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Original contribution

A unified framework for mapping individual interregional high-order morphological connectivity based on regional cortical features from anatomical MRI

Xun-Heng Wang[a,*], Yun Jiao[b], Lihua Li[a,*]

[a] Institute of Biomedical Engineering and Instrumentation, School of Automation, Hangzhou Dianzi University, Hangzhou 310018, China
[b] Jiangsu Key Laboratory of Molecular and Functional Imaging, Department of Radiology, Zhongda Hospital, Medical School of Southeast University, Nanjing 210009, China

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ABSTRACT

Building individual brain networks form the single volume of anatomical MRI is a challenging task. Furthermore, the high-order connectivity of morphological networks remains unexplored. This paper aimed to investigate the individual high-order morphological connectivity from anatomical MRI. Towards this goal, a unified framework based on six feature distances (euclidean, seuclidean, mahalanobis, cityblock, minkowski, and chebychev) was proposed to derive high-order interregional morphological features. The test-retest datasets and the healthy aging datasets were applied to analyze the reliability and the inter-subject variability of the novel features. In addition, the predictive models based on these novel features were established for age estimation. The proposed six neuroanatomical features exhibited significant high-to-excellent reliability. Certain connections were significantly correlated to biological age based on the six novel metrics ($p < .05$, FDR corrected). Moreover, the predicted age were significantly correlated to the original age in each regression task ($r > 0.5, p < 10^{-6}$). The results suggested that the novel high-order metrics were reliable and could reflect individual differences, which could be beneficial for current methods of individual brain connectomes.

1. Introduction

Morphological features from anatomical MRI have been widely applied in the brain science [1,2]. The morphological features could be potential biomarkers for brain maturation, cognitive performances, and brain disorders [3–5]. The conventional morphological features were univariate estimators that only reflect the voxel-wise, vertex-wise, or regional anatomical measures rather than brain networks. Of note, the human brain is a complex network that should be represented by neural connectivity between brain regions [6]. There were three kinds of brain networks (i.e., structural network, functional network and morphological network) that constructed from the diffusion MRI, resting state fMRI, and anatomical MRI [7–9]. The diffusion MRI is a non-invasive method that mapping the microstructure of water movements in the neurons [10]. The structural network can be modeled by tracking the neural fibers between the brain regions. The resting state fMRI is a common neuroimaging technique that probe the BOLD signals in the brain [11]. The functional network can be constructed using correlations between brain regions in grey matter. Complex and controversial processing steps were involved in diffusion MRI and resting state fMRI, because of the low signal-to-noise ratio (SNR) in these images [12,13]. The anatomical MRI which exhibited relatively higher SNR and higher test-retest reliability has been applied to investigate the brain topology [7,14]. Although the group-wise anatomical brain networks have been investigated using co-variance graphs, the individual morphological brain networks based on anatomical MRI remain largely unexplored.

Individual morphological connectivity has drawn significantly research interests in the field of brain connectome [15–17]. Building individual morphological connectivity from anatomical MRI was quite challenging, since only one 3-D volume of anatomical MRI was obtained for each subject. Different from the 4-D volumes of diffusion MRI or resting state fMRI, the 3-D volume contained limited information for the edge definitions in the individual brain networks. To solve this problem, several novel methods were applied for feature extraction of individual morphological connectivity in regional and voxel levels [15,17]. The complex brain networks based on the interregional morphological connectivity exhibited small-worldness properties and good test-retest reliability [16,18]. The node strengths of voxel-wise

* Corresponding authors.
E-mail addresses: xhwang@hdu.edu.cn (X.-H. Wang), lilh@hdu.edu.cn (L. Li).

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morphological network were also reliable and could reflect individual differences [15]. Moreover, the morphological connectivity exhibited discriminative power for brain disorder diagnosis [19,20]. Most of these methods were based on single modality of features (i.e., volume, or thickness). As far as we known, quite a few of current studies focused on building individual morphological network from multi-modality of cortical features. Furthermore, the above methods were designed for low-order morphological connectivity that indicated the pairwise relationships between brain regions. The high-order morphological connectivity and its reliability as well as variability remains largely unknown to date.

This paper aimed to provide a unified framework for feature extraction of individual high-order morphological connectivity from single volume of anatomical MRI and analyze the reliability as well as the variability. To this end, a cohort of subjects with test-retest anatomical MRI datasets and a cohort of subjects with normal aging anatomical MRI datasets were obtained from the NITRC websites. The raw datasets were preprocessed with Freesurfer to obtain regional morphological features (i.e., cortical thickness, volume size, mean curvature, and cortical area). The novel inter-regional high-order morphological connectivity was based on the correlation coefficients of feature distances (euclidean, seuclidean, mahalanobis, cityblock, minkowski, and chebychev). This unified framework provided a competitive method for building individual high-order morphological networks rather than low-order similarity or co-variance graphs. Therefore, the proposed features might open a new perspective for the brain connectome researches. To investigate the potential values of these metrics, we analyzed the reliability using test-retest datasets and inter-subject variability through normal aging datasets. In addition, predictive models for brain age were established based on machine learning to evaluate the individual differences of the proposed high-order morphological connectivity.

2. Methods

2.1. Participants and MRI protocols

Two datasets were selected for this research: to analyze the test-retest reliability of the proposed features and to investigate the inter-subject variability of the novel metrics. Both of the two datasets were open-accessed for academic usages.

2.1.1. Datasets 1

The test-retest reliability datasets were obtained from the Multi-Modal MRI Reproducibility Resource project [21] (http://www.nitrc.org/projects/multimodal). This project contained 21 healthy participants with test-retest multi-modal MRI scans, which were acquired using a 3T Philips Achieva MR scanner located at the Vanderbilt University, United States. The 21 adult participants were consisted of 11 males and 10 females with age from 22 to 61. The time gap between the two scan sessions was 1 h. The anatomical MRI datasets obtained through T1-weighted MPRAGE sequences were selected for analysis in this study. The parameters for the anatomical MRI scans could be found in previous studies [15,21].

2.1.2. Datasets 2

The normal aging datasets were downloaded from the ICBM sites of the 1000 functional connectome project (https://www.nitrc.org/projects/fcon_1000/). There were 85 healthy subjects in this dataset that contained structural MRI and resting state fMRI. The 85 adult subjects were consisted of 41 males and 44 females with age from 19 to 85. The anatomical MRI obtained via T1-weighted MPRAGE sequences were selected for investigating the inter-subject variability of the proposed neuroanatomical metrics. The detailed information of the MRI parameters could be found in a previous study [22].

2.2. Data preprocessing

The raw datasets were preprocessed using the Freesurfer package (https://surfer.nmr.mgh.harvard.edu/) to obtain regional morphological features [23]. The Freesurfer package was designed for anatomical MRI analysis as well as multimodal MRI integrations. The pipeline for surface-based morphology (SBM) contained the following key steps: non-brain tissue removal via skull-tripping; white matter and grey matter segmentation; affine registration to the MNI305 atlas; B1 bias field estimation; right and left hemispheres separation; white matter surface generation for each hemisphere; pial surface generation for each hemisphere; vertex-wise morphological features extraction; surface segmentation using the DK atlas; regional morphological features computation. Finally, four features (i.e., thickness, volume, area, and curvature) were derived for each anatomical brain regions in the Desikan-Killiany Atlas (DKA), which was a popular brain atlas for anatomical MRI. For each hemisphere, the DKA atlas divided the brain surface into 34 anatomical regions. The definitions and the abbreviations of the 68 whole-brain regions could be found in previous studies [19,24].

2.3. High-order morphological connectivity

In our previous studies, we found discriminative interregional morphological connectivity for ADHD identification [19]. Here, the original methods of low-order connectivity were extended to the high-order graph extraction. The high-order morphological connectivity for each subject was estimated in a unified framework: 1) obtain the regional morphological features; 2) construct a $68 * 4$ feature matrix; 3) compute the $1 * 2278$ feature distances (i.e., euclidean, seuclidean, mahalanobis, cityblock, minkowski, and chebychev); 4) get the $68 * 68$ feature distance matrix as low-order connectivity graph; 5) compute the linear correlations between each brain regions. Finally, the $68 * 68$ high-order morphological connectivity was obtained for each subject based on the correlation matrix of the feature distances. This paper provided a unified framework to derive high-order morphological connectivity compared to previous studies. To investigate the potential values of the proposed neuroanatomical metrics, we focused on the reliability and the variability of the original high-order morphological connectivity rather than the complex network estimators. The pipelines for high-order morphological connectivity extraction could be found in Fig. 1.

2.4. Test-retest reliability

The test-retest reliability was analyzed for whole-brain morphological connectivity. The reliability was measured by intraclass correlation coefficients (ICCs) [25]. Here, the ICC value equals to the ratio of inter-subject variance to the total variance in a random effects model according to previous studies [26]. The ICC values were divided into five levels: slight reliability ($ICC \leq 0.2$), fair reliability ($0.2 < ICC \leq 0.4$), moderate reliability ($0.4 < ICC \leq 0.6$), substantial reliability ($0.6 < ICC \leq 0.8$), almost perfect reliability ($0.8 < ICC \leq 1$) [27]. In addition, hypothesis tests were performed for the reliability with null hypothesis that the ICC value equals to the correlation coefficient. The irr package (https://cran.r-project.org/web/packages/irr/) was applied to compute the ICCs and p values. Significant ICCs were indicated by $p < .05$, corrected by the False Discovery Rate (FDR).

2.5. Inter-subject variability

The inter-subject variability for the proposed metrics were indicated by the correlations between brain features and normal aging. The inter-subject variability of the whole-brain morphological connectivity was analyzed in this paper. The inter-subject variability was evaluated using

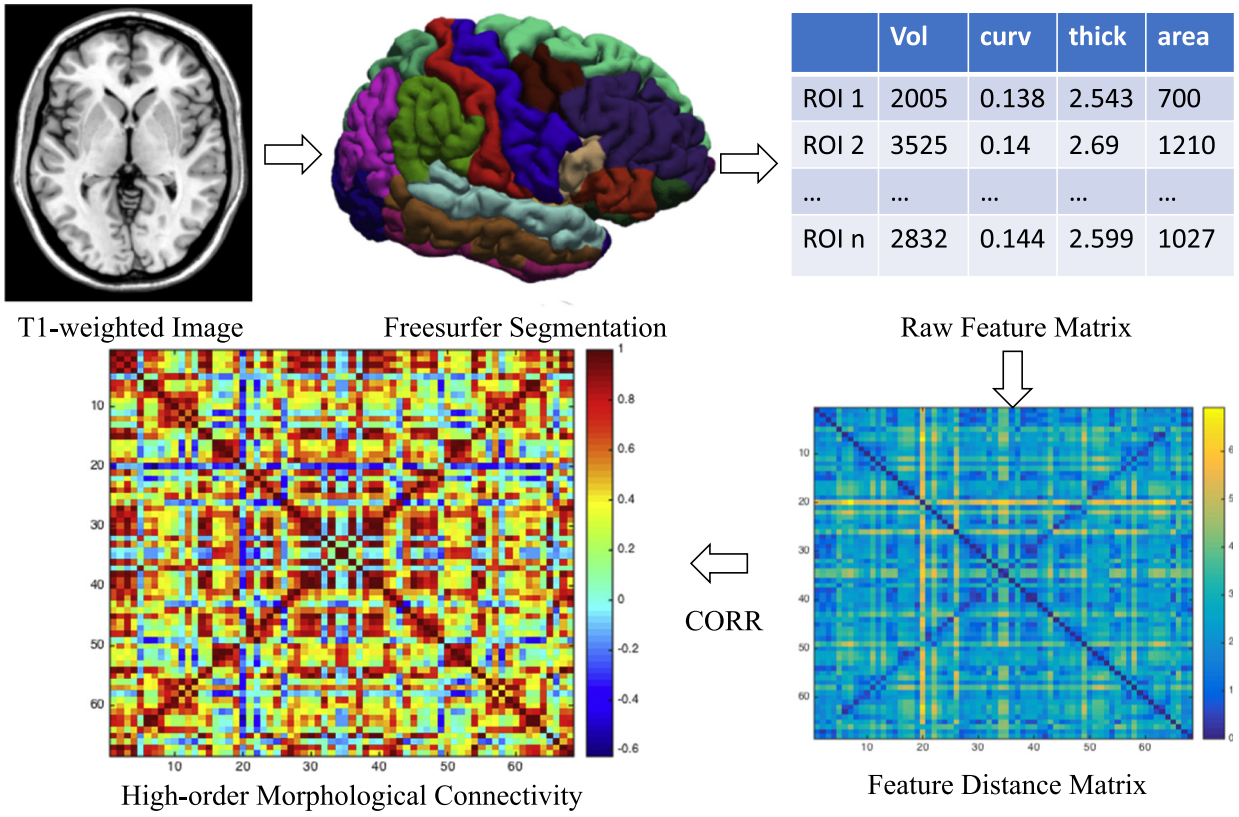

Fig. 1. Pipelines for computing high-order morphological connectivity. First, the raw T1-weigted MRI images are segmented by Freesurfer. Then, the feature matrix is obtained based on the regional features. Third, the feature distance matrix is computed based on the feature matrix. Finally, the high-order morphological connectivity matrix is obtain using the Pearson correlation coefficients.

linear correlation coefficients. The p values for the correlations were corrected by FDR.

Furthermore, we investigated the predictive power of the whole-brain morphological connectivity, which was applied as the raw features to estimate the brain age. The predictive models for age estimations were solved by the popular support vector regression (SVR). The performance of the predictive models was indicated by the linear correlation between the predicted age and the biological age through the leave-one-out cross-validation.

3. Results

3.1. Test-retest reliability

The proposed metrics exhibited substantial-to-perfect test-retest reliability. The significantly reliable brain networks ($p < .05$, FDR corrected) were indicated in Fig. 2. > 97% of the whole-brain networks measured using different distances were significantly reliable between the two scan sessions. More than 90% of the whole-brain networks measured using different distances exhibited significant substantial-to-perfect reliability (ICC $> 0.6, p < .05$, FDR corrected). The high-order features based on euclidean, cityblock, minkowski, and chebychev distances were more reliable than that based on seuclidean and mahalanobis distances (ICC > 0.8, $p < .05$, FDR corrected). The proportions of different levels of ICCs were presented in Table 1.

3.2. Inter-subject variability

Significant relationships were found between the high-order morphological connectivity and biological age, implying the fine inter-subject variability for statistical analysis. Fig. 3 represented the significant relationships ($p < .05$, FDR corrected). 30.82% of the connections in the proposed euclidean-based network were significantly correlate to biological age. 11.5% of the connections in the proposed seuclidean-based network were significantly correlate to biological age. 20.5% of the connections in the proposed mahalanobis-based network were significantly correlate to biological age. 22.08% of the connections in the proposed cityblock-based network were significantly correlate to biological age. 30.82% of the connections in the proposed minkowski-based network were significantly correlate to biological age. 32.7% of the connections in the proposed chebychev-based network were significantly correlate to biological age.

Significant correlations were found between the predicted brain age and the biological age, suggesting the potential predictive powers of high-order morphological connectivity for studies of individual differences. Fig. 4 represented the significant correlations indicated the performance of the predictive models. The performance of euclidean-based network was $r = 0.58$, $p < 10^{-8}$. The performance of seuclidean-based network was $r = 0.6$, $p < 10^{-8}$. The performance of mahalanobis-based network was $r = 0.65$, $p < 10^{-10}$. The performance of cityblock-based network was $r = 0.54$, $p < 10^{-6}$. The performance of minkowski-based network was $r = 0.58$, $p < 10^{-8}$. The performance of chebychev-based network was $r = 0.6$, $p < 10^{-8}$. The most predictive features were mahalanobis-related high-order morphological connectivity.

4. Discussion

In this paper, we proposed several novel metrics for individual high-order morphological connectivity in a unified framework. We also investigated the reliability and inter-subject variability of these neuroanatomical features. The results indicated that the proposed metrics were reliable and were significantly correlated to biological age. Moreover, the predictive powers of the novel metrics for age estimation

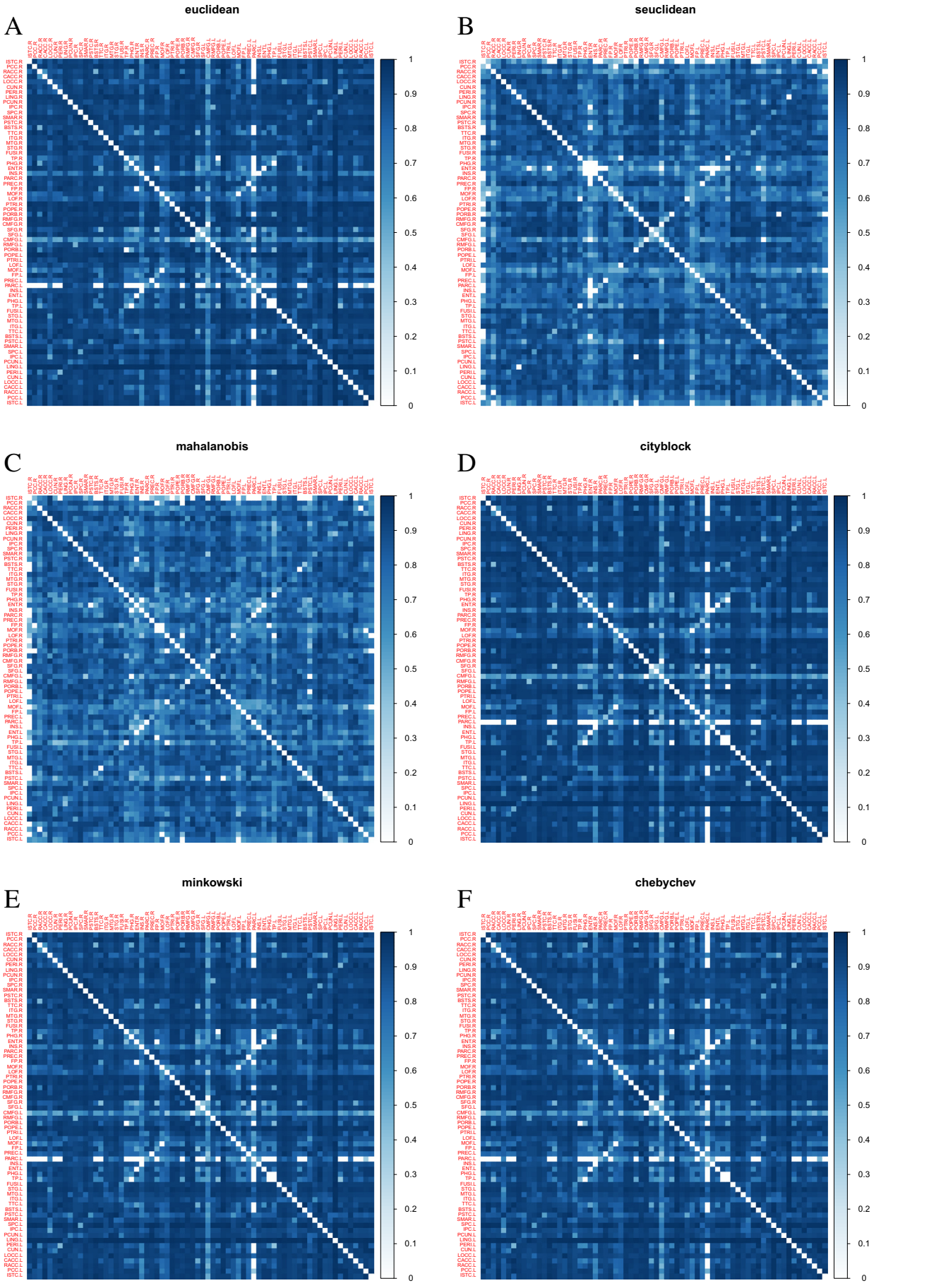

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Fig. 2. ICCs of the high-order morphological connectivity. Subfigure A denotes euclidean-related ICCs. Subfigure B denotes seuclidean-related ICCs. Subfigure C denotes mahalanobis-related ICCs. Subfigure D denotes cityblock-related ICCs. Subfigure E denotes minkowski-related ICCs. Subfigure F denotes and chebychev-related ICCs.

Table 1
Distributions of ICCs.

Features	Slight	Fair	Moderate	Substantial	Almost perfect
euclidean	1.67%	0.18%	3.25%	11.59%	83.32%
seuclidean	2.02%	0.48%	7.16%	29.76%	60.58%
mahalanobis	2.02%	0.57%	8.12%	32.92%	56.37%
cityblock	1.67%	0%	3.69%	10.4%	84.2%
minkowski	1.67%	0.18%	3.25%	11.59%	83.32%
chebychev	1.67%	0%	3.42%	11.9%	83.01%

were discovered using machine learning. The results suggested that the proposed reliable metrics could reflect individual differences, and could be applied in future brain network analysis.

High-order connectivity was a novel concept that investigated the multiple relationships among the nodes of the brain network. The high-order brain connectivity has been investigated through resting state fMRI [28,29]. The high-order functional connectivity was reliable and had discriminative powers for brain disorder classifications [28,30]. However, the high-order morphological connectivity remains unexplored. Previous studies applied regional image intensity distribution-based features to build individual low-order morphological connectivity [17]. Furthermore, the individual interregional morphological connectivity was proposed using the feature matrix of regional cortical features [19,31]. In this paper, we proposed a unified framework to derive individual high-order morphological connectivity rather than low-order connectivity features. A series of high-order brain networks were obtained in this unified framework. The proposed metrics were competitive to previous methods, and could be extended with other regional features and feature distances in this unified framework. The biological meanings of the proposed neuroanatomical metrics were unclear to date. One explanation was that the axon tension theory that anatomically connected brain regions should yield similar morphological features based on the mechanical force of neurons [17]. Another possible explanation was the information transmission theory that functionally connected brain regions should share similar morphological features for neural signal transmission [19]. In summary, the novel metrics for individual high-order morphological connectivity were proposed in a unified framework which has not been presented before. The inter-regional morphological connectivity could be supplementary features for current methods of brain connectome.

The test-retest reliability is one of the most significant indices for the neuroanatomical metrics [32,33]. The conventional anatomical features exhibited high reliability using different methods of brain morphology (i.e., volume, cortical thickness) [34]. Furthermore, the interregional morphological network and inter-voxel morphological network were reliable measured by low-order brain connectivity [15,31]. In this paper, we tested the hypothesis that high-order morphological connectivity was as reliable as the low-order connectivity. Our results indicated that the high-order morphological connectivity also exhibited substantial-to-perfect test-retest reliability using different features. Most of the whole-brain connections measured by the six connectivity metrics were significantly reliable between the two scan sessions. The connections with high reliability were located in over 90% of the cortical regions, including the hub areas. The above results suggested that the proposed high-order neuroanatomical metrics were as reliable as previous low-order features, and could be applied as additional features for clinical research.

The inter-subject variability is another important index for the neuroanatomical metrics [35]. The individual differences of a novel neural metrics can be applied to investigate the brain developments [36]. Previous studies found the developmental trajectories using anatomical or functional measures [37,38]. Although the brain functional network properties have been analyzed for healthy aging, the relationships between the morphological connectivity and the brain developments were still unclear. In this paper, we analyzed the correlations between the individual morphological connectivity and the biological age. The results found that a fraction of morphological connections was significantly correlated to the chronological age, suggesting the potential biological meanings of the proposed neuroanatomical metrics. Furthermore, predictive models based on the interregional high-order morphological connectivity were established for age estimation. Significant correlations were found between the predicted age and the original values. Although the performance of the predictive models based on interregional features was lower than previous studies based on regional features [39], the high-order morphological connectivity could provide a novel perspective for investigate the interregional brain morphological developments. In summary, the novel high-order metrics exhibited good inter-subject variability, and could be applied in statistical analysis of individual differences.

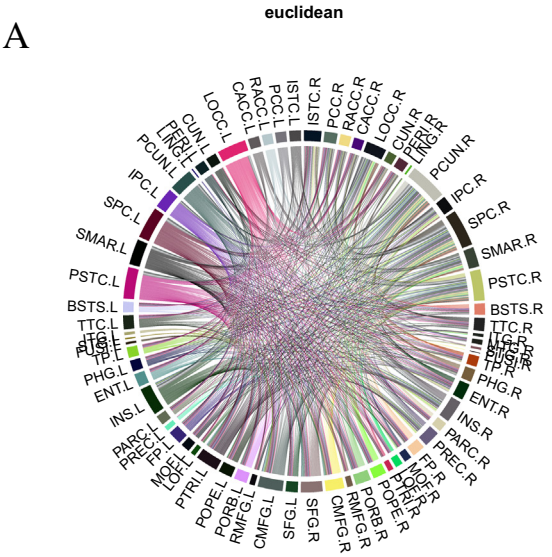
The advantage of this research was investigating the individual high-order morphological brain networks in a unified framework. To the best of knowledge, this is the first method that proposes six features in a unified framework for individual high-order morphological connectivity. The proposed individual high-order neuroanatomical metrics exhibited high reliability and good inter-subject variability, which was the two most significant properties for the novel features. The reliability of the morphological connectivity outperformed that of functional connectivity. The connections that significantly correlated to age confirmed with previous findings. In addition, the novel interregional features exhibited predictive powers in regression tasks for age estimations. The predicted ages based on the six novel neuroanatomical metrics were significantly correlated to the biological age. The results suggested that the individual high-order morphological connectivity was competitive to conventional group-wise covariance networks in statistical analysis and machine learning tasks, and the proposed metrics could be novel features for statistical analysis.

One limitation of this research was the interpretation of the novel high-order metrics. The biological meanings of these metrics should be explained using additional multimodal neuroimaging techniques (i.e., diffusion tensor imaging, resting state fMRI). Another limitation was the sparsity of the proposed brain networks. The morphological brain networks could be presented using novel sparse representations. The third limitation was we focused on the raw features of brain connectivity. The complex network measures (betweenness, small-worldness) should be tested in future study. The fourth limitation was the low-resolution interregional brain networks. Our methods can be extended to high-resolution interregional brain networks or inter-vertex brain networks. The last limitation was the MRI parameters of the anatomical datasets. The effects of field strengths, spatial resolutions, and scanners should be tested in future study.

5. Conclusions

Individual high-order morphological brain networks were proposed in a unified framework based on regional cortical features from anatomical MRI. The novel neuroanatomical metrics exhibited high test reliability and good inter-subject variability. Furthermore, the proposed features could reflect individual differences and exhibited predictive powers for age estimation. The results suggested that the reliable interregional morphological features could be additional metrics for individual brain connectome research.

A



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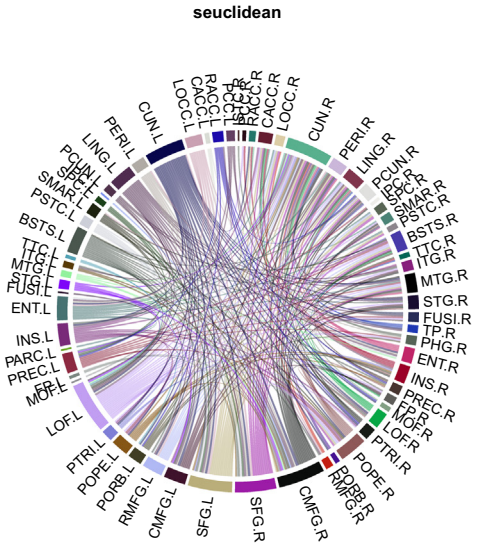

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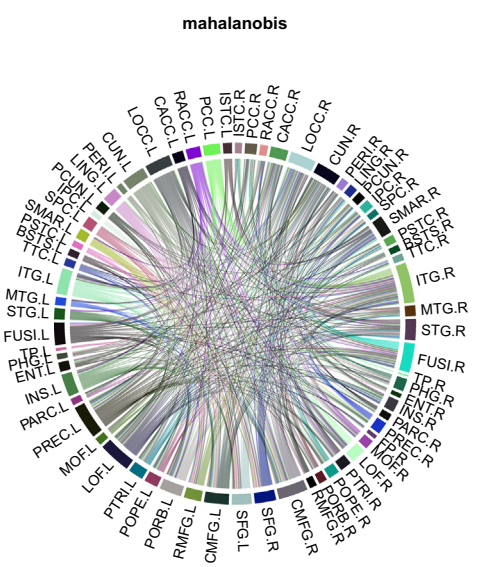

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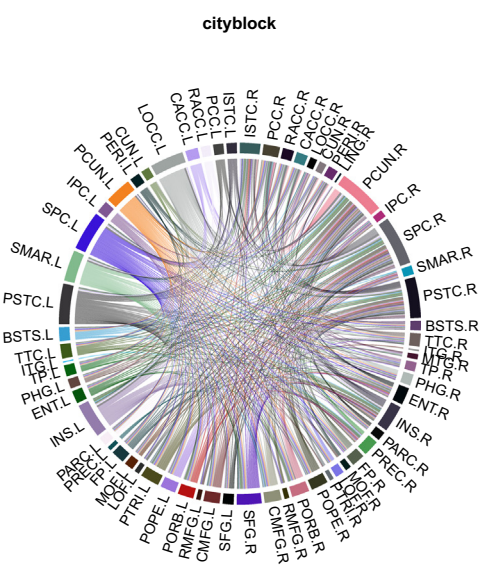

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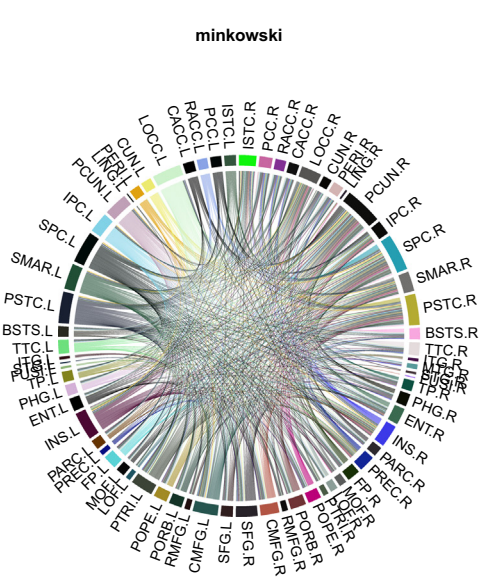

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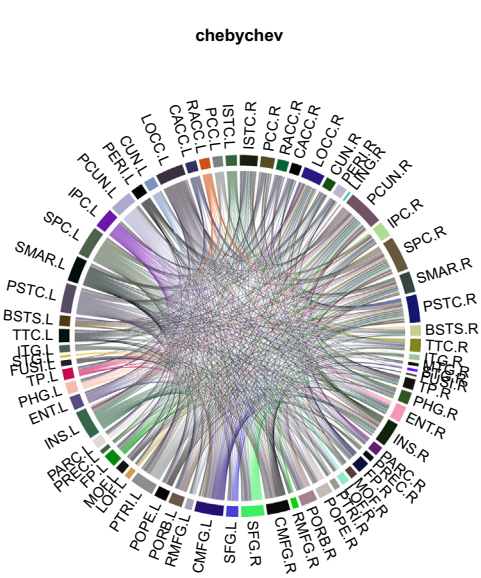

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Fig. 3. Significant relationships between the high-order morphological connectivity and age. Subfigure A denotes euclidean-related correlations. Subfigure B denotes seuclidean-related correlations. Subfigure C denotes mahalanobis-related correlations. Subfigure D denotes cityblock-related correlations. Subfigure E denotes minkowski-related correlations. Subfigure F denotes and chebychev-related correlations.

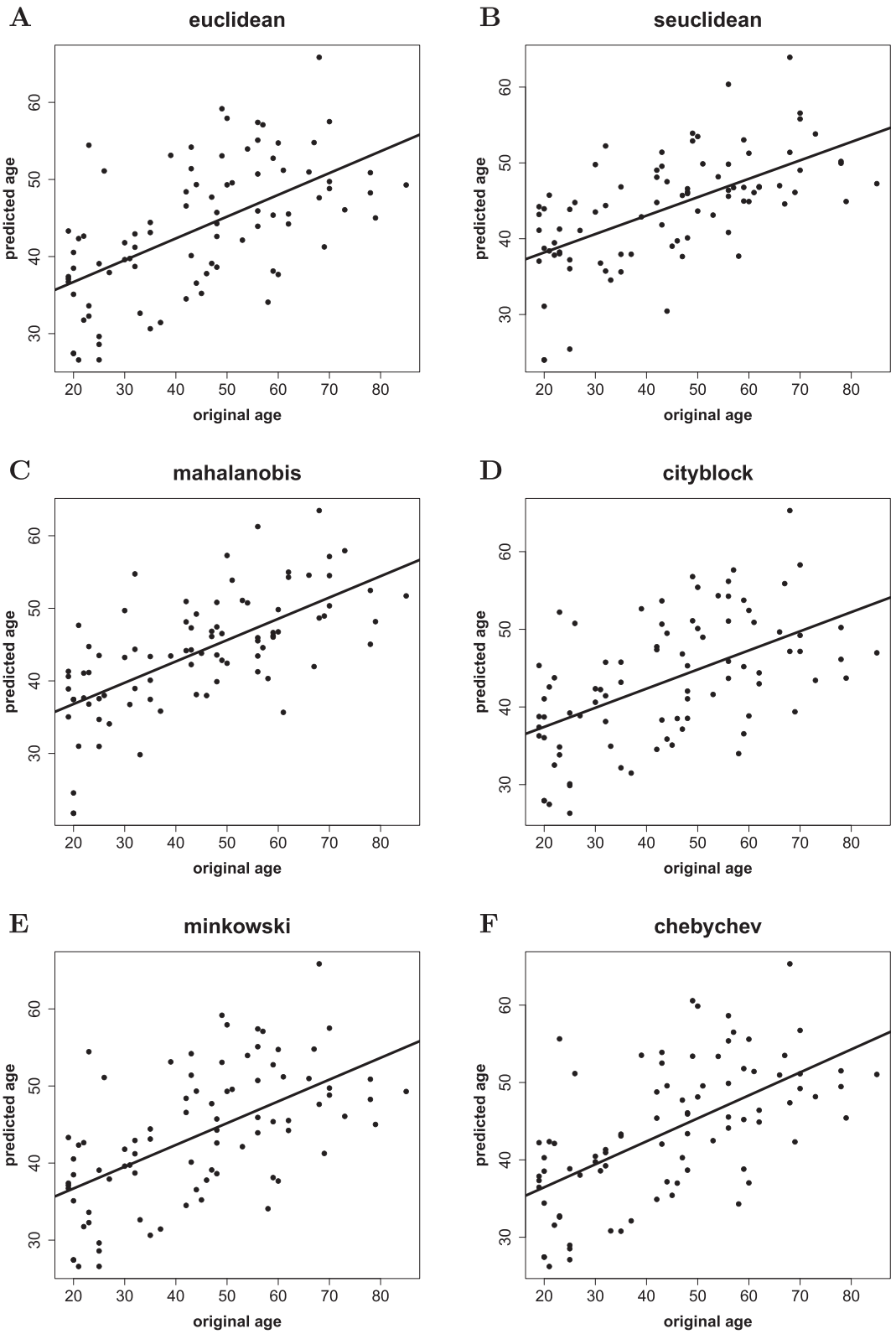

Fig. 4. Predictive models for brain age based on the high-order morphological connectivity. Subfigure A denotes euclidean-related models. Subfigure B denotes seuclidean-related models. Subfigure C denotes mahalanobis-related models. Subfigure D denotes cityblock-related models. Subfigure E denotes minkowski-related models. Subfigure F denotes and chebychev-related models.

Declaration of competing interest

The authors have no conflicts of interest to declare.

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