Curvature-based Methods for Brain Network Analysis

by

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Abstract

The human brain forms functional networks on all spatial scales. Modern fMRI scanners allow for resolving functional brain data in high resolution, enabling the study of large-scale networks that relate to cognitive processes. The analysis of such networks forms a cornerstone of experimental neuroscience. Due to the immense size and complexity of the underlying data sets, efficient evaluation and visualization pose challenges for data analysis.

In this study, we combine recent advances in experimental neuroscience and applied mathematics to perform a mathematical characterization of complex networks constructed from fMRI data. We use task-related edge densities [Lohmann et al., 2016] for constructing networks whose nodes represent voxels in the fMRI data and whose edges represent the task-related changes in synchronization between them. This construction captures the dynamic formation of patterns of neuronal activity and therefore efficiently represents the connectivity structure between brain regions.

Using geometric methods that utilize Forman-Ricci curvature as an edge-based network characteristic [Weber et al., 2017], we perform a mathematical analysis of the resulting complex networks. We motivate the use of edge-based characteristics to evaluate the network structure with geometric methods. Our results identify important structural network features including long-range connections of high curvature acting as bridges between major network components. The geometric features link curvature to higher order network organization that could aid in understanding the connectivity and interplay of brain regions in cognitive processes.

1 Introduction

The key idea of network analysis is to reduce a system to relations among its basic elements as means for understanding their interactions and commonalities. Recent technological advances in the natural sciences allow for the analysis and description of highly complex systems at increasingly smaller and more detailed scales. In the neurosciences, novel experimental technologies allow for the analysis of neural systems on the scale of specific brain regions or even on the single-neuron level. A landmark study, the Human Connectome Project (HCP) [Van Essen et al., 2013], provided the scientific community with the opportunity to study task-specific human brain activity measured with modern fMRI technology on an
unprecedented scale. The HCP and its follow up studies have produced a large body of knowledge about the inner workings of the brain that was unimaginable just a few years prior.

In the present study we bring together recent advances in Computational Neuroscience and Applied Mathematics to introduce a new approach in analyzing such large-scale neuro-scientific data sets. In [Lohmann et al., 2016], Lohmann et al. developed a method for analyzing fMRI data with a network-based approach called TED. The main idea behind TED is to compute large-scale, task-related changes in brain connectivity on the voxel level. In TED, task-related changes between a pair of voxels are defined as difference in synchronization between the respective time series. The advantage of this approach is that we do not depend on any specific hemodynamic response model. Critically, such changes in synchronization occur in dense packs around the spatial neighborhood of the voxel pair. Using nonparametric FDR-based statistics, large-scale networks can be derived using the TED method.

In a series of papers [Weber et al., 2017, Weber et al., 2016b, Weber et al., 2016a], Weber et al. introduced a new set of characteristics for network analysis. They show that information encoded in the edges yields novel insights into the local and global structure of the network as well as the direction and density of the information flow. These features are not captured in classic node-based network characteristics, such as the distribution of node degrees (i.e. the number of edges per node) and the average path length (minimal number of edges connecting any pair of two nodes) across a given network. The core component of this theory, a discrete Ricci-curvature introduced by R. Forman [Forman, 2003], gives rise to a corresponding Ricci flow that allows for the characterization of not only static networks, but also dynamic effects in the evolution of networks over time. Utilizing both Ricci curvature and its associated flows, this work suggests network-analytic methods with a wide range of possible applications to data mining. Essentially, the Forman-Ricci curvature measures the dispersion or divergence at the two ends or vertices of an edge. This measure provides an indication for the importance of an edge in the network.

By applying the TED method to fMRI data from the HCP, we construct TED networks for a curvature-based geometric analysis. The resulting fMRI TED networks are large, complex objects whose analysis with traditional tools presents a computational challenge. We analyze the geometry of the networks with the Forman-Ricci formalism, to give insights into the relation of network connectivity and functional features indicated by the underlying data. The curvature-based methods identify long-range connections with high curvature that span the network. With this, curvature can be linked to higher order network organization. This observation motivates the study of higher order structures in TED networks (the network’s backbone) and opens up possibilities for complexity reduction that could aid, more generally, in the computational analysis of large brain networks.

2 Methods

2.1 Forman-Ricci Curvature for Complex Networks

The early node-based approach employed in network analysis has proved incapable of capturing both the local and global behavior of complex networks. It has also proven to be ineffective in describing the interplay between large and small scales. In the search for new methods that could resolve this issue, certain properties that relate to the geometry of networks were found to be very useful. Such geometry, beyond simple and immediate metric properties, includes the notion of curvature. Various notions of discrete curvature have been explored on networks, starting with the combinatorial analogue of the classical Gauss curvature, in the guise of the, by now, ubiquitous clustering coefficient.

Among the different notions of curvature, Ricci curvature was found to be particularly powerful for developing a general notion of curvature on networks. While it is not the most general curvature concept, it has proved to be a tool strong enough to capture deep phenomena, but at the same time simple enough to be applied in various discrete settings. Two different discretizations of Ricci curvature have been shown to give efficient solutions for geometrizations of networks. The better known of these is Ollivier’s (coarse)
Ricci curvature [Ollivier, 2009, Ollivier, 2010], which has seen various applications in network analysis (see, e.g. [Sandhu et al., 2015, Gao et al., 2016]). The second one, based on Forman’s theoretical work on the so called weighted CW complexes [Forman, 2003], was proposed recently by some of the authors [Weber et al., 2017, Sreejith et al., 2016] as a tool for network analysis. From a computational point of view, the simple notion of Forman’s Ricci curvature is advantageous in terms of efficient computability that allows for large-scale complex networks.

The key advantage of Ricci curvature for network analysis is that it is edge-based rather than node-based. This resolves some of the issues with node-based network characteristics (e.g. node-degree biases in biological network analysis). As a discretization of the classical (smooth) notion, that “resides” on vectors, it gives rise to a natural measure of the discrete avatar of vectors: the network’s edges. Thus, a discrete notion of Ricci curvature is ideally suited for the study of edge-based network properties that capture the connectivity structure, such as weighted connections and directionality. By laying the focus on the relations (edges) between the system’s elements (nodes), the approach is especially suited for networks, where major information is encoded in the weighted connectivity structure of the network.

2.1.1 Definition

We denote a network graph by $G = \{V, E, \omega\}$ where $V := \{v \in G\}$ is the set of nodes (or vertices) and $E := \{e = (v_1, v_2) \forall v_1, v_2 \in G\}$ the set of edges connecting pairs of nodes. Let further $\omega := \{\omega(V), \omega(E)\}$ be the weighting schemes on nodes ($\omega(V)$) and edges ($\omega(E)$), both with values in $[0, 1]$.

![Figure 1: Local connectivity structure. Edge $e$ with adjacent vertices $v_1$ and $v_2$ and parallel edges $\{e'_v, e''_v, e'''_v\}$ (adjacent to $v_1$) and $\{e'_v, e''_v, e'''_v\}$ (adjacent to $v_2$).](image)

Then the Forman-Ricci curvature is defined by

$$Ric_F(e) = \omega(e) \left( \frac{\omega(v_1)}{\omega(e)} + \frac{\omega(v_2)}{\omega(e)} - \sum_{\substack{\omega(e_{v_1}) \sim e \\omega(e_{v_2}) \sim e}} \left( \frac{\omega(v_1)}{\sqrt{\omega(e)\omega(e_{v_1})}} + \frac{\omega(v_2)}{\sqrt{\omega(e)\omega(e_{v_2})}} \right) \right); \quad (1)$$

with edges $e = (v_1, v_2) \in E$ and $e_{v_1}, e_{v_2} \in E$ parallel edges adjacent to $e$ at vertices $v_1$ and $v_2$. This notion of Forman’s Ricci curvature is not restricted to combinatorial (unweighted) networks, but also applicable to weighted networks as the TED networks discussed in this article. Moreover, the definition can be easily extended to the case of directed networks. For each node, we evaluate the contributions of incoming and outgoing edges separately. $W$ denote the set of incoming and outgoing edges for a node $v$ by $E_{I,v}$ and $E_{O,v}$. We then define the In Forman curvature $Ric_I(v)$ and the Out Forman curvature...
Ric\(_O(v)\) by

\[
\text{Ric}_I(v) = \sum_{e \in E_{I,v}} \text{Ric}(e) \\
\text{Ric}_O(v) = \sum_{e \in E_{O,v}} \text{Ric}(e),
\]

summing over only the incoming or outgoing edges, respectively. Then the total amount of flow through a node \(v\) is

\[
\text{Ric}_{I/O}(v) = \text{Ric}_I(v) - \text{Ric}_O(v).
\]

The Forman-Ricci curvature defines an edge-based network characteristic that gives insights into community structure and directionality. In particular, it exhibits a "backbone effect" that we will discuss in the following section: Edges that form connections between major communities (the network’s "backbone") are characterized by high absolute Forman-Ricci curvature (see, e.g., [Weber et al., 2017]).

### 2.1.2 Curvature-based Network Analysis

Classic network analysis has focused on the elements of the system and their connectivity (node-based approach) rather than the relations (edges) between them. We propose an edge-based approach [Weber et al., 2017, Weber et al., 2016b]:

- evaluate not only binary, but also weighted networks;
- natural notion for directed networks;
- dynamic models for network evolution;
- generalization from pairwise to higher order interactions.

Our approach builds on a discrete version of the well-known concept of curvature in differential geometry. The edge-based Forman curvature and its associated geometric flow can be utilized to

- identify higher order connectivity structure;
- characterize local assortativity;
- detect structural anomalies.

### 2.1.3 Ricci flow and the "backbone effect"

In [Weber et al., 2017, Weber et al., 2016a], Weber et al. discuss the geometric relations between curvature and flow and construct a Ricci flow corresponding to Forman’s discrete Ricci curvature. The discrete Ricci flow introduced therein possesses the essential properties of the smooth Ricci flow. Its various applications in data mining include denoising and change detection of dynamic networks and the study of network evolution towards predicting long-time behavior of time-dependent complex networks [Weber et al., 2016b]. Together, curvature and flow capture the geometry of the network: Edges with high curvature evolve fast under the Ricci flow and therefore dominate the higher order network organization ("backbone effect"). The connection between high curvature values and the network’s backbone becomes evident when rewriting eq. 1:

\[
\text{Ric}_F = \omega(v_1) + \omega(v_2) - \sum_{e_{1,2} \sim e} \left[ \omega(v_1) \sqrt{\frac{\omega(e)}{\omega(e_{v_1})}} + \omega(v_2) \sqrt{\frac{\omega(e)}{\omega(e_{v_2})}} \right]
\]
We see that high absolute curvature occurs, if $v_1$ and $v_2$ have high degrees and if $\omega(e)$ is large compared to $\omega(e_{v_1})$ and $\omega(e_{v_2})$. This coincides with the notion of bridges, relating high curvature with the network’s backbone.

This backbone effect can be emphasized by applying the discrete Ricci flow. We iteratively scale edge weights according to curvature: A reverse Ricci flow acts on the edges and assigns high weights to edges with high curvature and low weights to low curvature edges. The iterative procedure highlights the backbone of the network and therefore lends itself as a tool for complexity reduction. By reducing the network to its much smaller backbone we can make large-scale networks accessible to computationally intense network analysis tools.

We construct a reverse Ricci flow on the edges by discretizing

$$\frac{\partial \omega(e,t)}{\partial t} = \text{Ric}_F(\omega(e,t))\omega(e,t)$$

(6)

to

$$\omega(e,t+1) = \omega(e,t) + \text{Ric}_F(\omega(e,t))\omega(e,t)$$

(7)

and renormalize after each step

$$\hat{\omega}(e,t+1) = \frac{\omega(e,t+1)}{\max_{e \in E} \omega(e,t+1)}$$

(8)

(Here, $\omega(e,t)$ denotes the weight of edge $e$ at time or iteration step $t$.)

We conclude with the remark, that the notion of Forman-Ricci curvature is not restricted to the pairwise interactions in classic networks. By extending the curvature notion to higher dimensions, we can study higher order interactions that might be represented as simplicial or, more general, polyhedral complexes.

### 2.2 Task-related edge densities for fMRI networks

#### 2.2.1 Data source

We analyze task-based fMRI data provided by the Human Connectome Project (HCP) and the WU-Minn Consortium [Van Essen et al., 2013, Barch et al., 2013]. More specifically, we analyze two functional task data sets from the HCP 1200 release by computing task-related network changes: An emotion task data set containing 1045 subjects and a motor task data set with 1079 subjects. For the motor task experiments, subjects were cued visually to tap their left or right fingers, squeeze their left or right toes, or move their tongue. Each block lasted 12 seconds (10 movements) and was preceded by a 3 second cue (for details see [Barch et al., 2013]). In the emotion task, subjects were cued to match two faces or two shapes with another face or shape shown at the bottom of the screen; the faces had either angry or fearful expressions. Each block consisted of 6 subsequent trials and lasted 21 seconds. All data sets were acquired with the following parameters: TR=720ms, TE=33.1ms, 2 mm isotropic voxel size, multiband factor 8.

#### 2.2.2 Method

Task-induced edge density (TED) [Lohmann et al., 2016] is a novel way for investigating changes in functional connectivity across a set of experimental conditions. It allows a whole-brain investigation into changes of connectivity and thus, it is not necessary to define a seeding region. Furthermore, the method operates on the voxel level, rendering pre-segmentations obsolete. TED relies on changes in synchronization between pairs of voxels and does not make assumptions on the haemodynamic response function.
The key idea behind TED is the observation that if two voxels change their synchronization, their spatial neighborhood also changes their connectivity to a much greater extent than it would be expected given the inherent spatial correlation between spatially adjacent voxels. The figure below exemplifies this effect, showing neighborhoods of voxels and their connectivity. The upper pair of neighborhoods (A) is more strongly connected than the lower one (B). This reflects on the TED value, which is defined as the number of connections divided by the number of theoretically possible connections (11/729 for A and 5/729 for B). The respective TED-value is then assigned to the central edge (shown in red). Statistical significance testing is established using permutation testing and controlling the false discovery rate.

2.2.3 Preprocessing with TED

We used minimally preprocessed HCP data (as described in [Glasser et al., 2013]), but constrained our analysis to runs with left-right phase encoding direction. To reduce dimensionality, we downsampled the data to $(3\,mm)^3$, applied a temporal high-pass filter (cutoff $1/100s$) and spatial smoothing with a 5mm kernel. For the motor task, we only investigated the left and right hand finger tapping condition, using the time course of the second trial as input for the TED analysis, resulting in 16 volumes. For the emotion task, we used fearful vs angry faces, resulting in 25 volumes. We computed TED networks for both tasks [Lohmann et al., 2016], using an initial fractional threshold $q=0.999$ for both tasks, implying we only computed edge density values for the top 0.1% of all edges. For both tasks we estimated statistical significance on the basis of 2000 permutations. The permutation and FDR procedure yielded an edge-density threshold of 0.1387 for the motor task, resulting in 109,328 significant edges. For the emotion task the edge-density threshold was 0.1235, resulting in 1,289,949 significant edges.

2.3 Correlation of curvature and TED

We evaluate the relation of curvature and task-related edge density through correlation tests. On both data sets we find significant correlations between both measures. This indicates that the curvature-defined backbone is partly, but not exclusively, characterized by edges that appear in dense packs.
Table 1: Results of a Pearson correlation test for edge densities and curvature values in two HCP data sets. The TED networks are constructed with \( q=0.999 \).

|                  | motor task | emotion task |
|------------------|------------|--------------|
| t-value          | 827.76     | 980.17       |
| correlation      | 0.62       | 0.65         |
| p-value          | \(< 2.2e^{-16}\) | \(< 2.2e^{-16}\) |

3 Results

We analyze task-based fMRI data provided by the Human Connectome Project with a focus on motor tasks using minimally preprocessed data of left-right phase-encoding runs. The curvature-based analysis of the resulting TED networks gives insight into the higher order network organization that can be linked to underlying functional structures.

3.1 Curvature-based Analysis.

We perform a curvature-based geometric analysis of TED networks built from task-based HCP data. For this, we compute the Forman-Ricci curvature (Eq. 1) across all edges of the network. We note that the sign of the curvature is negative across the network (see Fig. 4). In recent work (Weber et al., 2016b), some of the authors developed a curvature-based global classification scheme for networks, the so-called prototype networks. The TED networks analyzed here are of spherical type that exhibits a clique-like community structure.

Figure 4 shows curvature-colored plots for three different TED networks. The results illustrate the link between curvature and the network backbone as discussed in the previous section. A community structure is formed by clusters of vertices interconnected by bundles of ”long range” (inter-community) connections that form the ”backbone” of the network and have a high Forman-Ricci curvature. In a network-theoretic sense, these long-range connections act as ”bridges” (Jensen et al., 2016) between
Figure 4: Major network components (communities) are connected by dense bundles of edges with high curvature. They are displayed in red here; low curvature edges are shown in yellow (A-C). The geometry of the network is characterized by these (curvature-wise) dominating edges (backbone effect). Acting as bridges between major communities they determine the higher order structural organization of the network. See SI for details on visualization.

major network communities. Removing any of these bundles of high curvature edges would disconnect the network graph and remove major routes of "information transmission" in the network. The effects of high Forman curvature are comparable to a "dispersion", i.e. heavy branching out on one (or both) ends of the respective edge. This suggests Forman-curvature as a potential characteristic for the spread of information within a complex network.

The identification of key structural features (network backbone) is an essential part of network analysis: Networks built from empirical data suffer from experimental biases in the underlying measurements. Correlation-based construction methods such as TED might introduce additional bias through the choice of the threshold. In this context it is important to identify substructures that are strongly indicated by the data and robust against small variations in the systematic parameters (e.g. choice of threshold). With curvature-based methods, these key substructures are identified through high curvature and the "backbone effect".

This observation gives rise to a complexity reduction tool: If we restrict our analysis to the high-curvature edges and the vertices they connect (i.e., the network’s backbone) we reduce the complexity of the network significantly, making even very large network accessible for further computational analysis.

3.2 Neuro-Anatomical Analysis

For both the motor and emotion HCP experiments, we analyze the distribution of Forman-Ricci curvature across the TED networks. From the roughly 1 million edges, we extracted 20,000 edges with the highest and lowest curvature values (i.e. about 2% on each tail) for further analysis. For visualization, we use braingl and performed edge bundling using default parameters, as described in [Boettger et al., 2011].

In both HCP tasks, a similar pattern emerged: The top 2% of edges with highest curvature were condensed in very few brain areas, whereas edges with low curvature were distributed over more regions.
Figure 5: Task-based functional networks from the HCP that show voxel-wise changes in synchronization. The panel shows the HCP emotion task contrasting angry versus fearful faces (left) and the HCP motor task contrasting right hand versus left hand tapping (right). We computed the Forman-Ricci curvature for both tasks and extracted the edges with the highest (red) and lowest (blue) curvature. (see Fig. 5). More specifically, in the motor task, the highest edges were located in key motor regions, including the motor cortex, the cerebellum lobules VI and VIII, and the putamen. For the emotion task, the highest edges were located in the superior parietal cortex, the posterior cingulate gyrus, and visual cortex (see Fig. 6). The reported activities are in accordance with theoretical expectations. Edges with low curvature in both tasks were distributed diffusely throughout the brain. These results strengthen the theoretically established link between the network’s backbone (essential functional structure) and high curvature edges.

4 Discussion

In this paper we motivate the use of curvature-based methods, namely the discrete Forman-Ricci curvature and its associated geometric flow, for the analysis of complex brain networks. We demonstrate the formalism by studying fMRI networks constructed from task-related edge densities using the TED method.

Our analysis gives insights into structural properties of brain networks and allows for the characterization of their higher order organization. Low curvature-edges can be found within network communities whereas high curvature edges form connections between communities. This observation links curvature to
the network-theoretic notions of *bridges* and *network backbone*. We show both theoretically and empirically that edges with high Forman curvature span the network acting as bridges between major network communities. This core connectivity structure forms the backbone of the network and determines its higher order structure.

We present computational results for TED networks constructed from two HCP data sets, one for an underlying emotion task and one for a motor task. The empirical results support that the notion of Forman-Ricci curvature is indicative of brain network structure. We found that edges with high curvature differ drastically in structure from the ones with low curvature: High-curvature edges form denser bundles that span the network while low-curvature ones are widely distributed. For the motor task the high-curvature edges converged in areas of the core motor network (motor cortex, cerebellum, and putamen). For the emotion task, the edges with highest curvature are mainly located in default mode regions (posterior cingulate and superior parietal). The results suggest curvature as a potentially useful metric for brain network analysis. Future work is needed to establish the biological underpinnings of Forman-Ricci curvature in a systematic study on larger scale.

Recent advances in measurement technologies have enabled large-scale studies of neural systems with high resolution. With international landmark collaborations underway, new large-scale data resources for advances in the fast emerging field of Connectomics will become available over the course of the next years. These efforts include the *Human Brain Project* of the European Union, the *Blue Brain Project* of EPFL and IBM, and the US-lead *BRAIN initiative*. All of these projects aim to understand the complex interactions underlying human brain function on the scale of brain regions or even single neurons. Efficient tools are essential for the analysis of both the structural and functional features of the resulting complex brain networks and may eventually aid in establishing a deeper understanding of the all-important link between structure and function in the human brain. With the curvature-based formalism we hope to contribute to the growing toolbox of network-theoretic methods available to assists in these efforts.

**Supportive Information**

Details on computational methods and experiments can be found in the supplemental. All code is publicly available on GitHub.

![GitHub: MelWe/brainnet-curvature](https://github.com/MelWe/brainnet-curvature)
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Author contributions

Data analysis was performed by MW (curvature-based) and JS and GL (TED). MW, JS and AN performed data visualization. MW wrote the original draft with contributions from JS and ES. JJ and GL supervised the project.

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Supplemental Material: Curvature-based Methods for Brain Network Analysis

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1 Visualization

1.1 Network Visualization

The visualization incorporates the connectivity structure, the distribution of node degrees and the distribution of Forman-Ricci curvature across the set of edges. The algorithm draws the first node in the list, then its neighbors and the respective edges connecting them, then their neighbors and the corresponding edges, etc. Black dots represent nodes, their size being proportional to their respective degrees. Edges have the same width each, their color scales with the normalized Forman-Ricci curvature ranging from yellow (low value) to red (high value). For computing purposes, nodes with degree \(< 3\) are neglected.

1.2 Network Alignment

As part of this research, a MATLAB application was implemented and employed to sample and visualize brain network data. The main inputs are the node coordinates and the net connectivity data. Another input parameter employed in the visualization processes is a reference brain model of an individual (or MNI brain). Reference brain models can be represented by surface meshes or by voxels. In particular, we used cortical meshes as supplied in the non-linear MNI-ICBM152 atlas [Fonov et al., 2011].

We sample data according to specified minimal node rank and minimal edge probability parameters. Coordinates of sampled nodes are aligned with the reference brain model and the resulting net is colored according to its curvature, using a user-specified color scale function. Empirically, we have found that the best results are achieved with the logarithmic color scale. In order to depict core net structure, edge widths and edge transparencies are encoded according to edge probabilities (i.e. higher probabilities corresponding to wider and less transparent edges). Similarly, we depict nodes as dots of different sizes that correspond to node ranks.
Figure 1: Anatomically aligned network visualization: Test case showing the reduction, via the reverse Forman-Ricci flow, to high-curvature edges acting as bridge between major network communities.

2 Correlation of Curvature and Anatomical distance

We performed a brief analysis on the relation between Forman-Ricci curvature of edges and Euclidean distances measured between edge nodes (i.e. edge lengths). We computed distances directly from voxel and net connectivity data and the edge curvature was computed according to eq. 1, from the main text. The analysis reveals a minor negative correlation between anatomical distances and curvature values, suggesting the predominance of low curvature within communities and high curvature for the connections between between communities. This is consistent with the correspondence between high curvature and the network backbone.

Figure 2: Histogram plots of normalized distances (Dist) and normalized curvature values (Curv) on the main diagonal and Pearson correlation scatter plots between these values on the skew diagonal. (TED networks for emotion task (top) and motor task (bottom), both with $q=0.999$.)
References

[Fonov et al., 2011] Fonov, V., Evans, A. C., Botteron, K., Almli, C. R., McKinstry, R. C., Collins, D. L., Group, B. D., et al. (2011). Unbiased average age-appropriate atlases for pediatric studies. *Neuroimage*, 54(1):313–327.