EBRAINS Data Descriptor

TITLE

Parcellation-based structural and resting-state functional whole-brain connectomes of 1000BRAINS cohort (v1.1)

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ABSTRACT*

This dataset provides the individual whole-brain connectomes for 261 subjects from the 1000BRAINS cohort of healthy adults. For this, 20 different state-of-the-art cortical parcellations were used in this dataset to reconstruct the region-based empirical structural connectivity (representing the anatomy of axonal tracts) and functional connectivity (representing the temporal correlation between neuronal activity of brain regions) from diffusion-weighted (dwMRI) and resting-state functional magnetic resonance imaging (fMRI) data, respectively. In addition, the regional blood-oxygen-level-dependent (BOLD) signals used for the calculation of the resting-state functional connectivity are also included in this dataset. Connectivity patterns of brain networks are of special interest in contemporary brain research, as they may reflect communication in the brain at the structural and functional levels. Their extraction, however, is a complex process that requires deep knowledge of MRI data processing methods. Furthermore, there is no consensus as to which parcellation of the brain is most suitable for a given analysis. The provided data can thus be used to investigate structural and functional human connectomes and their interrelations for varying brain parcellations. Accordingly, the investigations can be also extended to the whole-brain models for further analyses of brain structure and function.

VERSION SPECIFICATIONS:

In this version of the dataset 18 MRI sessions were removed because of low-quality results of the data processing found after a detailed quality control. Accordingly, the sample size was reduced by 13 subjects, and one MRI session was removed for each of further 5 subjects that were represented by 2 MRI sessions in the previous version.

METHODS

The empirical connectomes included in this study were reconstructed for 261 healthy adults (140 males) aged between 21 and 86 years old (53.9 ± 15.7 years) from the 1000BRAINS cohort (Caspers et al., 2014). For 88 subjects (50 males) of this subject group 2 MRI sessions with diffusion-weighted and resting-state functional magnetic resonance imaging data (dwMRI and fMRI, respectively) were available, i.e., one additional dwMRI session as well as one additional resting-state fMRI scanning session was performed. This resulted in 261 + 88 = 349 MRI sessions in total and the same number of structural and functional connectomes included in this dataset. Here, we separately discuss the reconstruction of the structural connectivity (SC) and functional connectivity (FC) from the dwMRI and resting-state fMRI data, respectively, included in the mentioned 1000BRAINS cohort. We also present the 20 different state-of-the-art brain parcellations for which we extracted the cortical region-based connectomes. The same brain parcellations were used in the EBRAINS datasets (Domhof et al., 2022b, c) for derivation of the structural and functional connectomes and BOLD signals for the Human Connectome Project cohort(Van Essen et al., 2013), where more details can be found.

SC reconstruction from dwMRI data

We used a workflow developed in-house to reconstruct the SC from dwMRI data, see https://jugit.fz-juelich.de/inm7/public/vbc-mri-pipeline. This workflow consisted of four stages: (1) preprocessing of the T1-weighted and diffusion-weighted images, (2) computing the whole-brain tractography, (3) transformation of the atlas images to the subject's native space, and finally (4) reconstruction of the SC matrices. The pipeline can be regarded as a wrapper of functions included in the ANFI (Cox, 1996), ANTs (Tustison et al., 2010), FreeSurfer (Dale et al., 1999), FSL (Smith et al., 2004) and MRtrix3 (Tournier et al., 2019) software packages. Computations were performed on the JURECA high-performance computing cluster in Jülich Supercomputing Centre (Jülich Supercomputing Centre, 2021).

When preprocessing the images, FreeSurfer functions were used to perform (1) bias field correction, tissue segmentation, cortical (surface) reconstruction, volume-surface conversion and surface deformation on the T1-weighted images of the subjects. FreeSurfer functions were also used to perform head motion and eddy current distortion correction on the diffusion-weighted images, whereas MRtrix3 functions denoised them and performed bias field correction. The T1-weighted image was co-registered to the dwMRI by the linear transformation functions of FSL. Afterwards, tissue segmentation was also performed for the dwMRI. (2) Subsequently, the whole-brain tractography was computed on the basis of the preprocessed dwMRI by using MRtrix3 functions. The response functions for spherical deconvolution were estimated using a constrained deconvolution algorithm (Jeurissen et al., 2014). Through these response functions, the fibre-oriented distributions (FOD) were estimated from the dwMRI using spherical deconvolution. The whole-brain tractography was completed via a second-order integration over these distributions by means of a probabilistic algorithm (Tournier et al., 2010). We used the following tracking parameter settings: number of streamlines = 10M, step size = 1.2 mm, angle = 45°, min. length = 2.5 mm, max. length = 250 mm, FOD amplitude for terminating tract = 0.06, max. attempts per seed = 50, max. number of sampling trials = 1000 and down-sampling = 3 mm. (3) FSL function were used to linearly and nonlinearly transform the brain atlas images from the standard space to the subject's native space. (4) Eventually, the MRtrix3 function tck2connectome was used to derive the number of streamlines and their average length for all pairs of parcels included in a particular parcellation.

Derivation of the FC from the resting-state fMRI data

The preprocessing module of functional MRI performed slice time correction, head motion correction, re-slicing in a 2 mm iso-cubic voxel space, intensity normalization, de-trending with filtering of very slow fluctuations out (high pass), co-registration to the T1w image, and calculation of regressors for the white-

matter, cerebrospinal fluid (CSF), and brain global signals as well as for the head motion. The pipeline also transformed the labeled image of the brain parcellation generated in the standard T1w MNI space to the fMRI native space. Finally, we performed a nuisance regression with the prepared regressors (white-matter, CSF, and the brain global signals as well as head motions). Blood oxygen level dependent (BOLD) signals were extracted from the resting-state functional MRI data as processed by the mentioned pipeline. Then, the mean BOLD intensity was calculated for every brain region delineated according to a given brain parcellation by averaging across all voxels separately in each parcel. The result comprised one mean BOLD signal time series per parcel. Individual time series were linearly detrended. The FC matrix was subsequently reconstructed by calculating the Pearson correlation coefficients across the time series for all pairs of parcels.

Brain parcellations

The SC and FC of each subject were reconstructed on the basis of the 20 different brain atlases (or parcellations) included in Table 1. The used brain atlases are available for download provided by the corresponding publications cited in Table 1. In order to enhance the comparability between atlases, we modified the original atlas images so that they only covered the cerebral cortex (except for the Julich-Brain atlas, see Table 1) and were sampled to the MNI152 nonlinear template space. The details of these modifications vary across parcellations. The scripts performing their modifications were in the repository of the previous dataset publication (Domhof et al., 2022b, c).

These atlases were selected in order to balance between parcellations derived from functional data (Craddock et al. (2012), Shen et al. (2013), Schaefer et al. (2018) and Urchs et al. (2019)) and structural information, comprising the other brain atlases shown in Table 1. In addition, the considered parcellations were constructed via a variety of methodologies including boundary detection algorithms, histological stainings and diverse clustering approaches. This diversity in brain parcellation compilation paradigms enhanced the probability of finding parcellation-induced deviations. When available, we also included parcellations constructed through the same method in multiple granularities so that the effect of this quantity can be investigated as well.

Table 1. Overview of the used brain parcellation schemes with the number of parcels after atlas image modifications and associated publications.

Atlas name	Parcels	References
MIST	31 56 103 167	(Urchs et al., 2019)
Craddock	38 56 108 160	(Craddock et al., 2012)
Shen 2013	79 156	(Shen et al., 2013)
Schaefer	100 200	(Schaefer et al., 2018)
Harvard-Oxford	48 96	(Desikan et al., 2006; Frazier et al., 2005; Goldstein et al., 2007; Makris et al., 2006)
Desikan-Killiany	70	(Desikan et al., 2006)
von Economo-Koskinas	86	(Scholtens et al., 2018; von Economo and Koskinas, 1925)
AAL (version 2)	92	(Rolls et al., 2015; Tzourio-Mazoyer et al., 2002)
Destrieux	150	(Destrieux et al., 2010)
Brainnetome	210	(Fan et al., 2016)
Julich-Brain (version 2.9)	294	(Amunts et al., 2020)

TECHNICAL VALIDATION

The technical quality of the connectomes included in this repository highly depends on the quality of the neuroimaging data included in the 1000BRAINS cohort (Caspers et al., 2014). No ground truth exists for the SC and the FC. This is especially applicable to the FC derived from the resting-state fMRI data, where no references can be found to the observed dynamics as compared to, for example, the task-evoked activity. Our workflow used the freely available and broadly used software packages of FSL (Smith et al., 2004), FreeSurfer (Dale et al., 1999), ANTs (Tustison et al., 2010) AFNI (Cox, 1996), and MRtrix3 (Tournier et al., 2019). Finally, the Pearson correlation coefficients across the BOLD time series were calculated by Matlab R2020b. These procedures and tools have contributed to the quality and reliability of the connectomes included in this repository.

USAGE NOTES

As mentioned above, the connectivity matrices included in this repository comprise the individual SC and FC of 274 subjects with 367 sessions (two sessions for 93 subjects) for 20 different parcellations. The data are included as text files and hence can be processed by many different programming languages and software packages for further analyses. Examples of such analyses include atlas-induced variations in the structure-function relationship of individual subjects as estimated through diverging paradigms. Different methodologies include, but are not limited to, the statistical analysis of structure-function dependencies and dynamical whole-brain models (Suarez et al., 2020). In the latter paradigm, a network model is built on the basis of the SC, whereas the FC can be used to validate how well simulations of the constructed model replicate resting- state dynamics (Honey et al., 2009; Popovych et al., 2019). In particular, the presented data not only enable the investigation of atlas-induced group differences, but also parcellation-specific inter-subject variabilities. The BOLD signal time series of this repository can, for example, be used to study how different synchronization measures affect the functional connectivity of individuals and may also be used to extract personalized information that can complement the individualized connectomes at the derivation and validation of the whole-brain dynamical models (Domhof et al., 2022a).

SPATIAL ANCHORING:

All brain atlas images and the used MRI data were sampled in the volumetric MNI152 standard space included in FSL (MNI152 nonlinear 6th generation, see also https://fsl.fmrib.ox.ac.uk/fsl/fslwiki/Atlases). In addition, we ensured the parcellations only covered the cerebral cortex (except for the Julich-Brain atlas). We used the atlas images prepared in the previous dataset publications (Domhof et al., 2022b, c).

DATA RECORDS

In the repository the data are stored in the following directory structure:

… repository-root/
…… data-descriptor.pdf *[This data description file]*
…… <Number of parcels>-<Name of the atlas>/
…… BOLD/
…… <Subject ID>_<Session>_RestEmpBOLD.csv *[Mean BOLD signal across voxels in each cortical region]*
…… FC/
…… <Subject ID>_<Session>_RestEmpCorrFC.csv *[Pearson correlation of BOLD signals between regions]*
…… SC/
…… <Subject ID>_<Session>_Counts.csv *[Streamline counts between regions]*
…… <Subject ID>_<Session>_Lengths.csv *[Averaged path lengths of the given streamlines]*

The folders in the root directory are named after the atlas used for region-based BOLD signal extraction and are available as zip-files. The names of these files follow the format:

<Number of parcels>-<Name of the atlas>.zip.

Here, **<Subject ID>** indicates **anonymized subject ID** from **0001** to **0261** (261 subjects). **<Session>** indicates that session and has the format **session index.** The **session index** can either be **1** (day 1) or **2** (day 2).

CODE AVAILABILITY

The code used for the adaptation of these parcellation data can be found in the previous published datasets (Domhof et al., 2022b, c). The in-house pipeline we used for this dataset is also publicly available (https://jugit.fz-juelich.de/inm7/public/vbc-mri-pipeline). FreeSurfer (Dale et al., 1999), FSL (Smith et al., 2004), ANTs (Tustison et al., 2010), MRtrix3 (Tournier et al., 2019) and Python version 3 (Python Software Foundation, https://www.python.org/) are required to be installed on the system in order to run the software. The source code has been successfully tested on multiple Unix systems.

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Author contributions

S.B.E., O.V.P. and K.J. conceived the study; K.J. performed the MRI pipeline, extracted BOLD signals, and calculated FC and SC; O.V.P. contributed to technical validation and supervised the study; K.J. and O.V.P. both drafted the manuscript. All authors were involved in the preparation of the manuscript.

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