

1 **Functional Connectivity Prediction with Deep**
2 **Learning for Graph Transformation- Appendix**

3

4

5 **A Parameter Tuning**

6 Details on experimental setup for data splitting and hyperparameter tuning are included in this section.
7 We performed 5-fold cross-validation. This means the data was split into 5 subsets. The experiments
8 were done in 5 runs, and each time we selected one subset as the test set and the remaining 4 as the
9 training set. In the training set, 20% is randomly selected as validation for determining hyperparameters
10 automatically by a grid search.

11 We tuned three hyperparameters for each regularization setting and each dataset, including learning
12 rate (we assumed equal values for generator and discriminator), λ_2 , and number of epochs. We used the
13 grid search strategy to find the best combination of these on the validation dataset, which is the subset
14 of the training set. The searching space is as follows: i) learning rate is chosen between 0.001, 0.0001,
15 and 0.0005; ii) λ_2 is in $[10^0 \ 10^1 \ 10^2 \ 10^3 \ 10^4 \ 10^5 \ 10^6 \ 10^7]$; iii) number of epochs was between 1 to 500.
16 For the rest of hyper-parameters, we used the same values as commonly suggested and follows [15] and
17 did not tune any further.

18 **B Additional case studies and brain visualizations**

19 Here, we have included additional visualizations from Dataset 2. The predictions are provided by SF-GAN
20 Setting 1.

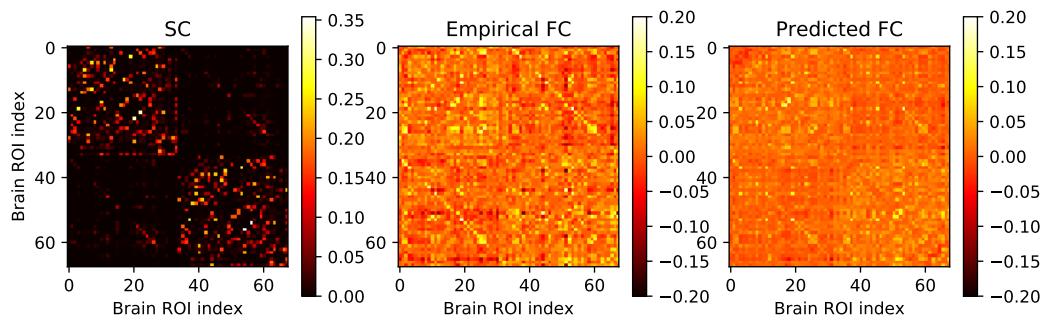


Figure B.1: Case study: subject 23

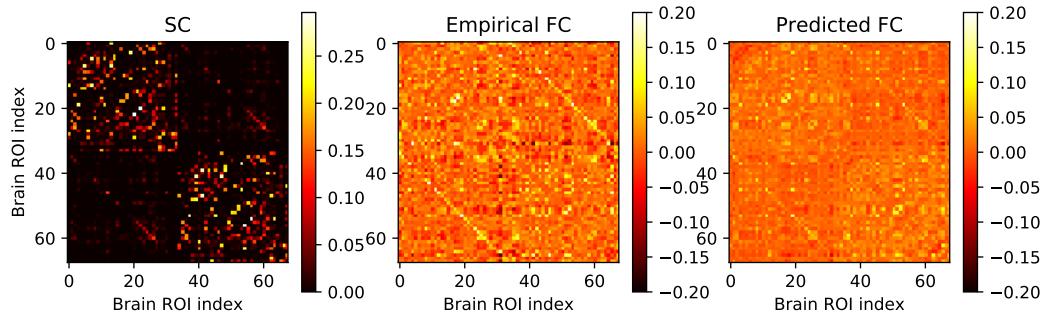


Figure B.2: Case study: subject 25

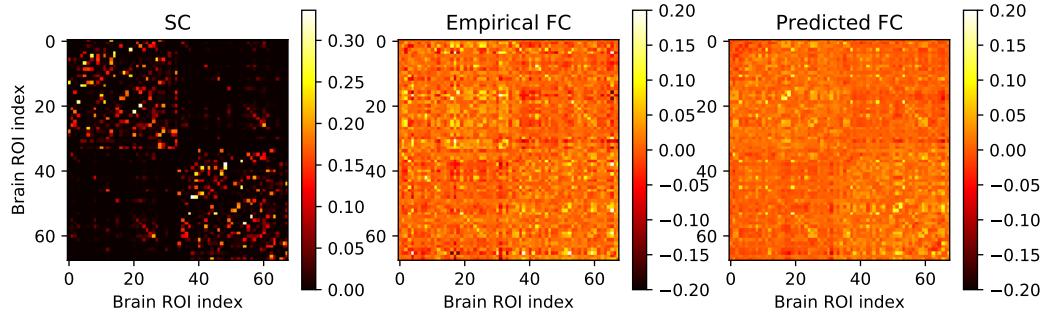


Figure B.3: Case study: subject 30

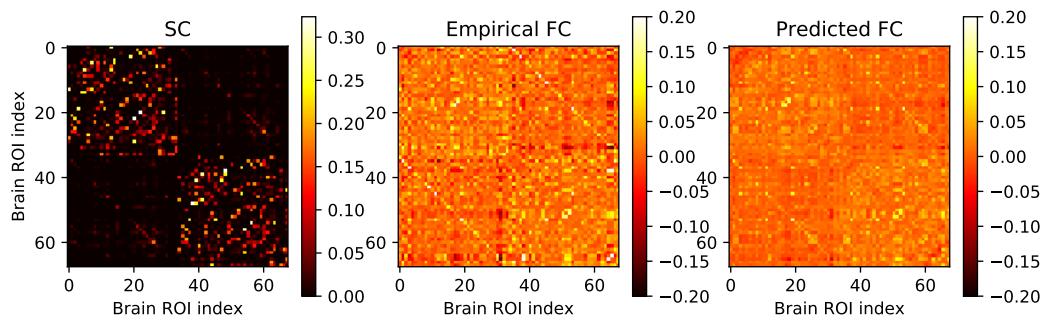


Figure B.4: Case study: subject 31

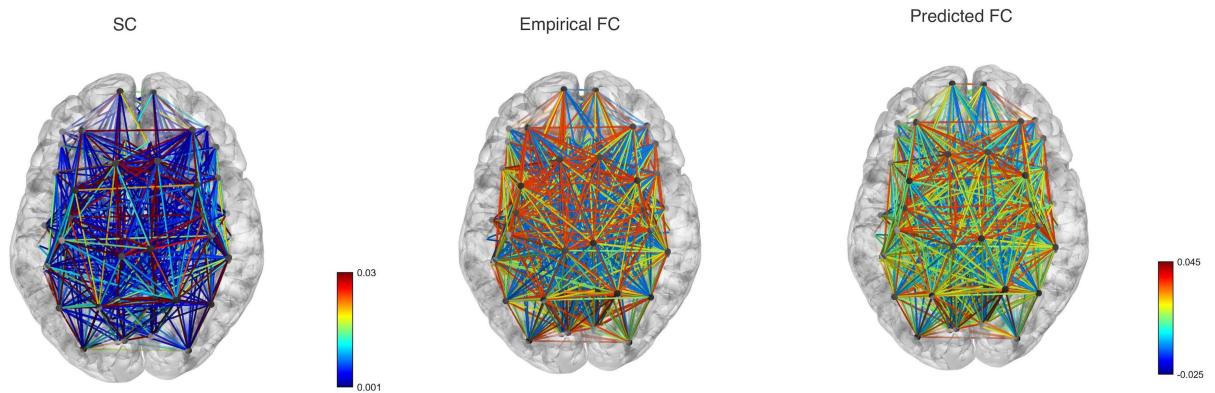


Figure B.5: Case study: subject 23

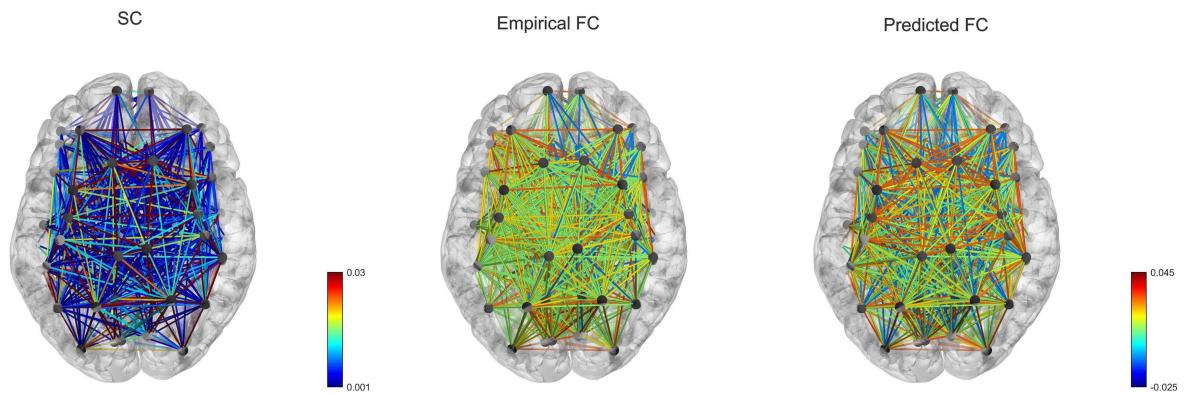


Figure B.6: Case study: subject 7

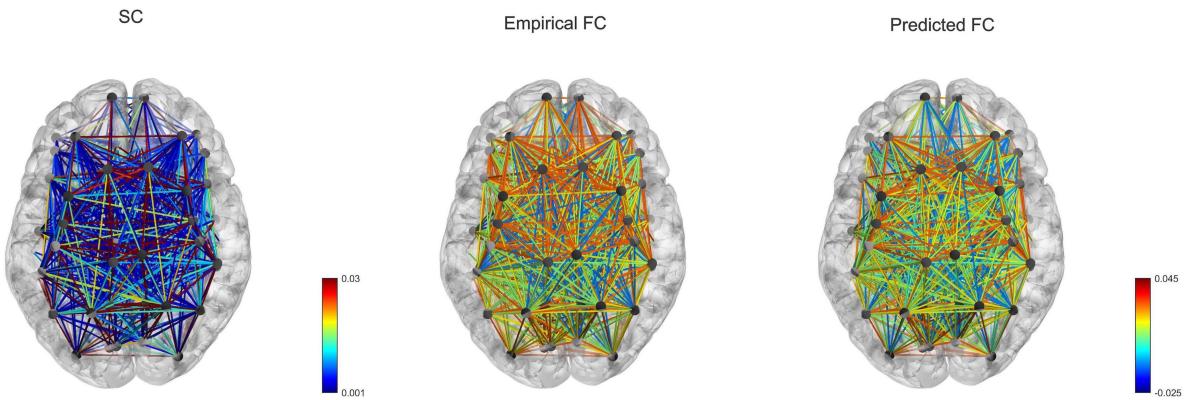


Figure B.7: Case study: subject 34

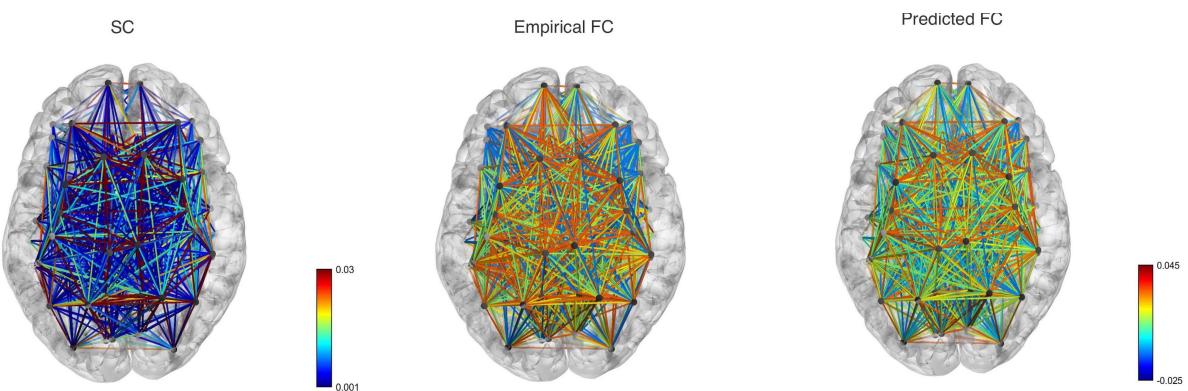


Figure B.8: Case study: subject 25

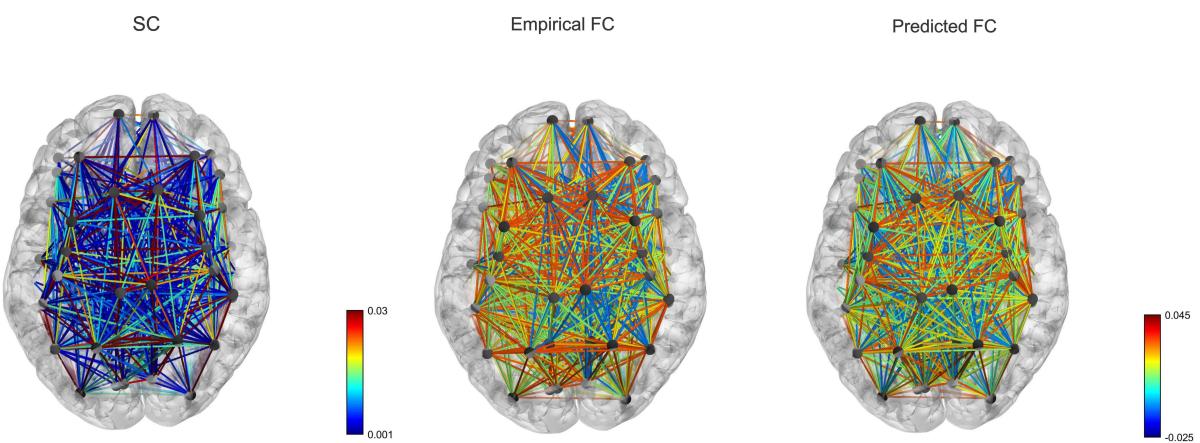


Figure B.9: Case study: subject 57

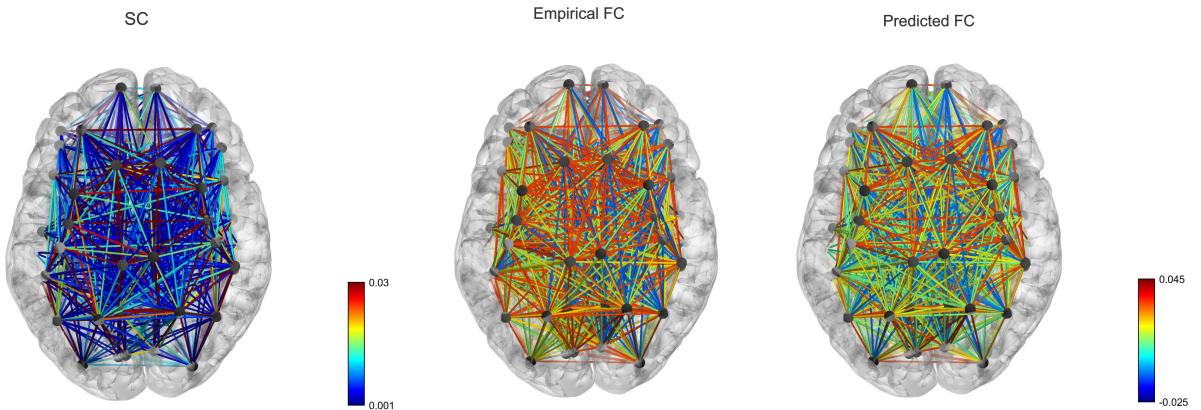


Figure B.10: Case study: subject 69

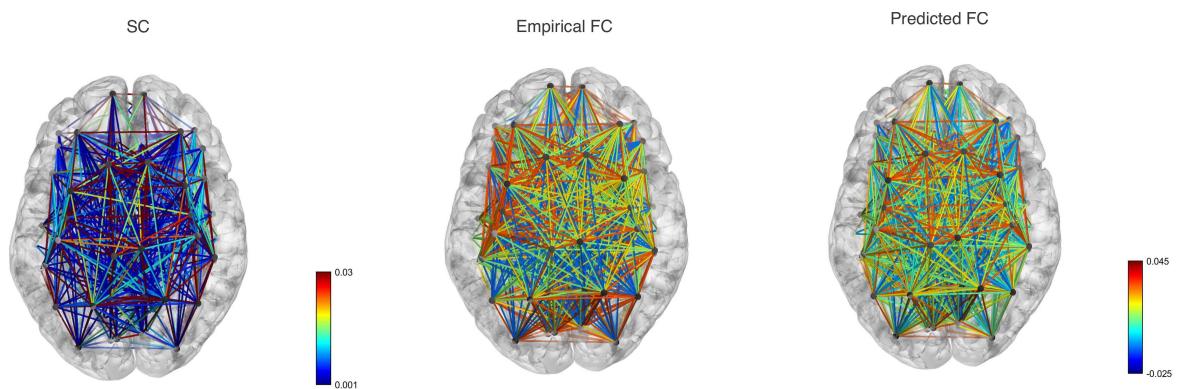


Figure B.11: Case study: subject 30

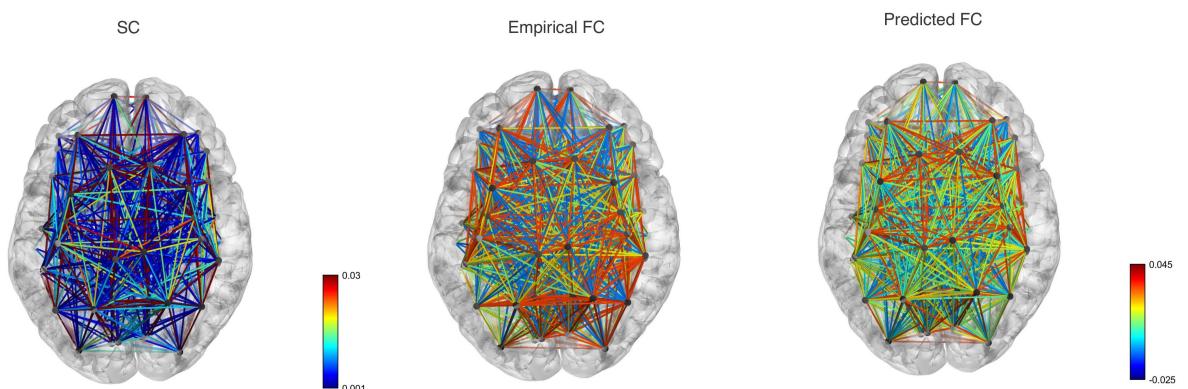


Figure B.12: Case study: subject 31

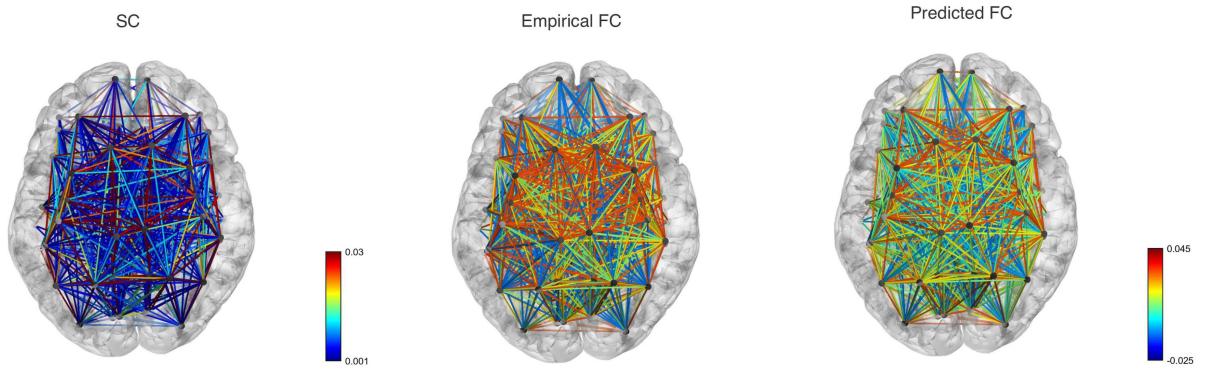


Figure B.13: Case study: subject 4

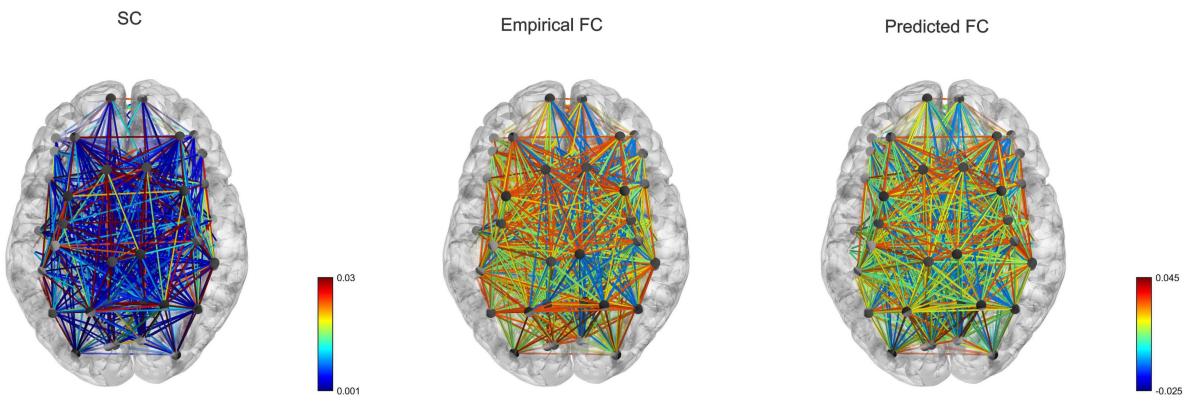


Figure B.14: Case study: subject 51

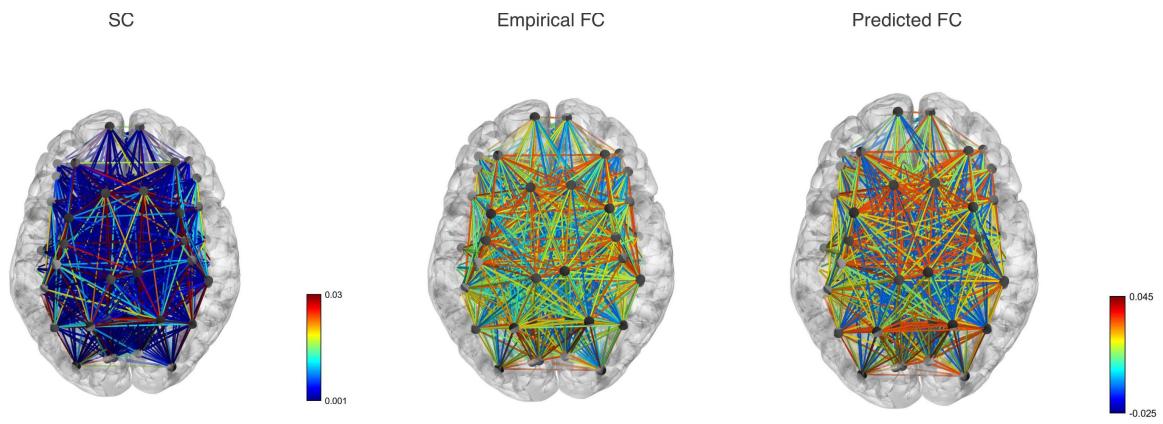


Figure B.15: Case study: subject 16

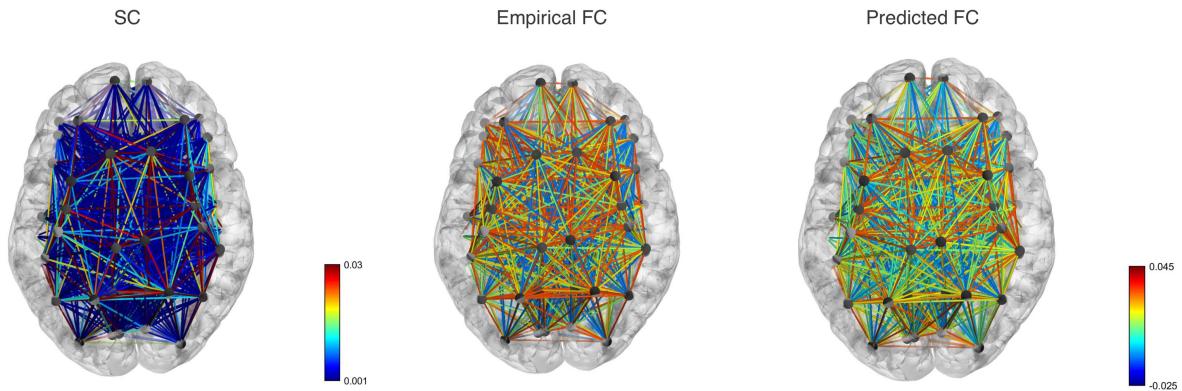


Figure B.16: Case study: subject 36

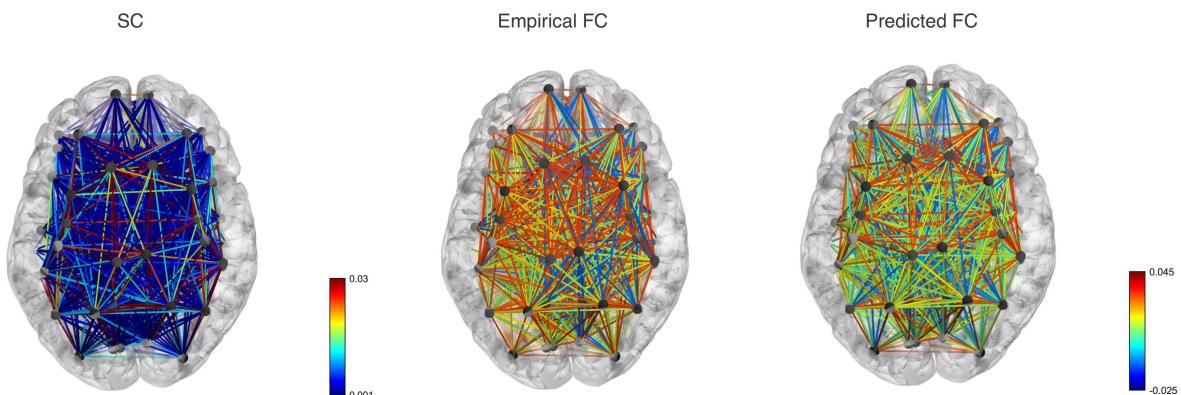


Figure B.17: Case study: subject 40

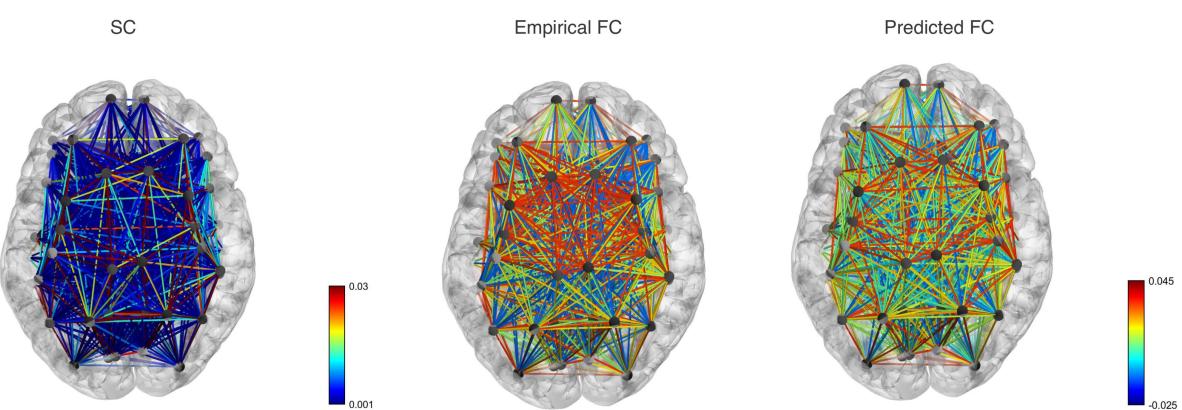


Figure B.18: Case study: subject 64

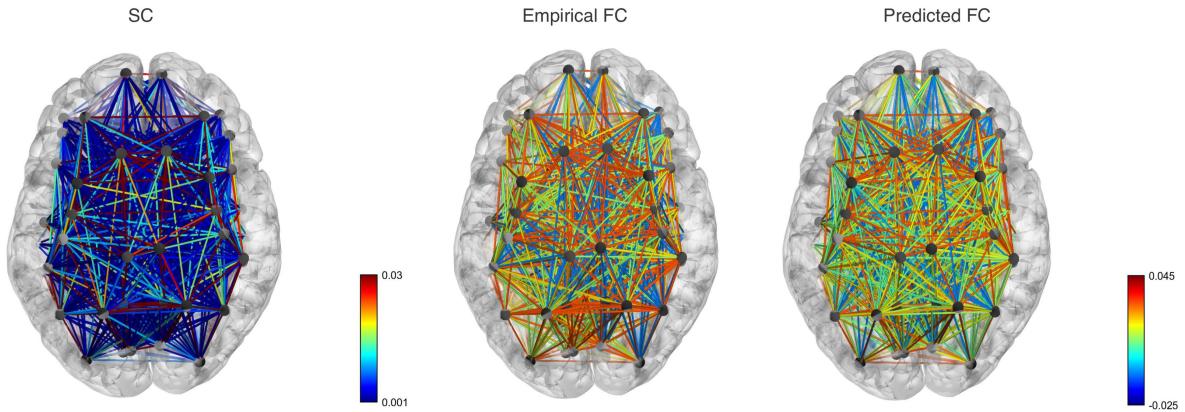


Figure B.19: Case study: subject 66

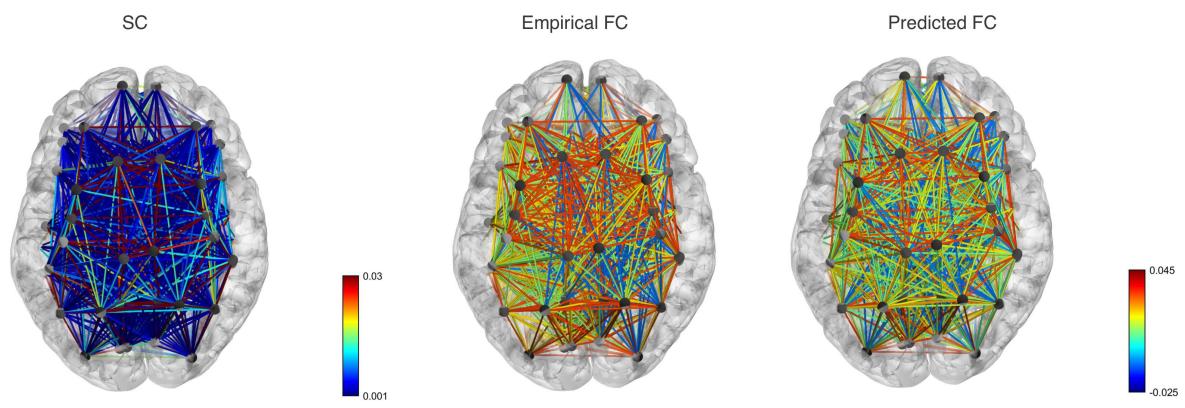


Figure B.20: Case study: subject 71

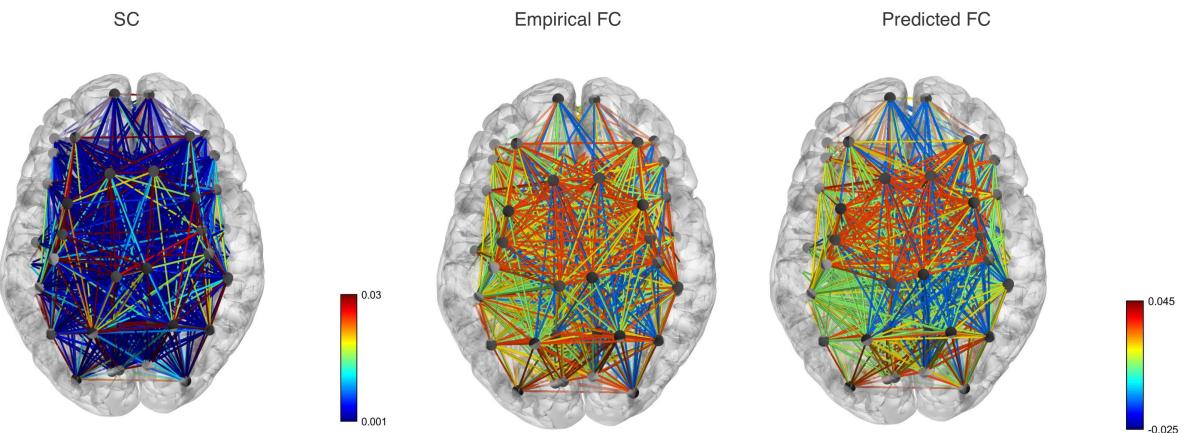


Figure B.21: Case study: subject 79

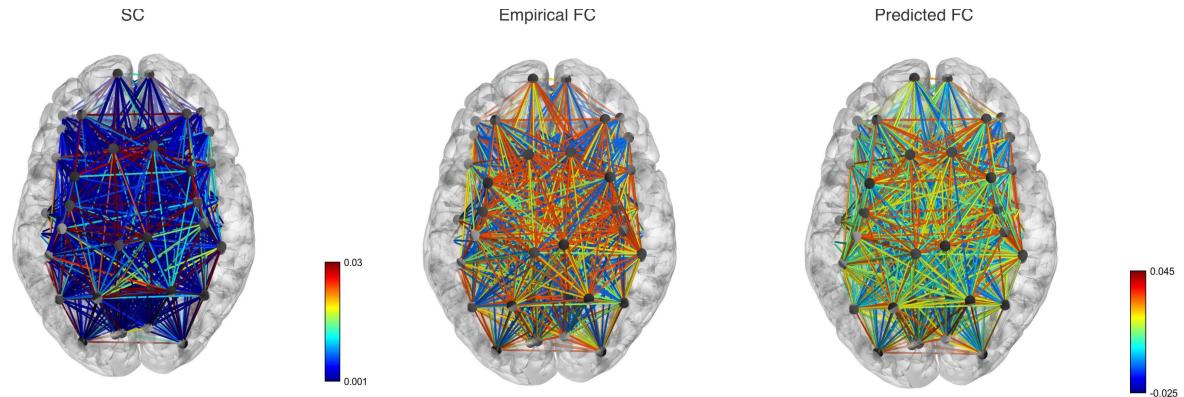


Figure B.22: Case study: subject 84

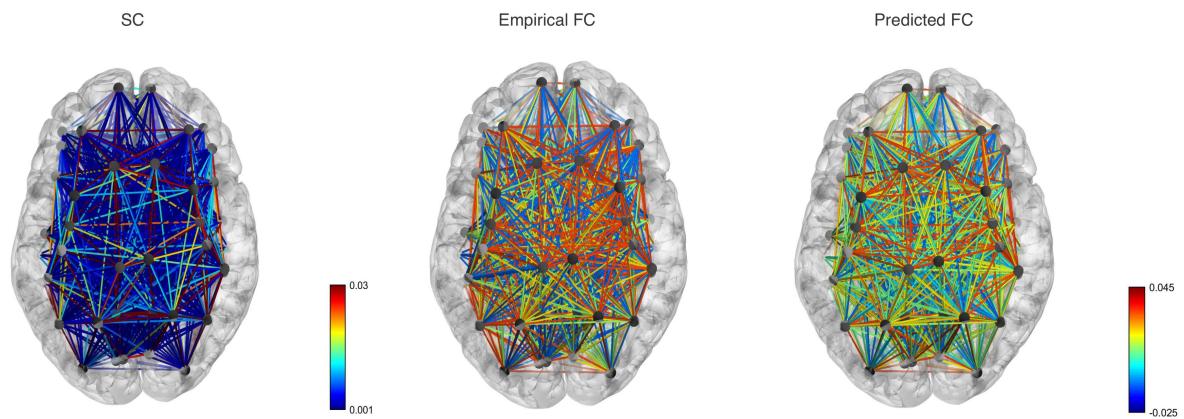


Figure B.23: Case study: subject 90

²¹ C Meta features

²² A list of meta features used in this work, is provided in Table C.1, and a list of the name of categories
²³ 1 to 5 is shown in Table C.2. Since the corresponding data is restricted due to patient confidentiality
²⁴ concerns, the actual subject meta data is not released here.

Table C.1: List of meta features and the corresponding categories

Feature	Category
Age of participant in Yrs	1
Ethnicity	1
Handedness from -100 to 100	1

Features	Category
employment status	1
Total household income	1
Years of education completed	1
Is respondent still in school for degree course?	1
Is respondent married or in live-in relationship?	1
Is respondent Missouri born?	1
Height (in Inches)	2
Weight (in Pounds)	2
BMI ($703 * weight(lb) / (heightin.^2)$)	2
Participant's current self-reported BMI category	2
Participant' self-reported BMI category for their heaviest period	2
Was blood drawn from participant	2
Blood sample 1 percentage of total blood volume that are red blood cells	2
Blood sample 2 percentage of total blood volume that are red blood cells	2
Systolic blood pressure of subject	2
Diastolic blood pressure of subject	2
If the participant's mother had schizophrenia or psychosis	2
If the participant's father had schizophrenia or psychosis	2
If the participant's mother had depression or psychosis.	2
If the participant's father had depression or psychosis.	2
If the participant's mother had bipolar disorder.	2
If the participant's father had bipolar disorder.	2
If the participant's mother had anxiety.	2
If the participant's father had anxiety.	2
If the participant's mother had drug/alcohol problems.	2
If the participant's father had drug/alcohol problems.	2
If the participant's mother had Alzheimer's Disease or dementia	2
If the participant's father had Alzheimer's Disease or dementia	2
If the participant's mother had Parkinson's Disease	2
If the participant's father had Parkinson's Disease	2

Features	Category
If the participant's mother had Tourette's Syndrome	2
If the participant's father had Tourette's Syndrome	2
None of the above - Mother	2
None of the above - Father	2
ASR Anxious/Depressed Raw Score	3
ASR Anxious/Depressed Gender and Age Adjusted Percentile	3
ASR Withdrawn Raw Score	3
ASR Withdrawn Gender and Age Adjusted T-score	3
ASR Somatic Complaints Raw Score	3
ASR Somatic Complaints Gender and Age Adjusted T-score	3
ASR Thought Problems Raw Score	3
ASR Thought Problems Gender and Age Adjusted T-score	3
ASR Attention Problems Raw Score	3
ASR Attention Problems Gender and Age Adjusted T-score	3
ASR Aggressive Behavior Raw Score	3
ASR Aggressive Behavior Gender and Age Adjusted T-score	3
ASR Rule Breaking Behavior Raw Score	3
ASR Rule Breaking Behavior Gender and Age Adjusted T-score	3
ASR Intrusive Raw Score (ASR_Intr_Raw)	3
ASR Intrusive Gender and Age Adjusted T-score	3
ASR Other Raw Score	3
ASR Critical Items Raw Score	3
ASR Internalizing Raw Score	3
ASR Internalizing Gender and Age Adjusted T-score	3
ASR Externalizing Raw Score	3
ASR Externalizing Gender and Age Adjusted T-score	3
ASR Sum of Thought, Attention, and Other Raw Score	3
ASR Total Raw Score	3
ASR Total Problems Gender and Age Adjusted T-score	3
ASR DSM Depressive Problems Raw Score	3

Features	Category
ASR DSM Depressive Problems Gender and Age Adjusted T-score	3
ASR DSM Anxiety Problems Raw Score	3
ASR DSM Anxiety Problems Gender and Age Adjusted T-score	3
ASR DSM Somatic Problems Raw Score	3
ASR DSM Somatic Problems Gender and Age Adjusted T-score	3
ASR DSM Avoidant Personality Problems Raw Score	3
ASR DSM Avoidant Personality Problems Gender and Age Adjusted T-score	3
ASR DSM AD/H Problems Raw Score	3
ASR DSM AD/H Problems Gender and Age Adjusted T-score	3
ASR DSM Inattention Problems Raw Score	3
ASR DSM Hyperactivity Problems Raw Score	3
ASR DSM Antisocial Personality Problems Raw Score	3
ASR DSM Antisocial Personality Problems Gender and Age Adjusted T-score	3
Childhood Conduct Problems	3
Non-diagnostic screen available to exclude possible cases of panic disorder	3
Non-diagnostic screen available to exclude possible cases of agoraphobia	3
Has the participant experienced a diagnosed DSMIV Major Depressive Episode over his/her lifetime?	3
Number of depressive symptoms over lifetime that meet DSMIV criterion for major depression.	3
Eye Used For Color Vision Test (Both (B)/Right (R)/Left (L))	4
EVA score - Numerator	4
EVA score - Denominator	4
Eyeglass correction	4
Any breathalyzer over .05	5
Any breathalyzer over .08	5
Positive test for Cocaine	5
Positive test for THC	5
Positive test for Opiates	5
Positive test for Amphetamines	5
Positive test for MethAmphetamine	5
Positive test for Oxycontin	5

Features	Category
Total drinks in past 7 days	5
Number days drank in past 7 days	5
Avg total weekday drinks/day in past 7 days	5
Avg total weekend drinks/day in past 7 days	5
Total drinks in past 7 days (Beer/Wine Coolers)	5
Avg total weekday drinks/day in past 7 days (Beer/Wine Coolers)	5
Avg total weekend drinks/day in past 7 days (Beer/Wine Coolers)	5
Total drinks in past 7 days (Malt Liquor)	5
Avg total weekday drinks/day in past 7 days (Malt Liquor)	5
Avg total weekend drinks/day in past 7 days (Malt Liquor)	5
Total drinks in past 7 days (Wine)	5
Avg total weekday drinks/day in past 7 days (Wine)	5
Avg total weekend drinks/day in past 7 days (Wine)	5
Total drinks in past 7 days (Hard Liquor)	5
Avg total weekday drinks/day in past 7 days (Hard Liquor)	5
Avg total weekend drinks/day in past 7 days (Hard Liquor)	5
Total drinks in past 7 days (Other Alcohol)	5
Avg total weekday drinks/day in past 7 days (Other Alcohol)	5
Avg total weekend drinks/day in past 7 days (Other Alcohol)	5
Number of DSM4 ALC Dependence Criteria Met	5
Participant meets DSM4 criteria for Alcohol Abuse	5
Number of symptoms participant has of DSM4 Alcohol Abuse	5
Participant meets DSM4 criteria for DSM4 Alcohol Dependence	5
Drinks consumed per drinking day in past 12 months	5
Frequency of any alcohol use in past 12 months	5
Frequency of drinking 5+ drinks in past 12 months	5
Frequency drunk in past 12 months	5
Max drinks consumed in a single day in the past 12 months	5
Age at first alcohol use	5
Drinks per day in heaviest 12-month drinking period of participant's lifetime	5

Features	Category
Frequency of any alcohol use in heaviest 12-month drinking period of participant's lifetime	5
Frequency of drinking 5+ drinks during heaviest 12-month drinking period of participant's lifetime	5
Frequency drunk in heaviest 12-month drinking period of participant's lifetime	5
Lifetime max drinks consumed in single day	5
Total times used/smoked ANY TOBACCO in past 7 days	5
Times used/smoked ANY TOBACCO TODAY	5
Number days smoked/used ANY TOBACCO in past 7 days	5
Avg total weekday ANY TOBACCO per day in past 7 days	5
Avg total weekend ANY TOBACCO per day in past 7 days	5
Total # CIGARETTES in past 7 days	5
Avg weekday CIGARETTES per day in past 7 days	5
Avg weekend CIGARETTES per day in past 7 days	5
Total # CIGARS in past 7 days	5
Avg weekday CIGARS per day in past 7 days	5
Avg weekend CIGARS per day in past 7 days	5
Total # PIPES in past 7 days	5
Avg weekday PIPES per day in past 7 days	5
Avg weekend PIPES per day in past 7 days	5
Times used CHEW in past 7 days	5
Avg weekday times used CHEW per day in past 7 days	5
Avg weekend times used Chew in past 7 days	5
Total times used Snuff in past 7 days	5
Avg weekday times used Snuff in past 7 days	5
Times used SNUFF in past 7 days	5
Total times used other tobacco in past 7 days	5
Avg weekday times used other tobacco in past 7 days	5
Avg weekend times used other tobacco in past 7 days	5
Smoking history	5
For those who were/are regular smokers, Is the participant still smoking?	5
Times used illicit drugs	5

Features	Category
Times used cocaine	5
Times used hallucinogens	5
Times used opiates	5
Times used sedatives	5
Times used stimulants	5
Ever used marijuana	5
Participant meets DSM criteria for marijuana dependence	5
Times used marijuana	5

Category number	Category name
1	Subject Information
2	Health and Family History
3	Psychiatric and Life Function
4	Sensory
5	Substance Use

Table C.2: Name of categories