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Corresponding author(s): Tatia M.C. Lee

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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	No software was used to collect the data. The behavioral data were collected through pencil- and-paper approach and the imaging data were collected using a 3T GE scanner with an eight-channel head coil.
Data analysis	The sampling strategy was conducted using G*Power 3.1.9.7 for power analysis. Behavioral data were analysed using the SPSS v.26. The resting-state functional imaging data were preprocessed using SPM 12 and DPABI 3.1. The diffusion tensor images were preprocessed using FSL 6.0. Diffusion tensor models were estimated using Diffusion Toolkit 0.6.4. Whole-brain fibre tracking was performed using TackVis 0.6.1. The connectome-based predictive modelling analysis was performed using MATLAB (MathWorks, 2017b), in which the code can be found at https://github.com/MengxiaGAO/Neuroimage2020. The connectivity figures were generated using gggraph (https://cran.r-project.org/web/packages/ggraph/index.html) on Rstudio 2022.02.1. The support vector machine classification was performed using the scikit-learn 0.32.2 package in Python 3.6.2. The MATLAB scripts for CPM analysis are available at https://github.com/YaleMRRC/CPM and https://github.com/MengxiaGAO/Neuroimage2020. The parameters of the CPM models are available at https://github.com/MengxiaGAO/LLD_suicide. Code for SVM analysis is available at https://scikit-learn.org/stable/modules/svm.html. The other custom codes for this study are available at https://github.com/MengxiaGAO/LLD_suicide.

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 Shen 268-node functional brain atlas is available at https://www.nitrc.org/frs/?group_id=51. The AAL-116 atlas is available at http://rfmri.org/dpabi (in the Templates folder). The minimum anonymized data that support the findings of this study are available upon reasonable request from the corresponding authors. The participants did not consent to the sharing of the raw data to the public. Source data are provided with this study.

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

Behavioural & social sciences study design

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

Study description	This study is a quantitative cross-sectional study.
Research sample	The research sample included 91 older adults (74 females, mean age = 66.39 years, SDage = 5.45, all Chinese; 17 males, mean age = 67.71 years, SDage = 6.70, all Chinese), who were diagnosed with major depressive disorder by certified psychiatrists using the DSM-5 criteria. None of the participants had been diagnosed with other comorbid major psychiatric disorders (e.g., bipolar disorder, psychotic disorders or substance-related disorder) or any major physical or neurological illness that considerably impaired their daily functioning. All of the participants were using medication at the time of the study. The patients were recruited in Taiwan. The research sample is representative. As depression is a major risk factor of suicide and suicidal actions are more lethal in older adults, people with late-life depression are at high risk of suicide and were chosen to be the study sample. Dataset 1 from Zhang et al. (2020) comprises rs- fMRI and DTI data from 44 middle-aged MDD patients (26 females, mean age = 30.12 years, SDage = 8.10, all Chinese; 18 males, mean age = 31.06 years, SDage = 9.91, all Chinese). Dataset 2 from Shao et al. (2021) comprises data from 24 middle-aged MDD patients (19 females, mean age = 51.16 years, SDage = 5.30, all Chinese; 5 males, mean age = 52.20 years, SDage = 5.19, all Chinese). Participants from two datasets provided written informed consent.
Sampling strategy	The sampling procedure was based on random and convenience. We recruited the patients from advertisement and bulletin in the hospital with specific inclusion and exclusion criteria on the poster. For the sample size, a post-hoc power analysis using G*Power 3.1.9.7 was conducted. For the CPM analysis using correlation between the predicted and observed values, we found that a sample size of N=91 and correlation coefficients = 0.3 can achieve a statistical power of 0.83 and a sample size of N=92 and correlation = 0.4 can achieve a statistical power of 0.98. Our sample size N=91 with the correlation coefficients from 0.3 to 0.6 obtained from the CPM models could achieve a statistical power from 0.83 to 0.98. The prediction performance (correlation coefficients) was similar to previously reported findings of studies that applied the CPM method on the resting-state fMRI data to predict behaviors [e.g. cognitive impairment in older adults (Lin et al., 2018), symptom improvement in patients with major depressive disorder (Ju et al., 2020), processing speed in older adults (Gao et al., 2020), and social abilities in clinical samples (Lake et al., 2019)]. For the group-comparison analysis, to achieve a large effect size of f=0.4 and a power of 0.92, the total sample size for the three groups estimated by G*Power was N=90. Our sample size was also comparable to recent studies that investigated suicidal behaviors in depressed patients using brain imaging (Cao et al., 2020; Cao et al., 2016; Dai et al., 2020; Du et al., 2017; Myung et al., 2016). In conclusion, our sample size fulfilled the requirement to achieve a relatively high effect size and statistical power. Cao, J., Ai, M., Chen, X., Chen, J., Wang, W., & Kuang, L. (2020). Altered resting-state functional network connectivity is associated with suicide attempt in young depressed patients. Psychiatry Research, 285, 112713. Cao, J., Chen, X., Chen, J., Ai, M., Gan, Y., Wang, W., Lv, Z., Zhang, S., Zhang, S., & Wang, S. (2016). Resting-state functional MRI of abnormal baseline brain activity in young depressed patients with and without suicidal behavior. Journal of Affective Disorders, 205, 252-263. Dai, Z., Shen, X., Tian, S., Yan, R., Wang, H., Wang, X., Yao, Z., & Lu, Q. (2020). Gradually evaluating of suicidal risk in depression by semi-supervised cluster analysis on resting-state fMRI. Brain Imaging and Behavior, 1-10. Du, L., Zeng, J., Liu, H., Tang, D., Meng, H., Li, Y., & Fu, Y. (2017). Fronto-limbic disconnection in depressed patients with suicidal ideation: a resting-state functional connectivity study. Journal of Affective Disorders, 215, 213-217. Gao, M., Wong, C. H., Huang, H., Shao, R., Huang, R., Chan, C. C., & Lee, T. M. (2020). Connectome-based models can predict processing speed in older adults. NeuroImage, 223, 117290. Ju, Y., Horien, C., Chen, W., Guo, W., Lu, X., Sun, J., Dong, Q., Liu, B., Liu, J., & Yan, D. (2020). Connectome-based models can predict early symptom improvement in major depressive disorder. Journal of Affective Disorders, 273, 442-452. Lake, E. M., Finn, E. S., Noble, S. M., Vanderwal, T., Shen, X., Rosenberg, M. D., Spann, M. N., Chun, M. M., Scheinost, D., & Constable, R. T. (2019). The functional brain organization of an individual allows prediction of measures of social abilities transdiagnostically in autism and attention-deficit/hyperactivity disorder. Biological Psychiatry, 86(4), 315-326.

Lin, Q., Rosenberg, M. D., Yoo, K., Hsu, T. W., O'Connell, T. P., & Chun, M. M. (2018). Resting-state functional connectivity predicts cognitive impairment related to alzheimer's disease. Frontiers in Aging Neuroscience, 10, 94.
Myung, W., Han, C., Fava, M., Mischoulon, D., Papakostas, G., Heo, J., Kim, K., Kim, S., Kim, D., & Kim, D. (2016). Reduced frontal-subcortical white matter connectivity in association with suicidal ideation in major depressive disorder. Translational Psychiatry, 6(6), e835-e835.

Data collection

Pen and paper were used to record the behavioral data, and the imaging data were collected using a 3T GE scanner with an eight-channel head coil. The researcher was present besides the participants while they were completing the behavioral assessments. The researcher was blind to the study hypothesis during data collection.

Timing

The sample was collected from October 2017 to July 2019.

Data exclusions

Participants were excluded due to the following criteria: 1) low scores (< 23) on the Mini-Mental State Examination (MMSE) indicating potential cognitive impairment (Tsai et al., 2012) (three participants); 2) missing resting-state fMRI, structural MRI or DTI image data due to technical issues (three participants); 3) missing behavioral score data (14 participants); and 4) excessive head motion: absolute head motion > 2 mm translation, > 2° rotation or mean frame-wise displacement (FD) > 0.3 mm (five participants). The exclusion criteria were pre-established.

Non-participation

No participants dropped out of the study.

Randomization

The participants were not allocated into experimental groups before or during the study. They were assigned to different groups in data analysis after completing the study. The participants were classified into three groups based on their suicide-related information collected during the clinical interviews: 37 patients without suicidal ideation, plans or attempts (NS); 24 patients with past and/or present suicidal ideation and/or plans (IP); and 30 patients with previous suicidal attempts (SA). Patients who had never thought of suicide or attempted suicide in their lifetime were in the NS group. Patients who had seriously thought about attempting suicide, and/or planned for suicide in their lifetime but without past history of suicide attempts were in the IP group. Patients who had ever attempted suicide in their lifetime were in the SA group. We further classified the patients in the IP group into two subgroups based on their scores on Item 3 of HAMD-17, which assessed whether the patients had suicide ideation/plan or attempts within the past week. Patients who scored >= 1 on Item 3 were considered as having current ideation. There were 10 patients with both current and past ideation (CPI group), and 14 patients with only past ideation (PI group). The allocation was not random because our study was an observational study and the participants did not receive any intervention. For group comparisons analysis, results were unchanged after controlling for sex, age, education, MMSE, HAMD/A, onset time of LLD, number of episodes of LLD, duration of LLD, the five types of medications, number of medication types, medication load, or mean FD.

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
☐	☒ Human research participants
☒	☐ Clinical data
☒	☐ Dual use research of concern

Methods

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

Human research participants

Policy information about studies involving human research participants

Population characteristics

See above

Recruitment

We recruited 116 older adults (aged 60–79 years old) diagnosed with major depressive disorder by two board-certified geriatric psychiatrists (C. Lin and S. Lee) through diagnostic interviews based on the DSM-5 criteria. Patients were recruited from psychiatric in- or out-patient services. During the interview, the Mini-International Neuropsychiatric Interview (M.I.N.I.) was carried out to evaluate the disease and suicide-related history and information.

We recruited the patients from advertisement and bulletin in the hospital with specific inclusion and exclusion criteria on the poster. We excluded patients who had severe underlying medical comorbidities, including renal failure, liver cirrhosis, heart failure, anemia, or chronic obstructive pulmonary disease, thyroid dysfunction, major neurological disorder or having malignancy. We acknowledge that our study has not considered patients who had suicide risk due to comorbidities and our results could not be generalized to this population before being validated. We have now added this point as a limitation: "Furthermore, we excluded patients with comorbid psychiatric disorders (other than GAD) or major medical illnesses to study a relatively homogenous sample. Importantly, patients with comorbidities had a higher suicide risk than those without comorbidities (Blasco-Fontecilla et al., 2016). Future studies are encouraged to verify the effect of comorbidities on suicide

	risk. Meanwhile, cautions must be taken when interpreting the generalizability of our results to clinical groups different from the current sample."
Ethics oversight	This study was approved by the Institutional Review Board of Chang Gung Memorial Hospital of Taiwan.

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

Magnetic resonance imaging

Experimental design

Design type	Resting-state design.
Design specifications	No experimental design was used.
Behavioral performance measures	No behavioral performance was recorded in the scanner.

Acquisition

Imaging type(s)	Functional resting-state fMRI images, T1-weighted structural images and diffusion tensor images.
Field strength	3T
Sequence & imaging parameters	We acquired MRI data using a 3T GE scanner with an eight-channel head coil. Resting-state fMRI images were acquired while the participants stayed awake but with their eyes closed. A total of 180 volumes were acquired using the following parameters: TR = 2,000 ms, TE = 30 ms, flip angle = 90°, field of view (FOV) = 220 × 220 × 144 mm3 and voxel size = 3.44 × 3.44 × 4 mm3. A total of 160 sagittal slices of the high-resolution T1-weighted structural images were acquired using the following parameters: TR = 8.2 ms, TE = 3.2 ms, flip angle = 12°, FOV = 250 × 250 × 160 mm3 and voxel size = 0.98 × 0.98 × 1 mm3. The DTI data were acquired in 32 diffusion-gradient directions (b = 1,000) with two non-diffusion-weighted (b = 0) references using the following parameters: TR = 7,500 ms, TE = 82.6 ms, flip angle = 90°, FOV = 220 × 220 × 136 mm3 and voxel size = 1.7 × 1.7 × 2.2 mm3.
Area of acquisition	A whole-brain scan was used.

Diffusion MRI ☒ Used ☐ Not used

Parameters	The DTI data were acquired in 32 diffusion-gradient directions (b = 1,000) with two non-diffusion-weighted (b = 0) references, single shell.

Preprocessing

Preprocessing software	The resting-state functional imaging data were preprocessed using SPM 12 (https://www.fil.ion.ucl.ac.uk/spm/) and DPABI 3.1 with the following procedures: 1) The first five volumes were deleted, followed by 2) slice-timing correction and 3) head motion correction. Then, 4) nuisance variables were regressed (Friston 24-motion parameters, white matter, cerebral-spinal fluid signals and global signals) with volumes with a mean frame-wise displacement (FD) > 0.5 mm. The volume prior to these volumes and the two volumes after these volumes were all added as covariates, as suggested by Power et al. (2013). Afterward, we conducted 5) spatial smoothing using a Gaussian kernel of 6 mm full width at half maximum (FWHM) and 6) band-pass temporal filtering using a 0.01–0.1 Hz frequency bandwidth. For each participant, DTI images were corrected for eddy current distortions and head motions using FMRIB's Diffusion Toolbox (FSL 6.0; http://www.fmrib.ox.ac.uk/fsl).
Normalization	The co-registered T1 images were normalized to standardized space using linear interpolation. The inverse deformation matrices generated from the previous step were used to transform the brain atlases from standardized space to individual space.
Normalization template	The template ICBM152 was used for normalization, which is defined as the group standardized space.
Noise and artifact removal	Nuisance variables including Friston 24-motion parameters, white matter, cerebral-spinal fluid signals and global signals were regressed out from the functional fMRI images.
Volume censoring	DPASRSF 4.4 Advanced Edition in the DPABI 3.1 was used for volume censoring. Volumes with a mean frame-wise displacement (FD) > 0.5 mm and the volume prior to these volumes and the two volumes after these volumes were all added as covariates, as suggested by Power et al. (2013).

Statistical modeling & inference

Model type and settings	This study did not use traditional modelling methods that include first and second levels. The connectome-based predictive modelling (CPM) method and leave-one-out cross-validation (LOOCV) were used, which were described in the Models & analysis section.
Effect(s) tested	This study is a resting-state design therefore no ANOVA or factorial design were used for the imaging analysis.

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

Statistic type for inference (See Eklund et al. 2016)	We used whole-brain analysis and defined ROIs based on previous studies. Permutation analysis was used to define the significance of the predictive models.
Correction	FDR correction was used to correct the number of comparisons when necessary.

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	Pearson correlation was used to calculate the functional connectivity between brain regions, and the functional connectivity matrices were z-transformed.
Multivariate modeling and predictive analysis	The connectome-based predictive modelling (CPM) method and leave-one-out cross-validation (LOOCV) were used. Independent variables were functional connectivity and structural connectivity. For each set of n-1 participants, we selected edges that were significantly positively and negatively correlated with their behavioral scores, controlling for age, sex and education. The selected edges were summed into two scores, namely positive network strength and negative network strength. The two scores were then fitted into two linear-regression models and coefficients were generated. The positive and negative network strength of the left-out participant were entered into the predictive models and predicted scores were generated using the coefficients. The prediction performance was assessed further using the coefficient of determination between the predicted values and the observed values. For model-significance testing, we randomized the observed behavioral variables and performed identical CPM analysis using the new generated scores for 5,000 times.