**ReadMe**

SC\_FC\_Coupling\_Task\_Personality

1. Scope

This repository contains scripts that were used to conduct the analyses in **"The Impact of Trait-Relevance: Predicting Personality from Structural-Functional Brain Network Coupling"** coauthored by Johanna L. Popp, Jonas A. Thiele, Joshua Faskowitz, Caio Seguin, Olaf Sporns and Kirsten Hilger (doi: will be updated after publication). In brief, we investigated the relationship between the Big Five Personality traits and structural-functional brain network coupling (SC-FC coupling) operationalized with similarity and network communication measures during resting state and seven different task conditions. The scripts found in this repository can be used to replicate all analyses or more generally, to study the association between intrinsic and task-induced SC-FC coupling and individual differences (e.g., in personality traits). In case you have questions or trouble with running the scripts, feel free to reach out under [johanna.popp@uni-wuerzburg.de](mailto:johanna.popp@uni-wuerzburg.de).

2. Data

For the main sample analysis, data from the S1200 sample of the Human Connectome Project funded by the National Institute of Health were used (HCP; Van Essen et al., 2013). For the replication of results, we used data from the PIOP1 and PIOP2 samples collected as a part of the Amsterdam Open MRI Collection (AOMIC; Snoek et al., 2021). All data analyzed in the current study can be accessed online:

**HCP**: <https://www.humanconnectome.org/study/hcp-young-adult/data-releases/>  
**AOMIC PIOP1**: <https://openneuro.org/datasets/ds002785>  
**AOMIC PIOP2**: <https://openneuro.org/datasets/ds002790>

3. Preprocessing

To conduct main analyses in the HCP sample, the minimally preprocessed resting-state fMRI data from the HCP (Glasser et al., 2013) were used. As additional denoising strategy, nuisance regression as explained in Parkes et al. (2018; strategy no.6) with 24 head motion parameters, eight mean signals from white matter and cerebrospinal fluid and four global signals was applied. For task-based data, basis-set task regressors in addition to the other nuisance regressors were used to remove mean task-evoked activations (Cole et al., 2019). Most of the fMRI preprocessing steps were conducted externally, and code can be found here: <https://github.com/faskowit/app-fmri-2-mat>. To assess individual structural connectivity, the minimally preprocessed DWI data provided by the HCP were used and we ran the MRtrix pipeline for DWI processing (Civier et al., 2019; Tournier et al., 2019; <https://github.com/civier/HCP-dMRI-connectome>). Probabilistic streamline tractography was employed (Smith et al., 2012) and only streamlines fitting the estimated white matter orientations from the diffusion image were kept. For the replication analysis, data from the AOMIC PIOP1 and PIOP2 samples was downloaded in minimally preprocessed form (using fMRIPrep version 1.4.1.; Esteban et al., 2019) and further processed similarly as in the main sample. Brain networks were constructed using a multimodal parcellation dividing the brain into 360 nodes (Glasser et al., 2016).

4. Structure and Script Description

4.1. HCP Data Prep

For the preparation of data from the HCP sample, the scripts should be run in the following order:

1. HCP\_MRI\_data\_import: Import of all MRI data from folder structure on local machine (SC matrices, resting-state fMRI and task fMRI time courses).
2. HCP\_prepare\_behavioral\_data: Import and preparation of HCP behavioral data (Output: HCP\_behavioral\_personality\_gscore).
3. HCP\_prepare\_SC\_data\_with\_subcortical: Preparation of structural connectivity matrices and creation of cell that is used for further analyses.
4. HCP\_prepare\_FC\_resting\_state\_data\_with\_subcortical: Preparation of resting-state functional connectivity matrices and creation of a cell that is used for further analyses. Included is: a) import of subject ID’s and time course data for all four runs (save in cell) b) exclusion of subjects that don’t have all four scans completed c) matching up node order according to node order of SC matrices d) computation of functional connectivity matrices from time courses e) averaging across all FC matrices for each subject and f) Fisher-z transformation of individual mean connectivity matrices.

*Motion Correction*

1. HCP\_motion\_data\_import\_resting\_state: Import of data for motion correction for 4 resting-state fMRI scans and creation of respective table.
2. HCP\_motion\_correction\_resting\_state: This script is used for motion correction with data from framewise displacement (FD). It includes a) definition of resting-state scans that need to be excluded b) computation of mean FD values across the remaining scans that are used for confound regression. Lastly, FC matrices are excluded based on the motion criteria and ultimately saved as final FC matrices and mean FD values in a table used for further analyses.
3. HCP\_motion\_data\_import\_task\_x: There is one script for each task condition: Import of data for motion correction for 2 task-based fMRI scans and creation of respective table.
4. HCP\_motion\_data\_correction\_task\_x: There is one script for each task condition used for motion correction with data from framewise displacement (FD). It includes a) definition of task-based scans that need to be excluded b) computation of mean FD values across the remaining scans that are used for confound regression. Lastly, FC matrices are excluded based on the motion criteria and ultimately saved as final FC matrices and mean FD values in a table used for further analyses.
5. HCP\_find\_subjects\_with\_complete\_data: Merging of all tables (behavioral data; SC matrices and FC matrices) and creation of final tables for subjects that have all data.

*Compute Coupling*

1. HCP\_compute\_coupling\_measures\_resting\_state: This script is based on a source script from Zamani Esfahlani et al. (2022) and was adjusted accordingly. It performs the computation of communication and similarity matrices based on SC connectivity matrices and calculates coupling measure specific coupling values by correlating regional connectivity profiles of the communication/similarity matrix with the respective FC matrix.
2. HCP\_compute\_coupling\_measures\_task\_x: This script is based on a source script from Zamani Esfahlani et al. (2022) and was adjusted accordingly. It calculates coupling measure-specific coupling values by correlating regional connectivity profiles of the communication/similarity matrix (computed with HCP\_compute\_coupling\_measures\_resting\_state) with the respective FC matrix.
3. HCP\_split\_lockbox\_sample: This script is used to partition the main sample (HCP) into a primary main sample (70%) and a lockbox sample (30%) to be able to conduct an initial replication. It takes into account the family structure in the HCP and makes sure that all families are in the same sample to keep them truly independent from one another.

4.2. Analysis Scripts

4.2.1. Scripts for HCP – Main Sample

In order to perform the analyses conducted in the main sample, the scripts should be run in the following order:

1. HCP\_region\_specific\_coupling\_all\_conditions: Computation of region-specific SC-FC coupling maps (measure that is able to explain the highest variance in FC across all participants most frequently).
2. HCP\_whole\_brain\_coupling\_plot\_across\_conditions: Computation of coupling measure-specific brain-average coupling values for all eight conditions, taking the mean across the four measure-specific coupling values per condition and creating the violin plot visualizing condition-specific differences in brain-average SC-FC coupling.
3. HCP\_whole\_brain\_coupling\_plot\_across\_coupling\_measures: Computation of coupling measure-specific brain-average coupling values for all eight conditions, taking the mean across the eight condition-specific coupling values per coupling measure and creating the violin plot visualizing coupling measure-specific differences in brain-average SC-FC coupling.
4. HCP\_whole\_brain\_coupling\_all\_conditions\_correlation\_personality: Computation of coupling measure-specific brain-average coupling values for all eight conditions and performance of partial correlations with individual personality scores.
5. HCP\_internal\_cross\_validation\_basic\_NMA\_prediction\_model: Conduction of the internal-cross-validation of the ‘Basic NMA Model’ that is built using two input predictor variables. The predictor variables are derived from individual’s coupling values and extracted by using group-based positive and group-based negative NMA masks. This script contains three parts: **Part 1** partitions the sample into five different folds (considering family relations and personality trait distribution) and creates positive and negative NMAs for each training sample and test sample. **Part 2** uses the NMAs created in part 1 to build multiple linear regression models that are then tested for their ability to predict personality scores in the test samples. **Part 3** assesses the significance of the prediction with a permutation test.
6. HCP\_internal\_cross\_validation\_expanded\_NMA\_prediction\_model: Conduction of the internal-cross-validation of the ‘Expanded NMA Model’ that is built using 14 input predictor variables (two from each of the seven task conditions). The predictor variables are derived from individual’s coupling values and extracted by using group-based positive and group-based negative NMA masks. This script contains three parts: **Part 1** partitions the sample into five different folds (considering family relations and personality distribution) and creates positive and negative NMAs for each training fold and test fold. **Part 2** uses the NMAs created in part 1 to build multiple linear regression models that are then tested for their ability to predict personality scores in the test samples. **Part 3** assesses the significance of the prediction with a permutation test.

*Latent NMA Prediction Models (only internal CV)*

This folder contains one script for each trait-specific model combining region-specific SC-FC coupling values from trait-relevant or trait-irrelevant tasks to predict individual personality scores.

1. HCP\_internal\_cross\_validation\_latent\_prediction\_model\_: Conduction of the internal-cross-validation of the ‘Latent NMA Model’ that is built using two input predictor variables. The predictor variables are derived from individual’s coupling values and extracted by using group-based positive and group-based negative NMA masks. This script contains three parts: **Part 1** partitions the sample into five different folds (considering family relations and personality distribution) and creates positive and negative NMAs for each training sample and test sample. **Part 2** uses the NMAs created in part 1 to build multiple linear regression models that are then tested for their ability to predict personality scores in the test samples. **Part 3** assesses the significance of the prediction with a permutation test.
2. HCP\_external\_validation\_basic\_NMA\_prediction\_model\_in\_HCP\_lockbox: Conduction of the external validation of the 'Basic NMA Model' that is built using two input predictor variables. The predictor variables are derived from individual's coupling values and extracted by using group-based positive and negative NMA masks. The script contains three parts: **Part 1** partitions the sample into five different folds (considering family relations and personality distribution) and creates a positive and negative NMAs for each training sample (4/5 folds) and test sample (lockbox sample in this case). **Part 2** uses the NMAs created in part 1 to build multiple linear regression models that are then tested for their ability to predict personality scores in the test samples (lockbox sample in this case). **Part 3** assesses the significance of the prediction with a permutation test.
3. HCP\_external\_validation\_expanded\_NMA\_prediction\_model\_in\_HCP\_lockbox: Conduction of the external validation of the ‘Expanded NMA Model’ that is built using 14 input predictor variables (two from each of the seven task conditions). The predictor variables are derived from individual’s coupling values and extracted by using group-based positive and group-based negative NMA masks. This script contains three parts: **Part 1** partitions the sample into five different folds (considering family relations and personality distribution) and creates positive and negative NMAs for each training sample (4/5 folds) and test sample (lockbox sample in this case). **Part 2** uses the NMAs created in part 1 to build multiple linear regression models that are then tested for their ability to predict personality scores in the test sample (lockbox sample in this case). **Part 3** assesses the significance of the prediction with a permutation test.

*Test Model Difference Personality vs. Intelligence*

7. HCP\_532\_test\_significance\_model\_difference: This script tests whether there are significant differences in prediction model performance between the internally cross-validated Basic NMA Model (using coupling data from all conditions separately) and Expanded NMA Model in the main sample when predicting intelligence scores vs. predicting personality scores. To do so, the actual difference in prediction performance is compared to differences in prediction performances based on permuted scores.

4.2.2. Scripts for HCP – Lockbox Sample

In order to perform the analyses conducted in the lockbox sample, the scripts should be run in the following order:

1. HCP\_lockbox\_region\_specific\_coupling\_all\_conditions: Computation of region-specific SC-FC coupling (measure that is able to explain the highest variance in FC across all participants most frequently).
2. HCP\_lockbox\_whole\_brain\_coupling\_plot\_across\_conditions: Computation of coupling measure-specific brain-average coupling values for all eight conditions, taking the mean across the four measure-specific coupling values per condition and creating the violin plot visualizing condition-specific differences in brain-average SC-FC coupling.
3. HCP\_lockbox\_whole\_brain\_coupling\_plot\_across\_coupling\_measures: Computation of coupling measure-specific brain-average coupling values for all eight conditions, taking the mean across the eight condition-specific coupling values per coupling measure and creating the violin plot visualizing coupling measure-specific differences in brain-average SC-FC coupling.
4. HCP\_lockbox\_whole\_brain\_coupling\_all\_conditions\_correlation\_personality: Computation of coupling measure-specific brain-average coupling values for all eight conditions and performance of partial correlations with individual personality scores.
5. HCP\_internal\_cross\_validation\_basic\_NMA\_prediction\_model: Conduction of the internal-cross-validation of the ‘Basic NMA Model’ that is built using two input predictor variables. The predictor variables are derived from individual’s coupling values and extracted by using group-based positive and group-based negative NMA masks. This script contains three parts: **Part 1** partitions the sample into five different folds (considering family relations and personality distribution) and creates positive and negative NMAs for each training sample and test sample. **Part 2** uses the NMAs created in part 1 to build multiple linear regression models that are then tested for their ability to predict personality scores in the test samples. **Part 3** assesses the significance of the prediction with a permutation test.
6. HCP\_lockbox\_internal\_cross\_validation\_expanded\_NMA\_prediction\_model: Conduction of the internal-cross-validation of the ‘Expanded NMA Model’ that is built using 14 input predictor variables (two from each of the seven task conditions). The predictor variables are derived from individual’s coupling values and extracted by using group-based positive and group-based negative NMA masks. This script contains three parts: **Part 1** partitions the sample into five different folds (considering family relations and personality distribution) and creates positive and negative NMAs for each training sample and test sample. **Part 2** uses the NMAs created in part 1 to build multiple linear regression models that are then tested for their ability to predict personality scores in the test samples. **Part 3** assesses the significance of the prediction with a permutation test.

4.3. Figures

1. Visualization\_distribution\_of\_personality\_scores: Creation of histograms depicting the distribution of personality scores in the main sample (HCP532) and the lockbox sample (HCP232).

2. Visualization\_HCP\_532\_NMAs\_whole\_sample\_conscientiousness: This script builds a positive and negative Node-Measure Assignment (NMA) for the complete main sample (HCP532, no cross-validation) and plots them.

3. Visualization\_prediction\_results: Creation of plots to visualize the results of the prediction analyses (bar graphs and matrices).

4.4. Functions

External functions and their licences can be found in this folder.

5. Software Requirements

* Matlab version 2021a

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Note that external functions have other licenses that are provided in the Functions folder.