

Attention-Deficit/Hyperactivity Disorder (ADHD) is a prevalent neurodevelopmental disorder widely hypothesized to stem from alterations in large-scale brain connectivity. However, neuroimaging studies have yielded inconsistent findings, motivating the need for advanced analytical methods capable of capturing the complex, dynamic nature of brain function. In this study, we apply Topological Data Analysis (TDA), specifically the Mapper algorithm, to resting-state functional magnetic resonance imaging (fMRI) data from the multi-site ADHD-200 dataset. We constructed graphical representations of brain state dynamics for participants with ADHD and typically developing controls (TDC) from three independent sites. The topological structure of these graphs was quantified using network centrality measures (betweenness, closeness, and degree). Our results reveal a significant increase in centrality measures in the ADHD group compared to TDC in three cohorts. Furthermore, we observed a weak but significant positive correlation between centrality and symptom severity in one of the cohorts. We conclude that TDA-derived centrality measures can detect alterations in the dynamical organization of brain activity in ADHD, potentially reflecting a less efficient or more rigid network topology.

Keywords: Topological Data Analysis, Mapper Algorithm, ADHD, Functional Connectivity, Brain Dynamics, Network Centrality, fMRI

1. Introduction

Attention-Deficit/Hyperactivity Disorder (ADHD) is a common neurodevelopmental disorder characterized by persistent patterns of inattention, hyperactivity, and impulsivity that interfere with development and functioning (Konrad and Eickhoff, 2010). Computational neuroscience aims to ground such clinical diagnoses in objective biological features, moving beyond purely symptom-based classifications (Saggar and Uddin, 2019). A prevailing neurobiological model posits that ADHD arises from atypical wiring and communication within and between large-scale brain networks (Gracia-Tabuenca et al., 2020; Konrad and Eickhoff, 2010). However, the functional connectivity literature in ADHD is marked by conflicting reports, with studies variously describing patterns of hyperconnectivity (abnormally strong connections) and hypoconnectivity (abnormally weak connections) (Tolonen T, 2023). These inconsistencies are often observed in key brain systems, including the Default Mode Network (DMN), fronto-parietal attention networks, and subcortical circuits, highlighting the complexity of the disorder and the challenges in identifying consistent neural markers.

A significant limitation of many traditional neuroimaging analyses is the practice of averaging data across time and space. Methods that compute functional connectivity across an entire scan session or average signals within predefined regions-of-interest inherently

collapse the data, potentially obscuring the rich, moment-to-moment fluctuations in brain activity that are fundamental to ongoing cognition (Saggar et al., 2018; Duman and Tatar, 2023). This spatiotemporal collapse may contribute to the inconsistent findings in the literature by masking the very dynamical properties that differentiate clinical populations from healthy controls.

To address these limitations, Topological Data Analysis (TDA) has emerged as a powerful mathematical framework for characterizing the underlying shape of complex, high-dimensional data (Carlsson, 2014; Singh et al., 2007). The Mapper algorithm, a key TDA technique, distills high-dimensional point cloud data into a simplified, yet topologically meaningful, graphical representation (Singh et al., 2007). A core advantage of Mapper, championed by researchers like Saggar and colleagues, is its ability to generate these representations at the single-participant level without collapsing the original temporal and spatial scales of the data (Saggar et al., 2018; Geniesse et al., 2019). This approach provides a data-driven lens into the brain's dynamical landscape, representing transient brain states as nodes in a graph and the transitions between them as edges. Foundational work by Saggar et al. (2018) demonstrated that Mapper could successfully reveal the dynamical organization of the brain during both task and rest states in fMRI data, with the resulting graph structures correlating with behavioral performance. The method has since been successfully applied to study pharmacological interventions, identify clinical subgroups in Fragile X syndrome, and analyze high-temporal-resolution MEG data (Saggar et al., 2022a; Romano et al., 2014; Duman and Tatar, 2023).

In this study, we apply the TDA-Mapper pipeline to the large, multi-site ADHD-200 resting-state fMRI dataset to investigate alterations in the topological structure of brain dynamics. We hypothesize that the brain state networks of individuals with ADHD will exhibit a more rigid and less efficient organization compared to typically developing controls (TDC). Specifically, we predict this will manifest as (1) higher network centrality in the Mapper-derived graphs of the ADHD group, and (2) that these topological alterations will be clinically relevant, showing a positive correlation with the severity of ADHD symptoms. By leveraging a multi-site dataset, we aim to not only identify potential topological biomarkers but also to critically assess their robustness and generalizability across different data acquisition environments.

2. Materials and Methods

2.1. Participants and Dataset

This study utilized data from the ADHD-200 Global Competition, a publicly available resource aggregated by the International Neuroimaging Datasharing Initiative (INDI) (The ADHD-200 Consortium, 2012; Bellec P, 2017). The full dataset comprises resting-state fMRI (rs-fMRI), structural MRI, and phenotypic data from 973 individuals across eight imaging sites (The ADHD-200 Consortium, 2012). For this analysis, we selected three sites with sufficient sample sizes and complete data: New York University (NYU), NeuroIMAGE (NI), and Oregon Health & Science University (OHSU). After excluding participants with poor quality data or missing phenotypic information, our final sample consisted of data from these three cohorts. Phenotypic data included diagnostic status (ADHD or TDC), age, sex, and scores from the ADHD Rating Scale IV, providing measures for an overall

ADHD Index, an Inattentive subscale, and a Hyperactive/Impulsive subscale (ADHD-200 Consortium, 2011). Participant demographics for each site are detailed in Table 3.

2.2. fMRI Data Acquisition and Preprocessing

Data were acquired at each site using 3T MRI scanners. Specific acquisition parameters varied by site and are detailed in the ADHD-200 documentation (The ADHD-200 Consortium, 2012). We used the preprocessed data provided by the Neuro Bureau initiative, which were processed using the Athena pipeline (Bellec P, 2017). This standardized pipeline included slice timing correction, 3D motion correction, spatial normalization to the MNI152 standard template, band-pass filtering (0.009–0.08 Hz), and regression of nuisance variables, including the six motion parameters, their derivatives, and signals from white matter and cerebrospinal fluid.

2.3. Topological Data Analysis: The Mapper Pipeline

We employed the Mapper algorithm to generate a compressed graphical representation of each participant's brain dynamics (Singh et al., 2007; Saggar et al., 2018). The pipeline consists of several sequential steps:

1. Input Data: For each participant, the preprocessed 4D rs-fMRI data was reshaped into a 2D matrix, where rows represent time points (volumes) and columns represent the BOLD signal intensity at each brain voxel. This matrix constitutes a high-dimensional point cloud, where each point is a snapshot of whole-brain activity.

2. Distance Metric: A pairwise distance matrix was computed between all time points using the Euclidean distance (L_2-norm). This metric quantifies the dissimilarity between any two whole-brain activation patterns and is a standard choice in prior neuroimaging applications of Mapper (Duman and Tatar, 2023; Kyeong et al., 2017).

3. Filter Function: We used Principle Component Analysis (PCA) to project the high-dimensional data into a 2D space. PCA is well-suited for visualizing the subtle, continuous transitions between brain states.

4. Covering and Binning: The resulting 2D PCA embedding was covered by a set of overlapping square bins. The number of bins (resolution) and the percentage of overlap (gain) are key hyperparameters that define the granularity of the resulting graph (Geniesse et al., 2019).

5. Partial Clustering: Within each bin, the corresponding time points were clustered in their original high-dimensional voxel space based on their Euclidean distances. This critical step groups temporally distinct but functionally similar brain states, forming the fundamental units of our network.

6. Graph Construction: A "shape graph" was constructed where each cluster from the previous step becomes a node. An edge is drawn between two nodes if their underlying clusters share at least one time point. The resulting undirected graph provides a topological summary of the brain's dynamical landscape, where nodes represent recurring brain states and edges represent transitions between them.

2.4. Graph-Theoretic Analysis of Brain State Networks

To quantify the topological structure of each participant's Mapper-derived shape graph, we computed three standard node centrality measures. In this context, nodes represent quasi-stable, recurring brain states, and centrality metrics quantify the importance of these states within the overall dynamical system.

- Degree Centrality: The number of edges connected to a node. A brain state with high degree centrality is a frequently visited "hub" state, acting as a common transition point to many other states.
- Betweenness Centrality: The fraction of all shortest paths in the network that pass through a given node. A high-betweenness state acts as a "bottleneck" or "bridge," and is critical for efficient communication between otherwise distant communities of brain states.
- Closeness Centrality: The reciprocal of the average shortest path distance from a node to all other nodes in the graph. A high-closeness state is one from which all other brain states can be reached quickly, suggesting a highly integrated and efficient processing state.

2.5. Statistical Analysis

For each participant, we calculated the mean of each centrality measure (degree, betweenness, closeness) across all nodes in their Mapper graph. To test for group differences, independent samples t-tests were conducted to compare the mean centrality scores between the ADHD and TDC groups within each of the three datasets separately. Given our directional hypothesis that ADHD would be associated with higher centrality, one-tailed p-values are reported. Cohen's d was computed to estimate the effect size of group differences. To examine the clinical relevance of these topological measures, we calculated Pearson's correlation coefficients between the mean centrality scores and the three clinical measures (ADHD Index, Inattentive, Hyper/Impulsive) across all participants within each dataset where data were available. One-tailed p-values are reported for the correlation analyses.

2.6. Code

The code can be found in the following github repository: https://github.com/duman-math/fMRI_Mapper

3. Results

3.1. Increased Network Centrality in ADHD at Select Sites

The parameters is determined using grid search on NYU dataset. The other two datasets are used as validation. Our TDA-Mapper analysis revealed significant differences in the topological structure of brain state networks between ADHD and TDC groups, but these findings were highly dependent on the dataset. The results from group comparisons are summarized in Figure 1, Figure 4, Figure 5, and Table 1.

In the NYU dataset, individuals with ADHD showed significantly higher mean centrality across their brain state networks compared to TDCs. This was observed for betweenness centrality ($p = 0.0039$, one-tailed) and closeness centrality ($p = 0.0137$, one-tailed). A trend towards higher degree centrality was also observed ($p = 0.0873$, one-tailed) (Figure 1).

Similarly, in the NeuroIMAGE dataset, the ADHD group exhibited significantly elevated centrality. The effect was strongest for degree centrality ($p = 0.0039$, one-tailed; Cohen's $d = 0.805$) and also significant for closeness centrality ($p = 0.0351$, one-tailed; Cohen's $d = 0.536$). A trend-level increase was found for betweenness centrality ($p = 0.0508$, one-tailed; Cohen's $d = 0.483$) (Figure 4).

In contrast, these clear group differences were not replicated in the other two sites. In the OHSU dataset, while the ADHD group showed numerically higher mean centrality on all measures, these differences did not reach statistical significance only for betweenness centrality ($p = 0.0577$, one-tailed; Cohen's $d = 0.376$) (Figure 5).

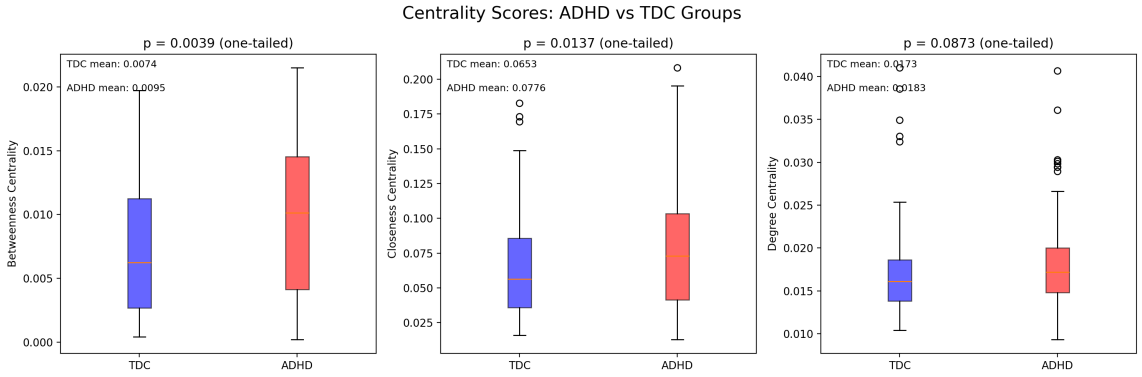

Figure 1: Group Differences in Centrality Scores for the NYU Dataset. Box plots compare betweenness, closeness, and degree centrality between Typically Developing Controls (TDC) and individuals with ADHD. The ADHD group shows significantly higher betweenness and closeness centrality.

Table 1: Summary of Group Differences in Centrality Measures Across Three Sites. One-tailed p-values and Cohen's d are reported for the comparison between ADHD and TDC groups.

	Betweenness		**Closeness**		**Degree**	
Site	**p-value**	**Cohen's d**	**p-value**	**Cohen's d**	**p-value**	**Cohen's d**
NYU	**0.0039**	0.371	**0.0137**	0.306	0.0873	0.188
NeuroIMAGE	**0.0508**	0.483	**0.0351**	0.536	**0.0039**	0.805
OHSU	**0.0577**	0.376	0.1003	0.305	0.1758	0.221

3.2. Centrality Correlates with Symptom Severity in the NYU Cohort

To assess the clinical relevance of the observed topological alterations, we examined the relationship between mean centrality scores and ADHD symptom severity. A consistent pattern of significant, positive correlations emerged in the NYU dataset, as shown in Figure 2 and summarized in Table 2. Specifically, higher betweenness centrality was associated with greater overall symptom severity as measured by the ADHD Index ($r = 0.154, p = 0.0126$, one-tailed), higher inattentive scores ($r = 0.122, p = 0.0378$, one-tailed), and higher hyperactive/impulsive scores ($r = 0.177, p = 0.0049$, one-tailed). Closeness centrality also showed trend-level positive correlations with the ADHD Index ($p = 0.0525$) and hyper/impulsive scores ($p = 0.0542$).

In the OHSU cohort, correlations between centrality measures and symptom scores were weaker with a trend level effect. (Figure 6).

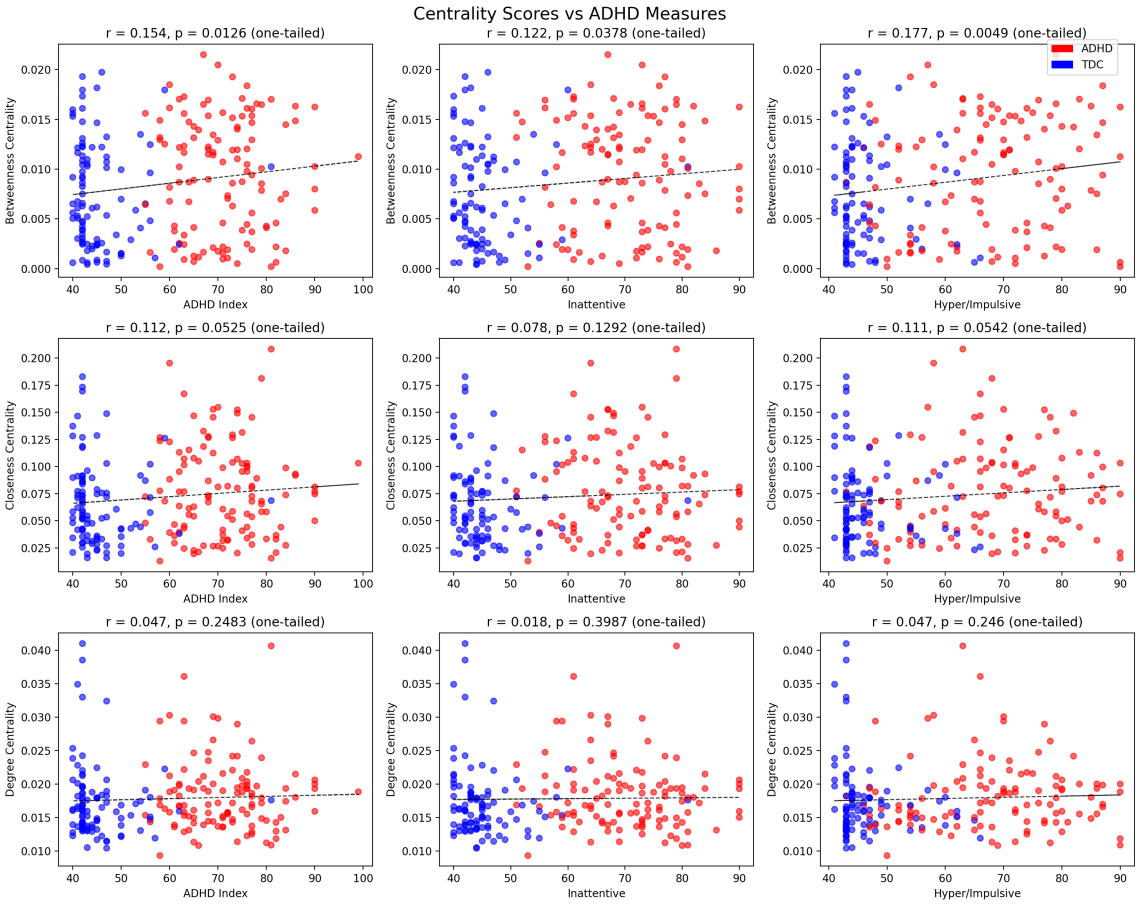

Figure 2: Correlations between Centrality Scores and ADHD Measures in the NYU Dataset. Scatter plots show the relationship between centrality measures (rows) and clinical scores (columns). Significant positive correlations are observed between betweenness centrality and all three clinical measures.

Table 2: Summary of Pearson's Correlations between Centrality and ADHD Symptoms (NYU Dataset). One-tailed p-values are reported.

	ADHD Index		**Inattentive**		**Hyper/Impulsive**	
Centrality Measure	**r**	**p-value**	**r**	**p-value**	**r**	**p-value**
Betweenness	0.154	**0.0126**	0.122	**0.0378**	0.177	**0.0049**
Closeness	0.112	0.0525	0.078	0.1292	0.111	0.0542
Degree	0.047	0.2483	0.018	0.3987	0.047	0.2460

4. Discussion

In this study, we applied the TDA-Mapper algorithm to a large, multi-site rs-fMRI dataset to investigate the topological organization of brain dynamics in ADHD. Our findings provide evidence for altered network centrality in individuals with ADHD, but also highlight the profound impact of inter-site heterogeneity on the robustness of these potential biomarkers.

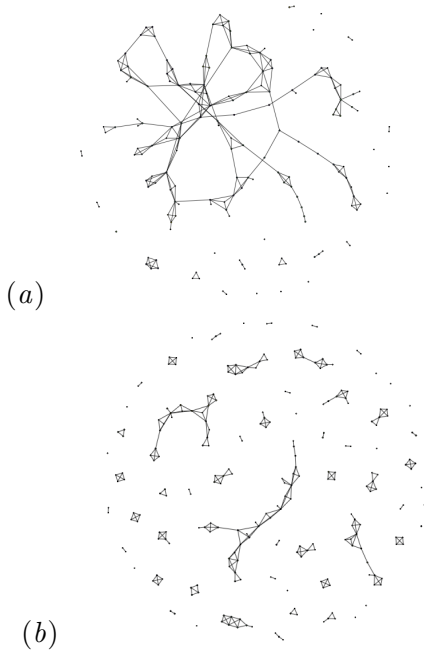

Figure 3: Example Mapper Graphs Illustrating Topological Differences. The graphs visualize the brain state networks for two representative participants from the NYU cohort. Panel (a) shows the shape graph from a participant with a high ADHD Index and high mean betweenness centrality, illustrating a highly interconnected core structure suggestive of a rigid dynamical system. Panel (b) shows the shape graph from a TDC participant with low mean betweenness centrality, displaying a more fragmented and peripheral structure, which may reflect a more flexible and exploratory traversal of brain states.

4.1. Increased Centrality as a Signature of Inefficient Brain Dynamics in ADHD

The primary finding in the NYU and NeuroIMAGE cohorts—that individuals with ADHD exhibit significantly higher centrality in their brain state networks—offers a novel perspective on the neurobiology of the disorder. A node in the Mapper graph represents a recurring, quasi-stable pattern of whole-brain activation. High centrality of these nodes suggests a dynamical system characterized by a densely interconnected core of states. Previous work has shown that such core-periphery structures are typical of cognitively demanding tasks, where brain activity is constrained to a specific set of relevant states (Saggar et al., 2018). In contrast, the resting state is typically associated with more peripheral, less-connected dynamics, reflecting a more flexible and exploratory traversal of the brain's functional repertoire (Saggar et al., 2018, 2022b). This topological difference is visually apparent when comparing the shape graph of a participant with high centrality to one with low centrality (see Figure 3).

Our observation of a more centralized graph structure in the ADHD group at rest suggests that their brains may not be efficiently exploring this diverse repertoire of states. Instead, they may be more rigidly locked into a constrained, repetitive pattern of transitions between a smaller set of hub-like states. This topological rigidity could be the neural substrate for the cognitive inflexibility, attentional lapses, and difficulty in shifting mental sets that are core clinical features of ADHD. This interpretation aligns with findings of reduced DMN regulation in ADHD, which may reflect an inability to appropriately disengage from a dominant network state (Harikumar et al., 2021). The significant positive correlation between centrality and symptom severity in the NYU cohort provides further support for this model, linking greater topological rigidity directly to more severe clinical impairment.

4.2. The Challenge of Inter-Site Heterogeneity

The failure to replicate these significant findings across all three sites is not merely a limitation but a critical result in its own right. It underscores a systemic challenge in psychiatric neuroimaging: the search for universal biomarkers in the face of clinical and methodological heterogeneity. The ADHD-200 dataset, while a landmark resource for open science, is known for its variability in scanners, acquisition protocols, and participant demographics across sites (Bellec P, 2017). Indeed, prior analyses of this dataset have explicitly reported high inconsistency in standard functional connectivity findings across the same sites we investigated (Tomasi and Volkow, 2012).

Our results demonstrate that even a sophisticated, data-driven method like TDA-Mapper, which is designed to be robust to certain types of noise, cannot fully overcome fundamental issues in the source data. This suggests that the ADHD cohorts at different sites may not be neurobiologically homogeneous. This is consistent with studies that have used TDA on clinical data to identify distinct patient subgroups, suggesting that ADHD itself may encompass several neurobiologically distinct profiles (Kyeong et al., 2017). Therefore, our mixed results likely reflect a combination of true biological heterogeneity within the ADHD diagnosis and methodological variance across imaging sites. This serves as a powerful cautionary tale: the quest for a single, universal biomarker for a complex disorder like ADHD from unharmonized, multi-site data is exceptionally challenging.

4.3. Comparison with Prior TDA and Connectivity Studies in ADHD

Our work contributes to a growing body of literature applying TDA to understand brain network alterations in ADHD. For instance, Gracia-Tabuenca et al. (2020), using persistent homology (a different TDA method that tracks the evolution of network components and loops), found evidence for over-synchronization, or hyper-connectivity, in the functional connectomes of children with ADHD. Our finding of increased centrality can be interpreted as a related phenomenon at the level of brain dynamics. A network of states with high centrality is one that is highly integrated, where hub states are densely interconnected. This could reflect the same underlying neurophysiology as a connectome with overly strong connections, resulting in a system that is less segregated and less capable of flexibly partitioning into specialized subnetworks. Our results, showing a pattern of increased centrality at some sites but not others, effectively encapsulate the broader debate in the standard connectivity literature, where both hyper- and hypo-connectivity have been reported in ADHD (Tolonen T, 2023).

4.4. Limitations and Future Directions

This study has several limitations. The primary limitation is our reliance on the ADHD-200 dataset with its inherent heterogeneity.

Future research should apply this TDA-Mapper pipeline to more recent, large-scale, and rigorously harmonized datasets, such as the Adolescent Brain Cognitive Development (ABCD) Study. This would provide a more robust test of the hypothesis that altered network centrality is a core feature of ADHD. Furthermore, exploring alternative filter functions (e.g., UMAP, t-SNE) or distance metrics (e.g., correlation, geodesic) could reveal different facets of the brain's dynamical organization (Geniesse et al., 2022). Finally, longitudinal applications of this method could be particularly powerful, allowing researchers to track how the topology of brain dynamics evolves with development or changes in response to clinical interventions.

5. Conclusion

This study demonstrates that Topological Data Analysis, via the Mapper algorithm, provides a powerful and sensitive method for examining the dynamical organization of brain activity in ADHD. Our findings from two large cohorts suggest that ADHD is associated with increased centrality of brain state networks at rest, a topological signature that may reflect an inefficient and rigid functional organization. However, our multi-site analysis also serves as a crucial reminder of the challenges posed by data heterogeneity, which remains a major obstacle for biomarker discovery in computational psychiatry. This work validates TDA as a promising methodology for capturing the complex, dynamic aspects of brain dysfunction while simultaneously highlighting the critical need for data harmonization to translate these advanced computational tools into reliable clinical applications.

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Appendix A. Supplemental Material

Table 3: Participant Demographics and Clinical Scores by Site. Values are presented as mean ± standard deviation for continuous variables and count (M/F) for sex.

Site & Group	N (M/F)	Age (years)	ADHD Index	Inattentive
NYU				
TDC	96 (65/31)	11.6 ± 3.3	45.4 ± 5.9	47.9 ± 6.3
ADHD	116 (87/29)	10.3 ± 2.4	67.2 ± 10.8	67.8 ± 10.7
NeuroIMAGE				
TDC	23 (13/10)	16.3 ± 3.0	N/A	N/A
ADHD	25 (23/2)	15.1 ± 2.8	N/A	N/A
OHSU				
TDC	37 (19/18)	9.8 ± 1.2	N/A	47.6 ± 5.9
ADHD	35 (24/11)	9.7 ± 1.3	N/A	62.4 ± 10.2

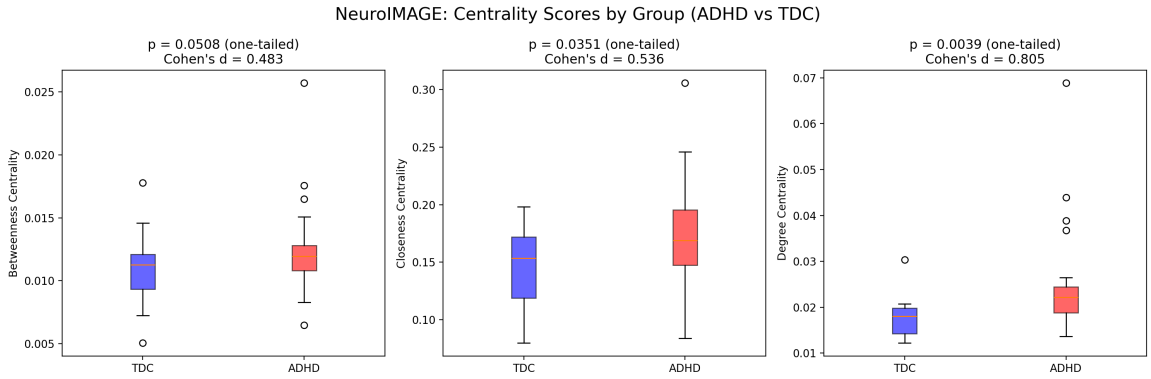

Figure 4: Group Differences in Centrality Scores for the NeuroIMAGE Dataset. The ADHD group shows significantly higher closeness and degree centrality, with a trend towards higher betweenness centrality, compared to the TDC group.

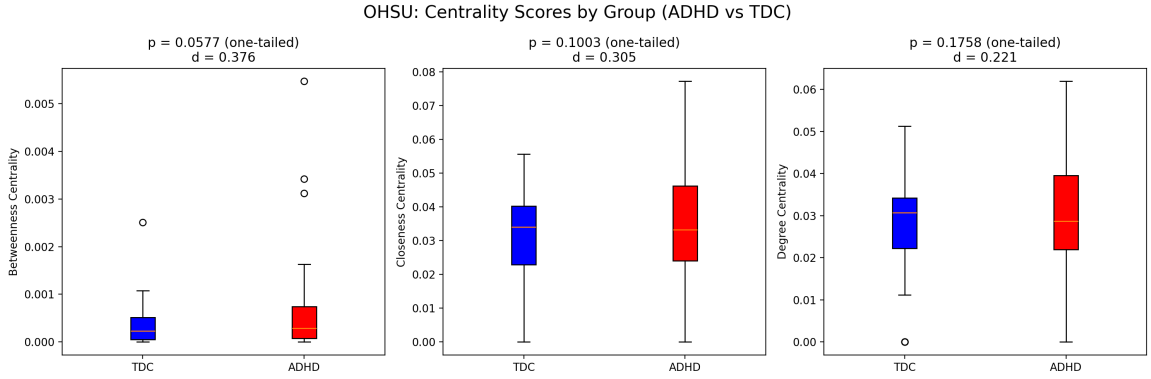

Figure 5: Group Differences in Centrality Scores for the OHSU Dataset. While the ADHD group shows numerically higher centrality scores, with betweenness centrality showing a trend-level effect.

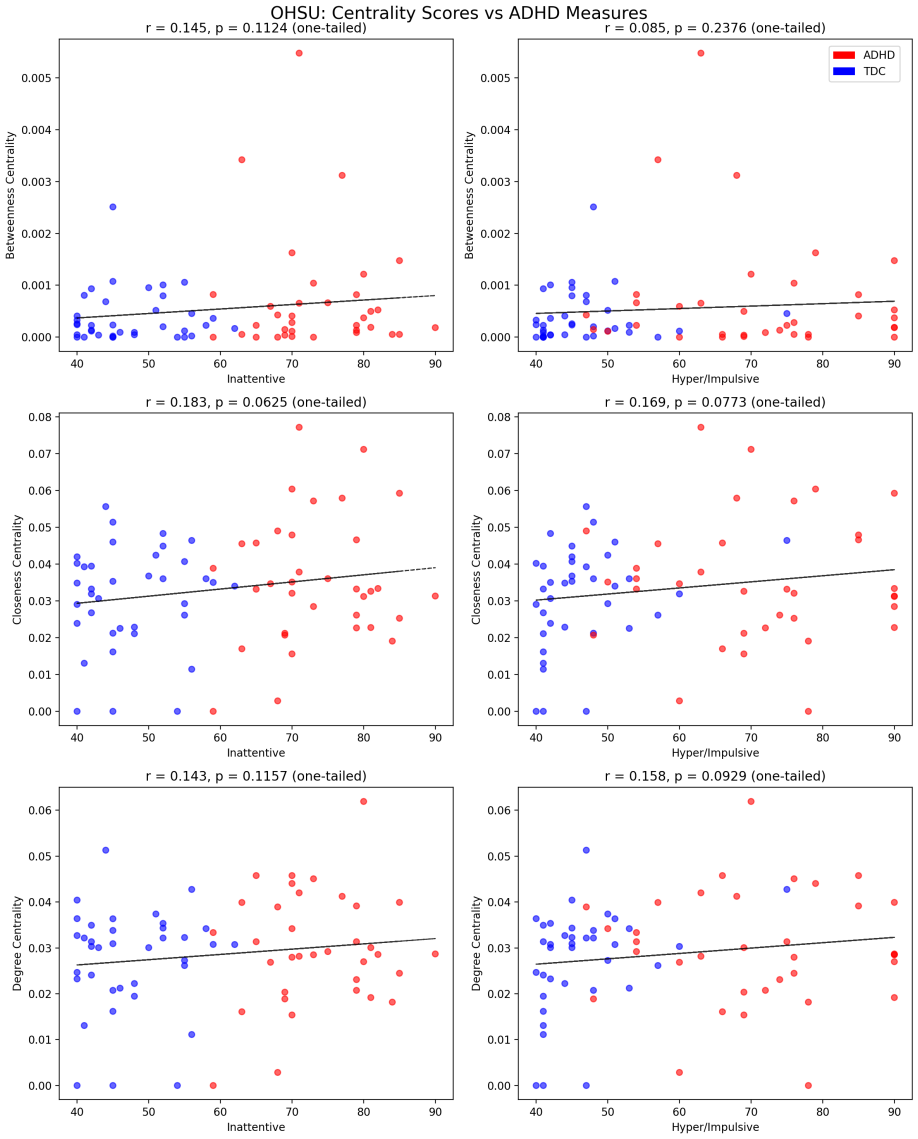

Figure 6: Correlations between Centrality Scores and ADHD Measures in the OHSU Dataset. In contrast to the NYU cohort, no significant correlations were found between centrality measures and available clinical scores.