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Reporting Summary

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Statistics

For all statistical analyses, confirm that the following items are present in the figure legend, table legend, main text, or Methods section.

n/a	Confirmed
☐	☒ The exact sample size (*n*) for each experimental group/condition, given as a discrete number and unit of measurement
☐	☒ A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly
☐	☒ The statistical test(s) used AND whether they are one- or two-sided *Only common tests should be described solely by name; describe more complex techniques in the Methods section.*
☐	☒ A description of all covariates tested
☐	☒ A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons
☐	☒ A full description of the statistical parameters including central tendency (e.g. means) or other basic estimates (e.g. regression coefficient) AND variation (e.g. standard deviation) or associated estimates of uncertainty (e.g. confidence intervals)
☐	☒ For null hypothesis testing, the test statistic (e.g. *F*, *t*, *r*) with confidence intervals, effect sizes, degrees of freedom and *P* value noted *Give P values as exact values whenever suitable.*
☒	☐ For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings
☒	☐ For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes
☐	☒ Estimates of effect sizes (e.g. Cohen's *d*, Pearson's *r*), indicating how they were calculated

Our web collection on statistics for biologists contains articles on many of the points above.

Software and code

Policy information about availability of computer code

Data collection	We presented all stimuli for task-based fMRI data collection using the PsychoPy software (Peirce, 2007).
Data analysis	The preprocessing of fMRI data was conducted using fMRIPrep 20.2.1. The features were extracted using the time-series analysis toolbox (hctsa) (Fulcher et al., 2013; Fulcher and Jones, 2017). Dimension reduction analysis was carried out using the Brainspace toolbox. For assessing spatial autocorrelation in our data, we implemented spin permutation tests via the BrainSMASH software. The classification analysis was performed using scikit-learn's (Pedregosa FABIANPEDREGOSA et al., 2011). The complete analysis code for this study is available at our GitHub repository: https://github.com/Xiuyi-Wang/Feature_similarity_Project.

For manuscripts utilizing custom algorithms or software that are central to the research but not yet described in published literature, software must be made available to editors and reviewers. We strongly encourage code deposition in a community repository (e.g. GitHub). See the Nature Portfolio guidelines for submitting code & software for further information.

Data

Policy information about availability of data

All manuscripts must include a data availability statement. This statement should provide the following information, where applicable:

- Accession codes, unique identifiers, or web links for publicly available datasets
- A description of any restrictions on data availability
- For clinical datasets or third party data, please ensure that the statement adheres to our policy

The HCP data is publicly available here https://www.humanconnectome.org/. The York data is not available due to insufficient consent. Researchers wishing to access the data should contact Elizabeth Jefferies or the Chair of the Research Ethics Committee of the York Neuroimaging Centre. Data will be released when this is possible under the terms of the UK GDPR.

Research involving human participants, their data, or biological material

Policy information about studies with human participants or human data. See also policy information about sex, gender (identity/presentation), and sexual orientation and race, ethnicity and racism.

Reporting on sex and gender	We recruited human participants of any sex for our experiments. Our study design did not specifically account for sex differences as our findings are intended to be generalizable across sexes. Participant sex was determined through self-reporting. Our participant demographic consisted of: York Semantic Task Group: 31 healthy adults (25 females). York Non-semantic Task Group: 31 healthy adults (26 females). HCP Sample: 245 healthy volunteers (115 females). Although sex-disaggregated data is provided, consent for sharing individual-level data was not obtained, adhering to ethical guidelines regarding participant privacy.
Reporting on race, ethnicity, or other socially relevant groupings	We did not collect data concerning race, ethnicity, or other socially relevant variables because we focused on cognitive functions that we anticipated would not be influenced by these variables. However, we acknowledge the importance of considering such factors in broader research contexts and plan to evaluate their relevance in future studies.
Population characteristics	Our participant demographic consisted of: York Semantic Task Group: 31 healthy adults (25 females; age: mean ± SD = 21.26 ± 2.93; range: 19 – 34 years). York Non-semantic Task Group: 31 healthy adults (26 females; age: mean ± SD = 20.60 ± 1.68; range: 18 – 25 years). HCP Sample: 245 healthy volunteers (115 females; age: mean ± SD = 28.21 ± 3.67; range: 23 – 35 years).
Recruitment	We recruited all participants based on specific inclusion criteria: right-handedness, native English-speaking ability, normal or corrected-to-normal vision, and no history of psychiatric or neurological illnesses. Each participant provided informed consent, adhering to ethical guidelines for human studies.
Ethics oversight	For the University of York datasets, the research was approved by the York Neuroimaging Centre and Department of Psychology ethics committees. For the HCP dataset, the study was approved by the Institutional Review Board of Washington University at St. Louis (Glasser et al., 2013).

Note that full information on the approval of the study protocol must also be provided in the manuscript.

Field-specific reporting

Please select the one below that is the best fit for your research. If you are not sure, read the appropriate sections before making your selection.

☒ Life sciences ☐ Behavioural & social sciences ☐ Ecological, evolutionary & environmental sciences

For a reference copy of the document with all sections, see nature.com/documents/nr-reporting-summary-flat.pdf

Life sciences study design

All studies must disclose on these points even when the disclosure is negative.

Sample size	We recruited 30 participants for each task fMRI experiment, aligning with common practices within the field. Task fMRI studies typically involve 20 to 30 participants, a range that effectively balances the need for detecting predefined effects with practical constraints such as time, financial resources, and participant availability. This sample size is generally considered the minimum required to achieve acceptable power levels for detecting moderate effect sizes. It helps in identifying typical brain activity patterns associated with the task without the complications associated with larger samples, such as increased logistical demands and costs. This approach ensures that our findings are robust yet sufficiently generalizable.
Data exclusions	Our exclusion criteria were pre-established to maintain the integrity of data analysis. 31 healthy adults performed the semantic tasks. A functional run was excluded if (I) relative root mean square (RMS) framewise displacement was higher than 0.2 mm, (II) more than 15% of frames showed motion exceeding 0.25 mm, or (III) the accuracy of the behaviour task was low (3SD below the mean). If only one run of a task was left for a participant after exclusion, all their data for that task were removed. Using the

exclusion criteria above for the semantic association task, there were 24 participants with 4 runs, 3 participants with 3 runs, and 3 participants with 2 runs. For the feature matching task, there were 23 participants with 4 runs, 4 participants with 3 runs, and 1 participant with 2 runs.

31 healthy adults performed the spatial working memory and math tasks. One participant with incomplete data was removed. These exclusion criteria above resulted in a final sample of 27 participants for both the spatial working memory task and the math task.

The HCP sample involved data from 245 healthy volunteers. Since not all participants completed all scans, we only included 339 unrelated participants from the S900 release. Subjects were considered for data exclusion based on the mean and mean absolute deviation of the relative root-mean-square motion across four rsfMRI scans, resulting in four summary motion measures. If a subject exceeded 1.5 times the interquartile range (in the adverse direction) of the measurement distribution in two or more of these measures, the subject was excluded. In addition, functional runs were flagged for exclusion if more than 25% of frames exceeded 0.2 mm frame-wise displacement (FD_power). The data of 91 participants was excluded because of excessive head motion and the data of another 3 participants was excluded because their resting data did not have all the time points. In total, the data of 245 participants was analyzed after exclusions.

Replication

Our study successfully replicated the finding that Regions belonging to the same intrinsic functional network have greater FS compared to regions in different networks (cf. Shafiei et al., 2020). Additionally, we replicated the first three connectivity dimensions described by Margulies et al. (2016). We extended these findings by demonstrating that feature similarity demonstrated greater sensitivity to task modulation than traditional functional connectivity (FC) and 46 out of 49 statistical measures of pairwise interactions (SPIs). These findings position FS as a powerful tool for capturing task-specific brain network dynamics and advancing our understanding of cognitive flexibility.

Randomization

We recruited two groups of participants, both meeting the same selection criteria: right-handedness, native English speaker, normal or corrected-to-normal vision, and no history of psychiatric or neurological illnesses. The first group was assigned to complete two semantic tasks (semantic association and semantic feature matching tasks), while the second group engaged in two non-semantic tasks (spatial working memory and math tasks). Our study mainly investigates whether feature similarity can show greater sensitivity to task modulation than traditional functional connectivity (FC) and most statistical measures of pairwise interactions (SPIs). We showed that in some contexts, FC and FS showed consistent patterns, but sometimes inconsistent patterns, excluding the difference is driven by individual participant differences.

Blinding

We recruited two groups of participants, both meeting the same selection criteria: right-handedness, native English speaker, normal or corrected-to-normal vision, and no history of psychiatric or neurological illnesses. The first group was assigned to complete two semantic tasks (semantic association and semantic feature matching tasks), while the second group engaged in two non-semantic tasks (spatial working memory and math tasks). Our study mainly investigates whether feature similarity can show greater sensitivity to task modulation than traditional functional connectivity (FC) and most statistical measures of pairwise interactions (SPIs). We showed that in some contexts, FC and FS showed consistent patterns, but sometimes show inconsistent patterns, excluding the difference is driven by individual participant differences. Although the investigators were aware of the group allocations during data collection and analysis, any conclusions drawn about the difference between feature similarity and functional connectivity are based on the data rather than observer bias.

Reporting for specific materials, systems and methods

We require information from authors about some types of materials, experimental systems and methods used in many studies. Here, indicate whether each material, system or method listed is relevant to your study. If you are not sure if a list item applies to your research, read the appropriate section before selecting a response.

Materials & experimental systems

n/a	Involved in the study
☒	☐ Antibodies
☒	☐ Eukaryotic cell lines
☒	☐ Palaeontology and archaeology
☒	☐ Animals and other organisms
☒	☐ Clinical data
☒	☐ Dual use research of concern
☒	☐ Plants

Methods

n/a	Involved in the study
☒	☐ ChIP-seq
☒	☐ Flow cytometry
☐	☒ MRI-based neuroimaging

Plants

Seed stocks

Report on the source of all seed stocks or other plant material used. If applicable, state the seed stock centre and catalogue number. If plant specimens were collected from the field, describe the collection location, date and sampling procedures.

Novel plant genotypes

Describe the methods by which all novel plant genotypes were produced. This includes those generated by transgenic approaches, gene editing, chemical/radiation-based mutagenesis and hybridization. For transgenic lines, describe the transformation method, the number of independent lines analyzed and the generation upon which experiments were performed. For gene-edited lines, describe the editor used, the endogenous sequence targeted for editing, the targeting guide RNA sequence (if applicable) and how the editor was applied.

Authentication

Describe any authentication procedures for each seed stock used or novel genotype generated. Describe any experiments used to assess the effect of a mutation and, where applicable, how potential secondary effects (e.g. second site T-DNA insertions, mosiacism, off-target gene editing) were examined.

Magnetic resonance imaging

Experimental design

Design type	This study analyzed the resting state fMRI data from the Human Connectome Project and two task fMRI datasets collected at the University of York, UK. The first task fMRI dataset involved two semantic control tasks: semantic association task and the semantic feature matching task. Semantic association task was presented in a rapid event-related design and the semantic feature matching task was presented in a mixed design. Each run consisted of four experimental blocks. In each block, 20 trials were presented in a rapid event-related design. The second task fMRI dataset involved two non-semantic tasks, spatial working memory task and math task, presented in a block design.
Design specifications	The semantic feature matching task included four runs and two conditions (two features: colour and shape), presented in a mixed design. Each run consisted of four experimental blocks (two 2 min 30 s blocks per feature), resulting in a total time of 10 min 12 s. In each block, 20 trials were presented in a rapid event-related design. To maximize the statistical power of the rapid event-related fMRI data analysis, the stimuli were presented with a temporal jitter randomized from trial to trial. The inter-trial interval varied from 3 to 5 s. Each trial started with a fixation, followed by the feature, probe word, and target word presented centrally on the screen, triggering the onset of the decision-making period. The feature, probe word, and target word remained visible until the participant responded, or for a maximum of 3 s. The semantic association task included four runs, presented in a rapid event-related design. Each run consisted of 80 trials, with about half being related and half being unrelated trials. The procedure of each trial was the same as the feature matching task except only two words were presented on the screen. In the spatial working memory task, participants were required to maintain four or eight sequentially presented locations in a 3×4 grid, giving rise to easy and hard spatial working memory conditions. Stimuli were presented at the center of the screen across four steps. Each of these steps lasted for 1s and highlighted one location on the grid in the easy condition, and two locations in the hard condition. This was followed by a decision phase, which showed two grids side by side (i.e., two-alternative forced choice (2AFC) paradigm). One grid contained the locations shown on the previous four steps, while the other contained one or two locations in the wrong place. Participants indicated their response via a button press and feedback was immediately provided within in 2.5s. Each run consisted of 12 experimental blocks (6 blocks per condition and 4 trials in a 32 s block) and 4 fixation blocks (each 16 s long), resulting in a total time of 448 s. In the math task, participants were presented with an addition expression on the screen for 1.45s and, subsequently made a 2AFC decision indicating their solution within 1s. The easy condition used single-digit numbers while the hard condition used two-digit numbers. Each trial ended with a blank screen lasting for 0.1s. Each run consisted of 12 experimental blocks (with 4 trials per block) and 4 fixation blocks, resulting in a total time of 316s.
Behavioral performance measures	We recorded the button pressed by each participant and the response time (RT) for each trial across all tasks. Our first analysis verified the effectiveness of our parametric manipulation of semantic task demands. To examine how semantic association strength influenced response time (RT) in the semantic association task, we built a linear mixed effect model. This model accounted for individual differences in the difficulty effect by including random intercepts and slopes. We compared a model incorporating a linear effect of semantic association strength with a model without this effect. The results showed that association strength significantly facilitated decision making for related trials ($z = -9.244$, $p < 0.0001$) but had no discernible effect on unrelated trials ($z = 0.018$, $p = 0.986$), after controlling for feature similarity and global similarity, the latter being the overall similarity of each word pair as rated by an independent group of 30 participants. We conducted a comparable analysis for the feature matching task to investigate how feature similarity influenced response times and accuracy. The results indicated that higher feature similarity facilitated decision-making for matching trials (RT: $z = -10.51$, $p < 0.0001$), but impeded decisions for non-matching trials (RT: $z = 11.97$, $p < 0.0001$) after controlling for association strength and global similarity. We also verified whether we manipulated the difficulty of the non-semantic tasks as expected by examining whether the more demanding conditions showed decreased accuracy and increased RT than the easy conditions. In the spatial working memory task, participants tracked locations presented in sequence, with the easy version involving one location per slide and the hard version two locations, thus increasing working memory load. In the more demanding version, both accuracy and RT were affected, showing decreased accuracy ($t(26) = -8.97$, $p = 7.31 * e-10$) and increased RT ($t(26) = 7.14$, $p = 7.20 * e-8$) compared to easier trials. Similarly, the math task ranged from single-digit additions in the easy version to double-digit additions in the hard version. The more demanding condition resulted in lower accuracy ($t(26) = -6.73$, $p = 2.19 * e-7$) and longer RTs ($t(26) = 12.06$, $p = 8.04 * e-13$) compared to easier trials.

Acquisition

Imaging type(s)	We analyzed the structural and functional fMRI data.
Field strength	For the York dataset, whole brain structural and functional MRI data were acquired using a 3T Siemens MRI scanner at York Neuroimaging Centre, University of York. For the HCP dataset, images were acquired using a customized 3T Siemens Connectome scanner.
Sequence & imaging parameters	Image acquisition of York Semantic dataset The functional runs were acquired using a multi-band multi-echo (MBME) EPI sequence, each 11.45 minutes long (TR=1.5 s; TE = 12, 24.83, 37.66 ms; 48 interleaved slices per volume with slice thickness of 3 mm (no slice gap); FoV =

24 cm (resolution matrix = 3x3x3; 80x80); 75° flip angle; 455 volumes per run; 7/8 partial Fourier encoding and GRAPPA (acceleration factor = 3, 36 ref. lines); multi-band acceleration factor = 2). Structural T1-weighted images were acquired using an MPRAGE sequence (TR = 2.3 s, TE = 2.3 s; voxel size = 1x1x1 isotropic; 176 slices; flip angle = 8°; FoV= 256 mm; interleaved slice ordering). We also collected a high-resolution T2-weighted (T2w) scan using an echo-planar imaging sequence (TR = 3.2 s, TE = 56 ms, flip angle = 120°; 176 slices, voxel size = 1x1x1 isotropic; Fov = 256 mm).

Image acquisition of York Non-semantic dataset
The scanning protocols included a T1-weighted MPRAGE sequence with whole-brain coverage. The structural scan used: acquisition matrix of 176×256×256 and voxel size 1×1×1 mm3, repetition time (TR) = 2300 ms, and echo time (TE) = 2.26 ms. Functional data were acquired using an EPI sequence with an 800 flip angle and using GRAPPA with an acceleration factor of 2 in 3 x 3 x 4 mm voxels in 64-axial slices. The functional scan used: 55 3-mm-thick slices acquired in an interleaved order (with 33% distance factor), TR = 3000 ms, TE = 15 ms, FoV = 192 mm.

Image acquisition of HCP dataset
MRI acquisition protocols of the HCP dataset have been previously described (Barch et al., 2013; Glasser et al., 2013). Participants underwent the following scans: structural (at least one T1-weighted (T1w) MPRAGE and one 3D T2-weighted (T2w) SPACE scan at 0.7-mm isotropic resolution), rsfMRI (4 runs ×14 min and 33 s), and task fMRI (7 tasks, 46.6 min in total). Briefly, whole-brain EPI acquisitions were acquired with a 32-channel head coil on a modified 3 T Siemens Skyra with TR = 720 ms, TE = 33.1 ms, flip angle = 52°, BW =2290 Hz/Px, in-plane FOV = 208 × 180 mm, 72 slices, 2.0 mm isotropic voxels, with a multi-band acceleration factor of 8. Spin echo phase reversed images were acquired during the fMRI scanning sessions to enable accurate cross-modal registrations of the T2w and fMRI images to the T1w image in each subject and standard dual gradient echo field maps were acquired to correct T1w and T2w images for readout distortion.

Area of acquisition

Whole brain structural and functional MRI data were acquired.

Diffusion MRI ☐ Used ☒ Not used

Preprocessing

Preprocessing software

Image pre-processing of York Semantic and Non-semantic dataset

The York datasets were preprocessed using fMRIPrep 20.2.1 [(Esteban et al., 2018), RRID:SCR_016216], which is based on Nipype 1.5.1 [(Gorgolewski et al., 2011), RRID:SCR_002502]. Post-processing of the outputs of fMRIPrep version 20.2.1 (Esteban et al., 2018) was performed using the eXtensible Connectivity Pipeline (XCP) (Satterthwaite et al., 2013; Ciric et al., 2018). The processed BOLD was smoothed using Connectome Workbench with a gaussian kernel size of 6.0 mm (FWHM). The T1w image was corrected for intensity non-uniformity (INU) with N4BiasFieldCorrection (Tustison et al., 2010), distributed with ANTs 2.3.3 [(Avants et al., 2008), RRID:SCR_004757], and used as T1w-reference throughout the workflow. The T1w-reference was then skull-stripped with a Nipype implementation of the antsBrainExtraction.sh workflow (from ANTs), using OASIS30ANTs as target template. Brain tissue segmentation of cerebrospinal fluid (CSF), white-matter (WM) and gray-matter (GM) was performed on the brain-extracted T1w using fast FSL 5.0.9 [(Zhang et al., 2001), RRID:SCR_002823]. Brain surfaces were reconstructed using recon-all from FreeSurfer 6.0.1 [(Dale et al., 1999a), RRID:SCR_001847], and the brain mask estimated previously was refined with a custom variation of the method to reconcile ANTs-derived and FreeSurfer-derived segmentations of the cortical gray-matter of Mindboggle [(Klein et al., 2017), RRID:SCR_002438].

The HCP data were preprocessed using HCP's minimal pre-processing pipelines (Glasser et al., 2013). A robust initial brain extraction is performed using an initial linear (FLIRT) and non-linear (FNIRT) registration of the image to the MNI template. The data were smoothed by a 2-mm FWHM kernel in the grayordinates space that avoids mixing data across gyral banks for surface data and avoids mixing areal borders for subcortical data.

Normalization

For the York datasets, volume-based spatial normalization to two standard spaces (MNI152NLin2009cAsym, MNI152NLin6Asym) was performed through nonlinear registration with antsRegistration (ANTs 2.3.3), using brain-extracted versions of both T1w reference and the T1w template.

For the HCP dataset, the average T1w and T2w images are aligned to the MNI space template (with 0.7 mm resolution for the HCP data) using a rigid 6 DOF transform, derived from a 12 DOF affine registration. After this, a robust brain extraction is performed using an initial linear (FLIRT) and non-linear (FNIRT) registration of the image to the MNI template.

Normalization template

For the York datasets, the following templates were selected for spatial normalization: ICBM 152 Nonlinear Asymmetrical template version 2009c [(Fonov et al., 2009), RRID:SCR_008796; TemplateFlow ID: MNI152NLin2009cAsym], FSL's MNI ICBM 152 non-linear 6th Generation Asymmetric Average Brain Stereotaxic Registration Model [(Evans et al., 2012), RRID:SCR_002823; TemplateFlow ID: MNI152NLin6Asym].

For the HCP dataset, a standard grayordinate space - CIFTI grayordinate space – was used. The resulting data were in CIFTI 64k-vertex grayordinate space. The left hemisphere had 29696 vertices and right hemisphere had 29716 vertices in total after removing the medial wall.

Noise and artifact removal

For the York datasets, several confounding time-series were calculated based on the preprocessed BOLD: framewise displacement (FD), DVARS (D refers to a derivative of fMRI time course, VARS refers to RMS variance) and three region-wise global signals. FD was computed using two formulations following previous work (absolute sum of relative motion; (Power et al., 2014), relative root mean square displacement between affines; (Jenkinson et al., 2002). FD and DVARS were calculated for each functional run, both using their implementations in Nipype (Power et al., 2014). Three global signals were extracted within the CSF, the WM, and the whole-brain masks. Additionally, a set of physiological regressors were extracted to allow for component-based noise correction (CompCor) (Behzadi et al., 2007) principal components were estimated after high-pass filtering the preprocessed BOLD time-series (using a discrete cosine filter with 128s cut-off) for two CompCor variants:

temporal (tCompCor) and anatomical (aCompCor). tCompCor components were then calculated from the top 2% variable voxels within the brain mask. For aCompCor, three probabilistic masks (CSF, WM and combined CSF+WM) were generated in anatomical space. Finally, these masks are resampled into BOLD space and binarized by thresholding at 0.99 (as in the original implementation). Components were also calculated separately within the WM and CSF masks. For each CompCor decomposition, the k components with the largest singular values were retained, such that the retained components' time series were sufficient to explain 50 percent of variance across the nuisance mask (CSF, WM, combined, or temporal). The remaining components were dropped from consideration. The head-motion estimates calculated in the correction step were also placed within the corresponding confounds file. The confound time series derived from head motion estimates and global signals were expanded with the inclusion of temporal derivatives and quadratic terms for each (Satterthwaite et al., 2013). Frames that exceeded a threshold of 0.5 mm FD or 1.5 standardized DVARS were annotated as motion outliers. All resamplings were performed with a single interpolation step by composing all the pertinent transformations (i.e., head-motion transform matrices, susceptibility distortion correction when available, and co-registrations to anatomical and output spaces). Gridded (volumetric) resamplings were performed using antsApplyTransforms (ANTs), configured with Lanczos interpolation to minimize the smoothing effects of other kernels (Lanczos, 1964).

Post-processing of the outputs of fMRIPrep version 20.2.1 (Esteban et al., 2018) was performed using the eXtensible Connectivity Pipeline (XCP) (Satterthwaite et al., 2013; Ciric et al., 2018). For each CIFTI run per subject, the following post-processing was performed: before nuisance regression and filtering any volumes with framewise-displacement greater than 0.3 mm (Satterthwaite et al., 2013; Power et al., 2014) were flagged as outliers and excluded from nuisance regression. In total, 36 nuisance regressors were selected from the nuisance confound matrices of fMRIPrep output. These nuisance regressors included six motion parameters, global signal, mean white matter, and mean CSF signal with their temporal derivatives, and the quadratic expansion of six motion parameters, tissue signals and their temporal derivatives (Satterthwaite et al., 2013; Ciric et al., 2017, 2018). These nuisance variables were accounted for in the BOLD data using linear regression - as implemented in Scikit-Learn 0.24.2 (Pedregosa et al., 2011). Residual timeseries from this regression were then band-pass filtered to retain signals within the 0.01-0.08 Hz frequency band.

For the HCP dataset, rest and task fMRI data were additionally identically cleaned for spatially specific noise using spatial ICA +FIX (Salimi-Khorshidi et al., 2014) and global structured noise using temporal ICA (Glasser et al., 2018).

Volume censoring

For the York datasets, frames that exceeded a threshold of 0.5 mm FD or 1.5 standardized DVARS were annotated as motion outliers. All resamplings were performed with a single interpolation step by composing all the pertinent transformations (i.e., head-motion transform matrices, susceptibility distortion correction when available, and co-registrations to anatomical and output spaces). Before nuisance regression and filtering any volumes with framewise-displacement greater than 0.3 mm (Satterthwaite et al., 2013; Power et al., 2014) were flagged as outliers and excluded from nuisance regression. In total, 36 nuisance regressors were selected from the nuisance confound matrices of fMRIPrep output. These nuisance regressors included six motion parameters, global signal, mean white matter, and mean CSF signal with their temporal derivatives, and the quadratic expansion of six motion parameters, tissue signals and their temporal derivatives (Satterthwaite et al., 2013; Ciric et al., 2017, 2018). These nuisance variables were accounted for in the BOLD data using linear regression - as implemented in Scikit-Learn 0.24.2 (Pedregosa et al., 2011).

Statistical modeling & inference

Model type and settings

We performed dimension reduction analysis (diffusion embedding) (Margulies et al., 2016) on the resting state FC matrix for the HCP dataset. We also calculated the network-based functional connectivity by calculating the temporal correlation of time series data and feature similarity by calculating the correlation of extracted features.

Effect(s) tested

We conducted paired-t tests for each task to examine the significance of the FC difference between network pairs. We further investigated whether the task influenced the FC difference between network pairs using the maximum/minimum permutation test.

Specify type of analysis: ☐ Whole brain ☒ ROI-based ☐ Both

Anatomical location(s)

We generated the individual-specific functional parcellations for each participant and then performed all subsequent analyses within the parcellation.

Statistic type for inference

We conducted a region of interest (ROI)-based analysis using the individual-specific parcellations.

(See Eklund et al. 2016)

Correction

We implemented multiple comparison corrections using the family-wise-error (FWE) and spin permutation techniques. The FWE correction was applied to control the expected proportion of incorrectly rejected null hypotheses (false discoveries), thereby balancing the need for sensitivity and specificity in our findings. Additionally, the spin permutation correction was utilized to address spatial autocorrelation in neuroimaging data, ensuring that our results are not unduly influenced by the anatomical proximity of analyzed regions.

Models & analysis

n/a	Involved in the study
☐	☒ Functional and/or effective connectivity
☒	☐ Graph analysis
☒	☐ Multivariate modeling or predictive analysis

Functional and/or effective connectivity

We calculated the resting-state and task-based functional connectivity for each run of each participant by

Functional and/or effective connectivity	demeaning the residual time series for each parcel and then calculating the Pearson correlations for each parcel pair.