Supplementary Information for

Outlier detection in multimodal MRI identifies rare individual phenotypes among more than 15,000 brains

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Supplementary Methods

Outlier detection and screening in the HCP dataset

Brain MRI data were obtained from the HCP 1200 Subjects Release (1113 subjects: 507 males and 606 females; age 22–37) (Glasser, Smith, et al., 2016). If available, each HCP subject’s T1w MPRAGE (N = 1113), T2w SPACE (N = 1094), and SE-EPI dMRI images (N = 1065) were used. The data were acquired on a 3 T Siemens Connectome Skyra MRI scanner, and the detailed acquisition protocols can be found elsewhere (Glasser et al., 2013). The HCP project was approved by the Institutional Review Board of Washington University, and informed consent was obtained from all participants.

The following four commonly used brain imaging phenotypes were extracted from the HCP imaging preprocessing outputs: VV, FA, MD, and CTh. Because of the lack of T2w FLAIR in the HCP data, and poor WMLV segmentation accuracy when only using T1w images (Hotz et al., 2021), WMLV was excluded from the outlier detection of the HCP dataset. The detailed imaging phenotype extraction procedures are described as follows. The raw T1w MPRAGE and T2w SPACE images were preprocessed by the HCP structural pipeline (v4) (Glasser et al., 2013) based on FreeSurfer (v6) (Fischl, 2012). VV and CTh were extracted from the pipeline outputs. CTh values were averaged within the ROIs of the HCP multimodal parcellation atlas (360 regions) (Glasser, Coalson, et al., 2016). The dMRI data underwent FSL eddy-current and head-movement correction (Andersson & Sotiropoulos, 2016), gradient distortion correction, diffusion tensor model fitting (Basser, Mattiello, & LeBihan, 1994), and TBSS analyses (Smith et al., 2006). The skeletonized FA and MD images were averaged within the ROIs from the Johns Hopkins...
University white matter atlas (Mori et al., 2008). The FA or MD maps of 27 major white matter ROIs (Table S2) were extracted.

Exclusion of poor quality data was carried out using the automatic quality control procedures described in Section 2.3 of the main text. Using the similar primary screening procedures described in Section 2.4 of the main text, outlier scores were calculated for each subject per imaging phenotype. Similar covariate control was performed, and this resulted in regressing out brain volume from VV. The total number of extreme outliers across all individual imaging phenotypes was 12. They were all distinct, because no subject was an outlier in more than one imaging phenotype. These outliers were checked individually using the similar secondary screening procedures described in Section 2.6 of the main text, and none of them were associated with data collection/processing errors. The structural images of all these outlier subjects were reviewed radiologically, and the cases that would be interesting for follow-up were highlighted in Figures 4c (the right panel), S5a (the first panel), S5b, and S6b (the second, third, and fourth panels). Table S4 summarizes the outlier detection and screening in the HCP dataset.

**Evaluation of impact of neuroimaging data processing software on outlier detection**

For each imaging phenotype, an additional neuroimaging data processing software different from the one used in the main Methods was used for obtaining an additional set of preprocessed data. The raw T1w MPRAGE images were preprocessed by the UKB T1 pipeline (Alfaro-Almagro et al., 2018), and VV values were extracted from the SIENAX outputs (Smith et al., 2002). The raw T1w MPRAGE and T2w FLAIR images
were processed by the UBO Detector (Dong et al., 2021; Jiang et al., 2018), a k-nearest-neighbor-based white matter hyperintensities segmentation toolbox, and WMLV values were extracted from the UBO Detector outputs. The raw dMRI data were preprocessed by the QSIprep pipeline (Cieslak et al., 2021), and diffusion tensor model fitting (b = 1000 shell) was performed by Scilpy (https://github.com/scilus/scilpy/) on the preprocessed data. The resulting FA and MD images were skeletonized by TBSS (Smith et al., 2006) and were averaged within the ROIs from the Johns Hopkins University white matter atlas (Mori et al., 2008). The FA or MD values of 27 major white matter ROIs (Table S2) were extracted. To calculate CTh, the raw T1w MPRAGE images were processed by the CAT12 toolbox (Dahnke, Yotter, & Gaser, 2013; Gaser & Dahnke, 2016). The resulting CTh values were then corrected for folding effects, resampled to the HCP 32k vertex standard mesh, and then averaged within the ROIs of the HCP multimodal parcellation atlas (360 regions) (Glasser, Coalson, et al., 2016). Similar outlier detection procedures described in the main Methods were carried out separately on this additional set of preprocessed data, and this generated an additional set of outlier scores and extreme outliers.

To evaluate whether a different data processing software could change the outlier detection results, this new set of outlier scores and extreme outliers were compared against the original set of outlier scores and extreme outliers reported in the main Results. For each imaging phenotype, Pearson correlation was evaluated between these two sets of outlier scores. In addition, Dice coefficient (DC) was used to assess the similarity between these two sets of extreme outliers. DC is defined as

\[ DC = \frac{2|S_1 \cap S_2|}{|S_1| + |S_2|} \]
where $|S_1 \cap S_2|$ is the number of same outliers between these two sets, and $|S_1|$ is the number of outliers in the original set and $|S_2|$ is the number of outliers in the new set.
Figure S1. Controlling the effects of covariates. The covariates with correlation $>0.3$ with VV, WMLV, or the autoencoder replication errors are shown here. (a) The scatterplots between VV and age, brain volume, and CAT12’s T1w image quality metric. Due to their correlations with VV, these metrics were included as covariates when calculating VV outlier scores. (b) The scatterplot between WMLV and age. Due to its correlation with WMLV, age was included as a covariate when calculating WMLV outlier scores. (c) The scatterplot between MD autoencoder replication error and age. Due to its correlation with MD autoencoder replication error, age was included as a covariate when calculating MD outlier scores. (d) The scatterplot between CTh autoencoder replication error and FreeSurfer’s Euler number. Due to its correlation with CTh autoencoder replication error, FreeSurfer’s Euler number was included as a covariate when calculating CTh outlier scores.
Figure S2. Beeswarm plots for showing outlier subjects' outlier score ranges. The outliers with data collection/processing errors are represented by red dots. The non-artifactual outliers reviewed by a neuroradiologist are represented by green dots. The non-artifactual outliers not sampled for radiologically check are represented by blue dots. (a) VV outliers. (b) WMLV outliers. (c) FA outliers. (d) MD outliers. (e) CTh outliers.
Figure S3. Additional information on low test-retest reliability of RSFC outlier scores. (a) The scatterplot of global signal amplitude (GSA) versus RSFC outlier score in the UKB discovery group (RSFC calculated using partial correlations). (b) The scatterplot of GSA versus RSFC outlier score in the UKB discovery group (RSFC calculated using full correlations after global signal regression [GSR]). Panels (c)-(h) show the assessment of test-retest reliability of RSFC outlier scores in the HCP dataset. The 3 T rsfMRI data of 795 HCP subjects using an improved image reconstruction algorithm “r227” were used. The data were preprocessed by the HCP functional pipeline (v3) (Glasser et al., 2013) and were denoised by ICA+FIX. Each HCP subject had two rsfMRI sessions, and the two runs within each session were demeaned, variance normalized, and concatenated temporally. Using the Gordon parcellation scheme (Gordon et al.,
RSFC was quantified by the Pearson cross-correlation coefficient with or without global signal regression, respectively. RSFC was also quantified using partial correlations with Tikhonov regularization ($p = 0.01$; FSLNets) (Pervaiz, Vidaurre, Woolrich, & Smith, 2020). The upper triangular parts of these RSFC matrices from each of the above three RSFC evaluation methods were extracted. The extracted RSFC data of the first sessions (aka “test”) were used to train an autoencoder, and this trained autoencoder was applied to the data of the second sessions (aka “retest”) to calculate retest outlier scores. (c) Test-retest reliability of RSFC outlier scores in the HCP dataset. Each subject’s outlier score of the first session is plotted against the outlier score of the second session. Red dashed line: $Q3 + 3 \times IQR$. (d) The scatterplot of test-retest GSA change versus test-retest RSFC outlier score change in the HCP dataset. (e) The scatterplot of GSA versus RSFC outlier score in the HCP dataset (RSFC calculated using full correlations). (f) The scatterplot of GSA versus RSFC outlier score in the HCP dataset after excluding the sessions with large head motion (RSFC calculated using full correlations). (g) The scatterplot of GSA versus RSFC outlier score in the HCP dataset (RSFC calculated using partial correlations). (h) The scatterplot of GSA versus RSFC outlier score (RSFC calculated using full correlations after GSR).
Figure S4. Representative types of data collection/processing errors occurred in the outliers. (a) Outliers with head motion artifact in T2w FLAIR images. (b) An outlier with wrong FOV in dMRI images. Missing the inferior part of the brain in dMRI images (second row) resulted in anomalously large negative FA deviations (first row) in these missing regions. (c) Outliers with incorrect segmentation in structural images. (d) An outlier with incorrect nonlinear registration. The FA images after the registration were severely distorted (second row) and this resulted in widespread anomalously large negative FA deviations (first row). The MRI images in this figure are reproduced by kind permission of UK Biobank ©.
Figure S5. Additional examples for VV outliers. (a) Structural images showing radiological findings in VV outlier subjects of a mega cisterna magna, an infarct, intraventricular nodules, and partial agenesis of the corpus callosum. The subject shown in the first panel is from the HCP dataset. The structural images in the second, third, and fourth panels are reproduced by kind permission of UK Biobank ©. (b) Structural images of other VV outlier subjects interesting for follow-up. These three subjects are from a family in the HCP dataset. One twin had large ventricles of unknown etiology, but the other twin and their non-twin brother had normal VV.
Figure S6. Additional information on outlier detection using white matter-based imaging phenotypes. (a) Regional MD deviation maps (overlaid on T2w FLAIR images) of an example of an MD outlier subject (left column) and an example of a normal MD subject (right column). An MD deviation map visualizes how the MD values in a subject deviate from the autoencoder-predicted MD values. (b) Regional deviation maps (overlaid on FA or MD images) of other FA or MD outliers appeared normal to the neuroradiologist. The subjects shown in the second, third, and fourth panels are from the HCP dataset. The MRI images in (a) and the first panel of (b) are reproduced by kind permission of UK Biobank ©.
Figure S7. Additional information on the relationship between outlier scores of different imaging phenotypes. (a) Bootstrapping results for comparing the subject densities in Zone I, II, and III in Figure 7b. (b) Bootstrapping results for comparing the subject densities in Zone I, II, and III in Figure 7c. (c) Structural images showing radiological findings in two subjects who were outliers in more than one imaging phenotype. These images are reproduced by kind permission of UK Biobank ©.
Figure S8. Autoencoder-derived outlier scores were significantly correlated with the amounts of deviations from the group averages. The amount of individual deviations was measured by the correlation distance between each subject and the group average. (a) The scatterplot of FA outlier score versus the amount of FA deviation from group average. (b) The scatterplot of MD outlier score versus the amount of MD deviation from group average. (c) The scatterplot of CTh outlier score versus the amount of CTh deviation from group average.
Figure S9. Outlier scores versus image quality metrics. Each small panel shows a scatterplot between the outlier score of an imaging phenotype (vertical axis) versus an image quality metric of that imaging phenotype (horizontal axis), and the Pearson correlation between the two quantities is shown above each scatterplot. (a) VV. (b) WMLV. (c) FA. (d) MD. (e) CTh. FD: framewise displacement.
Figure S10. Generalizability of outlier detection to new UKB subjects. (a) The distribution fitting of VV outlier scores of the UKB discovery group (red curve) overlaid on the distribution fitting of VV outlier scores of the UKB replication group (blue curve). (b) The distribution fitting of WMLV outlier scores of the UKB discovery group (red curve) overlaid on the distribution fitting of WMLV outlier scores of the UKB replication group (blue curve). (c) The UKB discovery group subjects’ FA outlier scores (first two panels): The first panel shows the distribution fitting of the outlier scores calculated using the autoencoder trained on the discovery group itself (red curve) overlaid on the distribution fitting of the outlier scores calculated using the autoencoder trained on the replication group (blue curve). The scatterplot in the second panel shows these two sets of outlier scores plotted against each other. The UKB replication group subjects’ FA outlier
scores (last two panels): The third panel shows the distribution fitting of the outlier scores calculated using the autoencoder trained on the replication group itself (red curve) overlaid on the distribution fitting of the outlier scores calculated using the autoencoder trained on the discovery group (blue curve). The scatterplot in the fourth panel shows these two sets of outlier scores plotted against each other. (d) The UKB discovery group subjects’ MD outlier scores (first two panels): The first panel shows the distribution fitting of the outlier scores calculated using the autoencoder trained on the discovery group itself (red curve) overlaid on the distribution fitting of the outlier scores calculated using the autoencoder trained on the replication group (blue curve). The scatterplot in the second panel shows these two sets of outlier scores plotted against each other. The UKB replication group subjects’ MD outlier scores (last two panels): The third panel shows the distribution fitting of the outlier scores calculated using the autoencoder trained on the replication group itself (red curve) overlaid on the distribution fitting of the outlier scores calculated using the autoencoder trained on the discovery group (blue curve). The scatterplot in the fourth panel shows these two sets of outlier scores plotted against each other. (e) The UKB discovery group subjects’ CTh outlier scores (first two panels): The first panel shows the distribution fitting of the outlier scores calculated using the autoencoder trained on the discovery group itself (red curve) overlaid on the distribution fitting of the outlier scores calculated using the autoencoder trained on the replication group (blue curve). The scatterplot in the second panel shows these two sets of outlier scores plotted against each other. The UKB replication group subjects’ CTh outlier scores (last two panels): The third panel shows the distribution fitting of the outlier scores calculated using the autoencoder trained on the replication group itself (red curve) overlaid on the distribution fitting of the outlier scores calculated using the autoencoder trained on the discovery group (blue curve). The scatterplot in the fourth panel shows these two sets of outlier scores plotted against each other.
Figure S11. Impact on outlier scores when processing the data using a different neuroimaging data processing software tool. In addition to the outlier detection results derived from the main pipeline outputs, the data were also processed using an additional pipeline for each imaging phenotype and outlier detection was performed on this additional set of preprocessed data. Each scatterplot shows these two sets of outlier scores plotted against each other in that imaging phenotype, and the Pearson correlation between the two sets of outlier scores is shown above each scatterplot. (a) VV. (b) WMLV. (c) FA. (d) MD. (e) CTh.
Figure S12. Impact on outlier scores when processing the CTh data using a different parcellation atlas. In addition to the CTh outlier detection results based on the HCP-MMP atlas, outlier detection was also performed on the CTh data parcellated using the Brainnetome atlas (Fan et al., 2016). This scatterplot shows these two sets of outlier scores plotted against each other.
Table S1. Summary of the demographic information of the main dataset.

| Type  | Initial number of subjects | Number of exclusions by automatic quality control | Final sample size | Gender | Age | mean ± SD |
|-------|-----------------------------|--------------------------------------------------|-------------------|--------|-----|-----------|
|       |                             |                                                  |                   |        |     |           |
| T1w   | 19406                       | 330                                              | 19076             | 40-49  | 776 | 62.4 ± 7.5|
|       |                             |                                                  |                   | 50-59  | 5999|           |
|       |                             |                                                  |                   | 60-69  | 8622|           |
|       |                             |                                                  |                   | 70-79  | 3676|           |
|       |                             |                                                  |                   | 80-89  | 3   |           |
|       |                             |                                                  |                   | mean   |     |           |
|       |                             |                                                  |                   | ± SD   |     |           |
| T2w FLAIR | 18462                       | 296                                              | 18166             | 40-49  | 710  | 62.4 ± 7.4|
|       |                             |                                                  |                   | 50-59  | 5728 |           |
|       |                             |                                                  |                   | 60-69  | 8224 |           |
|       |                             |                                                  |                   | 70-79  | 3501 |           |
|       |                             |                                                  |                   | 80-89  | 3   |           |
| dMRI  | 17942                       | 2510                                             | 15432             | 40-49  | 619  | 62.3 ± 7.4|
|       |                             |                                                  |                   | 50-59  | 4983 |           |
|       |                             |                                                  |                   | 60-69  | 7001 |           |
|       |                             |                                                  |                   | 70-79  | 2827 |           |
|       |                             |                                                  |                   | 80-89  | 2   |           |
| rsfMRI| 17218                       | 2052                                             | 15166             | 40-49  | 610  | 62.3 ± 7.4|
|       |                             |                                                  |                   | 50-59  | 4925 |           |
|       |                             |                                                  |                   | 60-69  | 6837 |           |
|       |                             |                                                  |                   | 70-79  | 2791 |           |
|       |                             |                                                  |                   | 80-89  | 3   |           |
Table S2. Twenty-seven white matter ROIs from the Johns Hopkins University white matter atlas (Mori et al., 2008) were used in the outlier detection of FA and MD.

| ROI name                                      |
|----------------------------------------------|
| Genu of corpus callosum                      |
| Body of corpus callosum                      |
| Splenium of corpus callosum                  |
| Right cerebral peduncle                      |
| Left cerebral peduncle                       |
| Right anterior limb of internal capsule      |
| Left anterior limb of internal capsule       |
| Right posterior limb of internal capsule     |
| Left posterior limb of internal capsule      |
| Right retrolenticular part of internal capsule |
| Left retrolenticular part of internal capsule |
| Right anterior corona radiata                |
| Left anterior corona radiata                 |
| Right superior corona radiata                |
| Left superior corona radiata                 |
| Right posterior corona radiata               |
| Left posterior corona radiata                |
| Right posterior thalamic radiation (include optic radiation) |
| Left posterior thalamic radiation (include optic radiation) |
| Right sagittal stratum (include inferior longitudinal fasciculus and inferior fronto-occipital fasciculus) |
| Left sagittal stratum (include inferior longitudinal fasciculus and inferior fronto-occipital fasciculus) |
| Right external capsule                       |
| Left external capsule                        |
| Right cingulum (cingulate gyrus)             |
| Left cingulum (cingulate gyrus)              |
| Right superior longitudinal fasciculus       |
| Left superior longitudinal fasciculus        |
Table S3. Summary of the demographic information of the UKB replication group used in this study.

| Type   | Initial number of subjects | Number of exclusions by automatic quality control | Final sample after the exclusions (UKB replication group) | Gender | Age | mean ± SD |
|--------|---------------------------|-------------------------------------------------|--------------------------------------------------------|--------|-----|-----------|
|        |                           |                                                 | Final sample size                                      | M      | F   | 40-49     | 50-59 | 60-69 | 70-79 | 80-89 |         |
|        |                           |                                                 |                                                        |        |     |           |       |       |       |       |          |
| T1w    | 19349                     | 166                                             | 19183                                                 | 8907   | 10276 | 104       | 5147  | 8111  | 5704  | 117   | 64.7 ± 7.4 |
| T2w FLAIR | 19349                     | 166                                             | 19183                                                 | 8907   | 10276 | 104       | 5147  | 8111  | 5704  | 117   | 64.7 ± 7.4 |
| dMRI   | 19349                     | 2295                                            | 17054                                                 | 7619   | 9435  | 96        | 4626  | 7272  | 4961  | 99    | 64.6 ± 7.4 |
Table S4. Summary of outlier detection and screening in the HCP dataset.

| Phenotype      | VV   | FA   | MD   | CTh  |
|----------------|------|------|------|------|
| Initial number of Subjects | 1113 | 1065 | 1065 | 1094 |
| Number of exclusions by automatic quality control | 0    | 85   | 85   | 82   |
| Final sample size | 1113 | 980  | 980  | 1012 |
| Skewness       | 1.50 | 0.97 | 0.64 | 0.38 |
| Kurtosis       | 6.64 | 4.63 | 3.72 | 3.74 |
| Number of outliers | 8   | 2    | 1    | 1    |
| (0.7%)         | (0.2%)| (0.1%)| (0.1%)|
| Outliers w/o data issue | 8   | 2    | 1    | 1    |
| Outliers read by neuroradiologist | 8   | 2    | 1    | 1    |
| Radiological comments |     |      |      |      |
| Normal         | 2    | 1    | 1    |      |
| Large ventricles | 8    |      |      |      |
| White matter lesions |      |      |      |      |
| Mass           |      |      |      |      |
| Cyst           |      |      |      |      |
| Infarct        |      |      |      |      |
| Encephalomalacia |    |      |      |      |
| Prominent sulci |    |      |      |      |
| Other findings | 2    |      |      |      |

Note: Empty entries are zeros.
Table S5. Comparison of outliers derived using two different neuroimaging data processing software.

| Imaging phenotype | VV  | WMLV | FA  | MD  | CTh |
|-------------------|-----|------|-----|-----|-----|
| Dice similarity coefficient | 0.83 | 0.65 | 0.71 | 0.71 | 0.13 |
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