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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 Data used was previously collected in prior studies indicated below.

Data analysis Preprocessing, All resting-state fMRI images were preprocessed by the DPARSF toolkit (<http://rfmri.org/DPARSF>). The MRI data processing was performed with Computational Anatomy Toolbox, CAT12 (<http://www.neuro.uni-jena.de/cat/>) and Statistical Parametric Mapping 12 (<https://www.fil.ion.ucl.ac.uk/spm/software/spm12/>). The meta-analytic decoding based on Neurosynth. All the above toolboxes/tools were implemented in MATLAB 2020a. NDM computations were conducted in Python 3.7.10 (Anaconda Distribution) with the following key dependencies: NumPy 1.21.0 (matrix operations), SciPy 1.7.0 (statistical functions), and Nilearn 0.8.0 (neuroimaging data I/O).

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 data that support the findings of this study are publicly available. The neuroimaging datasets are available from the Autism Brain Imaging Data Exchange I (ABIDE I) and Autism Brain Imaging Data Exchange II (ABIDE II) (http://fcon_1000.projects.nitrc.org/indi/abide/). Users must register with the NITRC and 1000 Functional Connectomes Project to gain access to ABIDE I and ABIDE II.

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

This project included both male and female participants, and the gender was determined based on self-report. In this project we did not perform specific gender-based analysis because our main aim was to identify atypical morphological development in autism spectrum disorder.

Reporting on race, ethnicity, or other socially relevant groupings

The project did not collect information about race and ethnicity from the participants.

Population characteristics

The ABIDE I and ABIDE II datasets contain 1,031 ASD subjects and 1,139 typically developing controls. Following the study exclusion criteria there were ASD (N=301, aged 12.82±2.70 years; 49 females) and typically developing controls (N=375, aged 12.45±2.73 years; 63 females).

Recruitment

This study was performed on existing datasets (ABIDE I and ABIDE II) and did not include any further recruitment of subjects.

Ethics oversight

This study was performed on existing datasets (ABIDE I and ABIDE II) and study protocols for the scanning sites can be found in the data repositories.

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](https://www.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

No sample size calculation was performed. Sample size was based on the number of subjects collected in the existing data sets.

Data exclusions

(1) all participants were under 18 years of age;
(2) all participants underwent both resting-state functional magnetic resonance imaging (rs-fMRI) and T1-weighted structural brain imaging;
(3) participants exhibited minimal head motion (maximum translation < 2 mm and rotation < 2°, with less than 50% of frames showing high mean framewise displacement);
(4) participants had complete cortical coverage during scanning;
(5) for the ASD and typically developing children (TDC) group, an additional criterion required at least 20 participants in each one-year age interval to ensure representative age distribution and adequate statistical power.

Replication

More details are described in detail in the Methods (see sections 'Statistics and Reproducibility', and 'Null models', and). To validate the robustness reproducibility of our findings, we repeated the analyses using brain parcellation templates comprising 200 and 400 regions, and by restricting the dataset to a single large site (New York University, NYU) and to male-only participants.

Randomization

The authors conducted analysis of an existing dataset, so subject randomization was not applicable.

Blinding

The authors conducted analysis of an existing dataset, so blinding was not applicable.

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, mosaicism, off-target gene editing) were examined.

Magnetic resonance imaging

Experimental design

Design type	Resting-fMRI and T1-weighted structural
Design specifications	All details for the 41 different scan sites can be found at the public dataset repository: http://fcon_1000.projects.nitrc.org/indi/abide/ .
Behavioral performance measures	None.

Acquisition

Imaging type(s)	Functional and Structural
Field strength	3T for all subjects
Sequence & imaging parameters	All details for the 41 different scan sites can be found at the public dataset repository: http://fcon_1000.projects.nitrc.org/indi/abide/ .
Area of acquisition	Whole-brain scan was used for all subjects.
Diffusion MRI	☐ Used ☒ Not used

Preprocessing

Preprocessing software	SPM12 Cat 12
Normalization	Nonlinear deformation based on anatomical data
Normalization template	3 mm MNI atlas template (group standardized space)
Noise and artifact removal	Denoising steps included linear de-trending and nuisance regression (5 principle components from eroded white matter and

Noise and artifact removal	cerebrospinal fluid masks from the aforementioned tissue segmentation; 6 motion parameters and first-order temporal derivatives; and pointregressors to censor time points with mean frame-wise displacement > 0.2 mm). Residual time-series were band-pass filtered ($0.01 \text{ Hz} < f < 0.08 \text{ Hz}$) after regression to avoid reintroduction of nuisance-related variation in the time-series.
Volume censoring	Temporal masks were created to flag motion-contaminated frames for scrubbing. High-motion volumes were identified by framewise displacement (FD) calculated as the sum of absolute values of the differentials of the three translational motion parameters and three rotational motion parameters. Motion was censored with a 0.2 mm threshold and volumes preceding high motion were also censored. More detail is provided in the Methods.

Statistical modeling & inference

Model type and settings	Group differences in age were analyzed using an independent two-sample t-test for demographic data, while chi-square test was applied to assess differences in sex. For the NDM (Network Diffusion Model) fitting procedure, we employed non-parametric permutation testing to evaluate statistical significance.
Effect(s) tested	Spatial permutation test ("spin test") to determine whether the observed correlation was specific to the actual DEV pattern rather than being influenced by the spatial autocorrelation of DEV described fully in the Methods section.
Specify type of analysis:	☐ Whole brain ☒ ROI-based ☐ Both
Anatomical location(s)	The fMRI volumes were registered to the MNI template and partitioned into 246 nodes regions of interest (ROIs) based on the Brainnetome Atlas.
Statistic type for inference (See Eklund et al. 2016)	All variables were carefully examined for outliers, data entry errors, and missing values. Group differences in age were analyzed using an independent two-sample t-test for demographic data, while chi-square test was applied to assess differences in sex. Pearson correlation coefficients were calculated to examine the relationships between DEV and FC edges. Statistical significance was set at $p < 0.05$, and all tests were two-tailed unless otherwise specified.
Correction	We evaluated a null model using a spatial permutation test ("spin test") to determine whether the observed correlation was specific to the actual DEV pattern rather than being influenced by the spatial autocorrelation of DEV.

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 correlations between regional BOLD time series were used to represent functional connectivity.
Multivariate modeling and predictive analysis	We used two multivariate models in this study. 1. we proposed a DEV method that integrates the expected value (see Supplementary Figure S2) and KL divergence to quantify developmental changes in brain regions. 2. We used the NDM to investigate whether the DEV of atypical developmental brain regions spreads throughout the brain via a diffusion process. NDM simulates the dynamic propagation of pathology across nodes in a weighted network through a diffusion process (see Fig. S1).