***eLife’s* transparent reporting form**

We encourage authors to provide detailed information *within their submission* to facilitate the interpretation and replication of experiments. Authors can upload supporting documentation to indicate the use of appropriate reporting guidelines for health-related research (see [EQUATOR Network](http://www.equator-network.org/%20)), life science research (see the [BioSharing Information Resource](https://biosharing.org/)), or the [ARRIVE guidelines](http://www.plosbiology.org/article/info:doi/10.1371/journal.pbio.1000412) for reporting work involving animal research. Where applicable, authors should refer to any relevant reporting standards documents in this form.

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**Sample-size estimation**

* You should state whether an appropriate sample size was computed when the study was being designed
* You should state the statistical method of sample size computation and any required assumptions
* If no explicit power analysis was used, you should describe how you decided what sample (replicate) size (number) to use

Please outline where this information can be found within the submission (e.g., sections or figure legends), or explain why this information doesn’t apply to your submission:

Explicit power analysis is not applicable for the model construction, since the methods proposed novel approach. Recent study on predictive modeling of a single specific task performance using fMRI connectivity has reported comparable sample size (N = 14 in Baldassarre et al., 2012, PNAS; N = 25 in Rosenberg et al., 2016, Nat Neurosci).

For the generalization tests using independently collected cohorts, we used the largest sample size for each group (N = 474, 118, 140, 96, and 140) available when the analysis was performed. These sample sizes were also comparable to or even larger than recent generalization test analysis (N = 112 in Rosenberg et al., 2016, Nat Neurosci).

**Replicates**

* You should report how often each experiment was performed
* You should include a definition of biological versus technical replication
* The data obtained should be provided and sufficient information should be provided to indicate the number of independent biological and/or technical replicates
* If you encountered any outliers, you should describe how these were handled
* Criteria for exclusion/inclusion of data should be clearly stated
* High-throughput sequence data should be uploaded before submission, with a private link for reviewers provided (these are available from both GEO and ArrayExpress)

Please outline where this information can be found within the submission (e.g., sections or figure legends), or explain why this information doesn’t apply to your submission:

The current study shows generalizability of a prediction model to independently collected cohorts beyond large variation, such as psychiatric diagnoses. For each dataset, inclusion/exclusion criteria are explicitly described in Materials and Methods. Outliers identified in Multiple Psychiatric Diagnoses Dataset were removed from analysis as described in Materials and Methods.

**Statistical reporting**

* Statistical analysis methods should be described and justified
* Raw data should be presented in figures whenever informative to do so (typically when N per group is less than 10)
* For each experiment, you should identify the statistical tests used, exact values of N, definitions of center, methods of multiple test correction, and dispersion and precision measures (e.g., mean, median, SD, SEM, confidence intervals; and, for the major substantive results, a measure of effect size (e.g., Pearson's r, Cohen's d)
* Report exact p-values wherever possible alongside the summary statistics and 95% confidence intervals. These should be reported for all key questions and not only when the p-value is less than 0.05.

Please outline where this information can be found within the submission (e.g., sections or figure legends), or explain why this information doesn’t apply to your submission:

Throughout the results, we have justified and described the statistical tests used. Exact values of N, definitions of center, methods of multiple test correction, and dispersion and precision measures, and effect size are reported in results and figure legends. Exact p-values and 95% confidence intervals are reported.

(For large datasets, or papers with a very large number of statistical tests, you may upload a single table file with tests, Ns, etc., with reference to sections in the manuscript.)

**Group allocation**

* Indicate how samples were allocated into experimental groups (in the case of clinical studies, please specify allocation to treatment method); if randomization was used, please also state if restricted randomization was applied
* Indicate if masking was used during group allocation, data collection and/or data analysis

Please outline where this information can be found within the submission (e.g., sections or figure legends), or explain why this information doesn’t apply to your submission:

Group allocation was applied in Multiple Psychiatric Diagnoses Datasets. Their group (healthy/typically developed vs patients) was based on the psychiatric diagnosis performed by the psychiatrists.

**Additional data files (“source data”)**

* We encourage you to upload relevant additional data files, such as numerical data that are represented as a graph in a figure, or as a summary table
* Where provided, these should be in the most useful format, and they can be uploaded as “Source data” files linked to a main figure or table
* Include model definition files including the full list of parameters used
* Include code used for data analysis (e.g., R, MatLab)
* Avoid stating that data files are “available upon request”

Please indicate the figures or tables for which source data files have been provided:

The ATR dataset, Multiple Psychiatric Diagnoses Dataset, and MATLAB Code used for data analysis is available from our institute website (<https://bicr.atr.jp/dcn/en/download/database-wmp/>). HCP dataset is available from ConnectomeDB (<https://db.humanconnectome.org)>.