

A review of two network curvature measures

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Abstract The curvature of higher-dimensional geometric shapes and topological spaces is a natural and powerful generalization of its simpler counterpart in planes and other two-dimensional spaces. Curvature plays a fundamental role in physics, mathematics and many other areas. However, graphs are discrete objects that do not necessarily have an associated natural geometric embedding. There are many ways in which curvature definitions of a continuous surface or other similar space can be adapted to graphs depending on what kind of local or global properties the measure is desired to reflect. In this chapter, we review two such measures, namely the Gromov-hyperbolic curvature measure and a geometric measure based on topological associations to higher-dimensional complexes.

1 Introduction

Useful insights for many complex systems are often obtained by representing them as graphs¹ and analyzing them using graph-theoretic and combinatorial tools [50]. For analyzing graphs, researchers have proposed and evaluated a number of established graph-theoretic measures such as the *degree-based measures*, (e.g., degree distributions), *connectivity-based measures*, (e.g., clustering coefficients), *geodesic-*

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¹ In this chapter, we use the two use the two terms “graph” and “network” interchangeably.

based measures (e.g., betweenness centralities) and other more novel graph-theoretic measures such as in [2, 6, 41]. To simplify exposition for this chapter, our input is an undirected weighted or unweighted graph $G = (V, E)$ of n nodes v_1, \dots, v_n ; the adjacency matrix for G is denoted by $A(G) = [a(G)_{i,j}]$ where $a(G)_{i,j} = 1$ (resp., $a(G)_{i,j} = 0$) if $\{v_i, v_j\} \in E$ (resp., if $\{v_i, v_j\} \notin E$). The notations $\overline{u, v}$ and $\text{dist}_H(u, v)$ denote a *shortest path* between nodes u and v , and the distance between nodes u and v in graph H , respectively.

The graph-theoretic measure discussed in this chapter is an appropriate notion of “network curvature”. A curvature for a graph G for this chapter is a scalar function $\mathfrak{C} : G \mapsto \mathbb{R}$. Curvatures are very natural measures of the anomaly of higher dimensional objects used in mainstream physics and mathematics [10, 13]. However, graphs are discrete objects that do *not* necessarily have an associated natural geometric embedding. There are many ways in which curvature definitions of a continuous surface or other similar space can be adapted to graphs depending on what kind of local or global properties the measure is desired to reflect. More specifically, we discuss *Gromov-hyperbolic* curvature (based on the properties of geodesics and higher-order connectivities) and *geometric curvatures* (based on identifying network motifs with geometric complexes), both of which encode non-trivial *higher-order* correlation among nodes. Some important characteristics of these two curvature measures are as follows.

- ▶ They depend on *non-trivial global* network properties, as opposed to measures such as *degree distributions* or *clustering coefficients* that are *local* in nature or *dense subnetworks* that use *only* pairwise correlations.
- ▶ They can mostly be computed efficiently in polynomial time, as opposed to NP-complete measures such as *cliques* [28], *densest-k-subgraphs* [28], or some types of community decompositions such as *modularity maximization* [20].
- ▶ When applied to real-world networks, these curvature measures can explain many phenomena one frequently encounters in real graph-theoretic applications that are *not* easily explained by other measures.

2 Gromov-hyperbolic Curvature

This type of measure for a metric space was originally suggested by Gromov in the context of group theory [32] by observing that many results concerning the fundamental group of a Riemann surface hold true in a more general context. The measure was first defined for *infinite* continuous metric space via properties of geodesics (e.g., see the textbook [13]), but was later also adopted for *finite* graphs. Usually the measure is defined via *geodesic triangles* in the following manner.

Definition 1 (Gromov curvature measure via geodesic triangles). A graph G has a Gromov curvature (or Gromov hyperbolicity) of $\delta \stackrel{\text{def}}{=} \delta(G)$ if and only if for every three ordered triple of shortest paths $(\overline{u, v}, \overline{u, w}, \overline{v, w})$, $\overline{u, v}$ lies in a δ -neighborhood

of $\overline{u, w} \cup \overline{v, w}$, i.e., for every node x on $\overline{u, v}$, there exists a node y on $\overline{u, w}$ or $\overline{v, w}$ such that $\text{dist}_G(x, y) \leq \delta$.

Definition 2 (the class of δ -Gromov-hyperbolic graphs). An infinite collection \mathcal{G} of graphs belongs to the class of δ -Gromov-hyperbolic graphs (or, simply δ -hyperbolic graphs) if and only if any graph $G \in \mathcal{G}$ has a Gromov curvature of at most δ .

Informally, any infinite metric space has a finite value of δ if it behaves metrically in the large scale as a *negatively curved* Riemannian manifold, and thus the value of δ can be related to the standard scalar curvature of a hyperbolic manifold. For example, a simply connected complete Riemannian manifold whose sectional curvature is below $\alpha < 0$ has a value of $\delta = O((-\alpha)^{-1/2})$ (see [58]). This is a justification of using the value δ as a notion of curvature of any metric space.

For the purpose of designing computational algorithms, it is often useful to consider another alternate but *equivalent* (“up to a constant multiplicative factor”) way of defining Gromov curvature for a graph G via the following 4-node conditions.

Definition 3 (equivalent definition of Gromov curvature via 4-node conditions). For a set $\{u_1, u_2, u_3, u_4\}$ of four nodes, let $(\pi_1, \pi_2, \pi_3, \pi_4)$ be a permutation of $\{1, 2, 3, 4\}$ denoting a rearrangement of the indices of nodes such that

$$\begin{aligned} \text{dist}_G(u_{\pi_1}, u_{\pi_2}) & & \text{dist}_G(u_{\pi_1}, u_{\pi_3}) & & \text{dist}_G(u_{\pi_1}, u_{\pi_4}) \\ + \text{dist}_G(u_{\pi_3}, u_{\pi_4}) & \leq & + \text{dist}_G(u_{\pi_2}, u_{\pi_4}) & \leq & + \text{dist}_G(u_{\pi_2}, u_{\pi_3}) \\ = S_{u_1, u_2, u_3, u_4} & & = M_{u_1, u_2, u_3, u_4} & & = L_{u_1, u_2, u_3, u_4} \end{aligned}$$

Let $\widehat{\delta} = \widehat{\delta}(G) = \max_{u_1, u_2, u_3, u_4 \in V} \{L_{u_1, u_2, u_3, u_4} - M_{u_1, u_2, u_3, u_4}\} / 2$. Then, if \mathcal{G} is a δ -Gromov-hyperbolic graph then $\delta/c \leq \widehat{\delta} \leq c\delta$ for some absolute constant $c > 0$.

In order to account for the fact that sometimes the value of $\widehat{\delta}(G)$ may be a rare deviation from typical values of $L_{u_1, u_2, u_3, u_4} - M_{u_1, u_2, u_3, u_4}$ that one would obtain for most combinations of nodes $\{u_1, u_2, u_3, u_4\}$, the authors in [3] defined the *average Gromov-curvature* of a graph G as $\delta_{\text{ave}}(G) = \sum_{u_1, u_2, u_3, u_4 \in V} (L_{u_1, u_2, u_3, u_4} - M_{u_1, u_2, u_3, u_4}) / \binom{n}{4}$ such that $\delta_{\text{ave}}(G)$ is the expected value of $L_{u_1, u_2, u_3, u_4} - M_{u_1, u_2, u_3, u_4}$ when the four nodes u_1, u_2, u_3, u_4 are picked independently and uniformly at random from the set of all nodes.

It is easy to see that if G is a tree then $\delta(G) = \widehat{\delta}(G) = 0$, and $\widehat{\delta}(G) \leq D/2$ where D is the diameter of the given graph. Other examples of graph classes for which $\delta(G)$ and $\widehat{\delta}(G)$ are small constants include *chordal* graphs, *cactus of cliques*, *AT-free* graphs, *link graphs of simple polygons*, and *any class of graphs with a fixed diameter*. On the other hand, theoretical investigations have revealed that *expanders*, *vertex-transitive* graphs and (for certain parameter ranges) classical *Erdős-Rényi* random graphs are δ -hyperbolic only for $\delta = \omega(1)$ [7–9, 44, 47].

2.1 Topological characteristics of Gromov-hyperbolicity measure

The Gromov-hyperbolicity measure $\delta(G)$ enjoys *many* non-trivial topological characteristics. Some examples are as follows.

- ▷ The “ $\delta = o(n)$ ” property is not hereditary (and thus also not monotone). For example, removing a single node or edge can increase/decrease the value of δ *very* sharply.
- ▷ A small value of δ does *not* necessarily imply that the graph is a tree. For example, *all* bounded-diameter graphs have $\delta = O(1)$ irrespective of whether they are tree or not (however, graphs with $\delta = O(1)$ need *not* be of bounded diameter). In general, even for small δ , the metric induced by a δ -hyperbolic graph may be quite far from a tree metric [17].
- ▷ A similar popular measure used in both the bioinformatics and theoretical computer science literature is the *tree-width* measure first introduced by Robertson and Seymour [57]. However, as observed in [45] and elsewhere, the two measures are *not* correlated.

We end this section with a very important topological consequence of small Gromov-hyperbolicity values of a graph, popularly known as the “divergence of geodesic rays” property. The result appears in several forms in prior works such as [3, 7, 13, 32, 44]; we state two such versions. Let $\mathcal{B}(u, r)$ denote the set of nodes contained in a *ball* of radius r centered at node u in graph G , i.e., $\mathcal{B}(u, r) = \{v \mid \text{dist}_G(u, v) \leq r\}$

Fact 1 (Cylinder removal around a geodesic) *Assume that G is a δ -hyperbolic graph. Let p and q be two nodes of G such that $\text{dist}_G(p, q) = \beta > 6$, and let p', q' be nodes on a shortest path between p and q such that $\text{dist}_G(p, p') = \text{dist}_G(p', q') = \text{dist}_G(q', q) = \beta/3$. For any $0 < \alpha < 1/4$, let \mathcal{C} be set of nodes at a distance of $\alpha\beta - 1$ of a shortest path $\overline{p', q'}$ between p' and q' , i.e., let $\mathcal{C} = \{u \mid \exists v \in \overline{p', q'} : \text{dist}_G(u, v) = \alpha\beta - 1\}$. Let $G_{-\mathcal{C}}$ be the graph obtained from G by removing the nodes in \mathcal{C} . Then, $\text{dist}_{G_{-\mathcal{C}}}(p, q) \geq (\beta/60)2^{\alpha\beta/\delta}$.*

Fact 2 (Exponential divergence of geodesic rays) *Assume that G is a δ -hyperbolic graph. Suppose that we are given the following:*

- three integers $\kappa \geq 4$, $\alpha > 0$, $r > 3\kappa\delta$, and
- five nodes v, u_1, u_2, u_3, u_4 such that $\text{dist}_G(v, u_1) = \text{dist}_G(v, u_2) = r$, $\text{dist}_G(u_1, u_2) \geq 3\kappa\delta$, $\text{dist}_G(v, u_3) = \text{dist}_G(v, u_4) = r + \alpha$, and $\text{dist}_G(u_1, u_4) = \text{dist}_G(u_2, u_3) = \alpha$.

Consider any path \mathcal{Q} between u_3 and u_4 that does not involve a node in $\bigcup_{0 \leq j \leq r+\alpha} \mathcal{B}(v, j)$. Then, the length $|\mathcal{Q}|$ of the path \mathcal{Q} satisfies $|\mathcal{Q}| > 2^{\frac{\alpha}{6\delta} + \kappa + 1}$.

For example, these facts are used by Benjamini in [7] to show that graph classes with a constant value of δ *cannot* be expanders and also by Malyshev in [44] to show that expander graphs must have Gromov-hyperbolicity *at least* proportional to their diameter. Further works on the effect of the hyperbolicity measure δ on expansion and cut-size bounds on graphs and its algorithmic implications are reported in [22].

2.2 Gromov curvature of real-world networks

Recently, there has been a surge of empirical works measuring and analyzing the Gromov curvature δ of networks, and many real-world networks (*e.g.*, preferential attachment networks, networks of high power transceivers in wireless sensor networks, communication networks at the IP layer and at other levels) were observed to have a small constant value of δ [5, 34, 36, 46, 55]. Moreover, extreme congestion at a small number of nodes in a large traffic network that uses the shortest-path routing was shown in [37] to be caused by a small value of δ of the network. The authors in [3] computed Gromov hyperbolicity values for 11 biological networks (3 transcriptional regulatory, 5 signalling, 1 metabolic, 1 immune response and 1 oriented protein-protein-interaction networks) and 9 social networks. They reported that the hyperbolicity values of all except one network are small and statistically significant. They also reported several interesting experimentally-validated implications of these hyperbolicity values, such as

- ▷ Independent pathways that connect a signal to the same output node (*e.g.*, transcription factor) are rare, and if multiple pathways exist then they are interconnected through cross-talks.
- ▷ All the biological networks have central influential small-size node neighborhoods that can be selected to find knock-out nodes to cut off specific up- or down-regulation.

2.3 Efficient computation of Gromov curvature

Using Definition 3 directly one can compute $\delta(G)$ in $O(n^4)$ time, but this time complexity is prohibitive for large graphs. For faster computation, one needs to define Gromov curvature via an equivalent but more algorithmically amenable formulation as follows.

Definition 4 (equivalent definition of Gromov curvature via Gromov product nodes). [32] For any three nodes u, v and r , the Gromov-product of u and v anchored at r is defined by

$$(u|v)_r = \frac{1}{2} \left(\text{dist}(u, r) + \text{dist}(v, r) - \text{dist}(u, v) \right)$$

Define the value of Gromov-hyperbolicity “anchored” at a node r as:

$$\delta_r = \max_{u,v,w} \left\{ \min \{ (u|w)_r, (v|w)_r \} - (u|v)_r \right\}$$

Then, the value of Gromov-hyperbolicity of a graph G is defined as

$$\delta \stackrel{\text{def}}{=} \delta(G) = \max_r \{ \delta_r \}$$

The value of $\delta(G)$ computed via Definition 4 is identical to the one computed via geodesic triangles in Definition 1. It was also shown in [32] that $\delta(G) \leq \delta_r \leq 2\delta(G)$ for any r . Let ω be the value such that two $n \times n$ matrices can be multiplied in $O(n^\omega)$ time; the smallest current value of ω is 2.373 [62]. The (max, min)-matrix multiplication of two $n \times n$ matrices A and B , denoted by $A \otimes B$, is defined as:

$$A \otimes B[i, j] = \max_k \min \{ A[i, k], B[k, j] \}$$

Duan and Pettie in [23] showed that $A \otimes B$ can be computed in $O(n^{(3+\omega)/2}) = O(n^{2.688})$ time. Subsequently, Fournier, Ismail and Vigneron [26] showed that computation of δ_r can be cast as computing a (max, min)-matrix multiplication problem; as a result, one can compute $\delta(G)$ and a 2-approximation of $\delta(G)$ in $O(n^{(5+\omega)/2}) = O(n^{3.69})$ and in $O(n^{(3+\omega)/2}) = O(n^{2.69})$ time, respectively. Faster less accurate approximation is also known, *e.g.*, Chalopin *et al.* [14] showed that a 8-approximation of $\delta(G)$ can be computed in $O(n^2)$ time. On the other hand, an exact computation of $\delta(G)$ involves computing the "all-pairs-shortest-path" problem which is widely conjectured to take at least $\Omega(n^3)$ time (and, can be done in $O(n^3)$ time [19]).

2.4 Algorithmic implications of small Gromov curvature

A small value of Gromov curvature δ is often crucial for algorithmic designs; for example, several routing-related problems or the diameter estimation problem become easier for graphs with small δ values [16–18, 29]. DasGupta *et al.* in [22] discussed further implications of small values of δ for several graph-theoretic problems. In particular, they showed that a large family of s - t cuts having at most $d^{O(\delta)}$ cut-edges can be found in polynomial time in δ -hyperbolic graphs of n nodes when d is the maximum degree of any node except s, t and any node within a distance of 35δ of s and the distance between s and t is at least $\Omega(\delta \log n)$, and used such a result to design an approximation algorithm for minimizing bottleneck edges in a graph.

2.5 Statistical validation of Gromov curvature via "scaled" version

Suppose that $\delta(G)$ has been computed for a given graph G of n nodes and it is indeed a small value compared to the size of the graph. One major task for empirical researchers is then to determine more precisely if $\delta(H)$ is indeed a small number independent of the size of H for every graph H in the *class of graphs* \mathcal{G} to which G belongs (as opposed to $\delta(H)$ being small specifically only for the particular graph $H = G$ in \mathcal{G}). For this purpose, we can make use of a "scaled" version of Gromov curvature [35, 36, 46]. The basic idea is to "scale" the values of

Name	Notation	μ_{u_1, u_2, u_3, u_4}	ϵ
diameter-scaled curvature	$\delta^{\mathcal{D}}$	$\max_{i, j \in \{1, 2, 3, 4\}} \{\text{dist}_G(u_i, u_j)\}$	0.2929
L -scaled curvature	δ^L	L_{u_1, u_2, u_3, u_4}	$\frac{\sqrt{2}-1}{2\sqrt{2}}$
$(L+M+S)$ -scaled curvature	δ^{L+M+S}	$L_{u_1, u_2, u_3, u_4} + M_{u_1, u_2, u_3, u_4} + S_{u_1, u_2, u_3, u_4}$	0.0607

Fig. 1 [35] Various scaled Gromov curvatures.

$L_{u_1, u_2, u_3, u_4} - M_{u_1, u_2, u_3, u_4}$ in Definition 3 by a suitable scaling factor μ_{u_1, u_2, u_3, u_4} such that there exists a constant $0 < \epsilon < 1$ with the following property:

the maximum achievable value of $(L_{u_1, u_2, u_3, u_4} - M_{u_1, u_2, u_3, u_4}) / \mu_{u_1, u_2, u_3, u_4}$ is ϵ in the standard hyperbolic space or in the Euclidean space, and $(L_{u_1, u_2, u_3, u_4} - M_{u_1, u_2, u_3, u_4}) / \mu_{u_1, u_2, u_3, u_4}$ goes beyond ϵ in positively curved spaces .

By using theoretical or empirical calculations, the authors in [35] provide the bounds shown in Fig. 1. Following the ideas espoused in [3, 35], assuming G is a connected graph we can use the following criterion to determine if $\delta(H)$ is indeed a small number independent of the size of H for every graph $H \in \mathcal{G}$:

Let $0 < \eta < 1$ be a value indicating the confidence level of our criterion. Then, $\delta(H)$ is a small number independent of the size of H for every graph $H \in \mathcal{G}$ if and only if

$$\forall Y \in \{\mathcal{D}, L, L+M+S\} : \Delta^Y(G) = \frac{\text{number of subset of four nodes } \{u_i, u_j, u_k, u_\ell\} \text{ such that } \delta_{u_i, u_j, u_k, u_\ell}^Y > \epsilon}{\binom{n}{4}} < 1 - \eta$$

In the above criterion, larger values of η indicate better confidence levels. An alternative method would be to use the procedure outlines in Section 3.7.

3 Geometric Curvature

There are many well-known measures of curvature of a continuous surface or other similar spaces (*e.g.*, curvature of a manifold) that are widely used in many branches of physics and mathematics. In section 2 we discussed how to relate Gromov curvature to such other curvature notions indirectly via introduction of its scaled version. In this section, we describe a notion of geometric curvatures of graphs by using a correspondence with topological objects in *higher dimension*.

3.1 Basic topological concepts

In this section we review some basic concepts from topology; see introductory textbooks such as [27, 33] for further information. For concreteness of exposition, let

the underlying metric space be the r -dimensional real space \mathbb{R}^r be for some integer $r > 1$. See Fig. 2 for some illustrations of these concepts in \mathbb{R}^3 .

- ▷ A subset $S \subseteq \mathbb{R}^r$ is *convex* if and only if for any pair $x, y \in S$, the *convex combination* of x and y is also in S (i.e., $\lambda x + (1 - \lambda)y \in S$ for any real $0 \leq \lambda \leq 1$).
- ▷ A set of $k + 1$ points $x_0, \dots, x_k \in \mathbb{R}^r$ are called *affinely independent* if and only if for all $\alpha_0, \dots, \alpha_k \in \mathbb{R}$ $\sum_{j=0}^k \alpha_j x_j = 0$ and $\sum_{j=0}^k \alpha_j = 0$ implies $\alpha_0 = \dots = \alpha_k = 0$.
- ▷ The k -*simplex* generated by a set of $k + 1$ affinely independent points $x_0, \dots, x_k \in \mathbb{R}^r$ is the subset of \mathbb{R}^r $\mathcal{S}(x_0, \dots, x_k) = \{ \sum_{j=0}^k \alpha_j x_j \mid \forall j: \alpha_j \geq 0 \text{ and } \sum_{j=0}^k \alpha_j = 1 \}$ generated by *all* convex combinations of x_0, \dots, x_k . For example, the equation of a k -simplex with *unit intercepts* is given by $\sum_{j=0}^k x_j = 1$ with $x_j \geq 0$ for all $0 \leq j \leq k$.
 - ▶ Each $(\ell + 1)$ -subset $\{x_{i_0}, \dots, x_{i_\ell}\} \subseteq \{x_0, \dots, x_k\}$ defines the ℓ -simplex $\mathcal{S}(x_{i_0}, \dots, x_{i_\ell})$ that is called a *face* of dimension ℓ (or a ℓ -*face*) of $\mathcal{S}(x_0, \dots, x_k)$. A $(k - 1)$ -face, 1-face and 0-face is called a *facet*, an *edge* and a *node*, respectively.
- ▷ A (closed) *halfspace* is a set of points satisfying $\sum_{j=1}^r a_j x_j \leq b$ for some $a_1, \dots, a_r, b \in \mathbb{R}$. The convex set obtained by a bounded non-empty intersection of a finite number of halfspaces is called a *convex polytope* (called a *convex polygon* in two dimensions).
 - ▶ If the intersection of a halfspace and a convex polytope is a subset of the halfspace then it is called a *face* of the polytope. Of particular interests are faces of dimensions $r - 1$, 1 and 0, which are called *facets*, *edges* and *nodes* of the polytope, respectively.
- ▷ We can define a partial order relation \prec_f between faces of various dimensions of a simplex or a convex polytope in the usual manner: a ℓ -face f^ℓ is a parent of a ℓ' -face $\hat{f}^{\ell'}$ (denoted by $\hat{f}^{\ell'} \prec_f f^\ell$) if $\hat{f}^{\ell'}$ is contained in f^ℓ . Similarly, two ℓ -faces f^ℓ and $\hat{f}^{\ell'}$ are *parallel* (denoted by $f^\ell \parallel_f \hat{f}^{\ell'}$) if they have either at least one common *immediate predecessor* or at least one common *immediate successor* (in the partial order \prec_f) *but not both*.
- ▷ A *simplicial complex* (or just a complex) is a topological space constructed by the union of simplexes via topological associations.

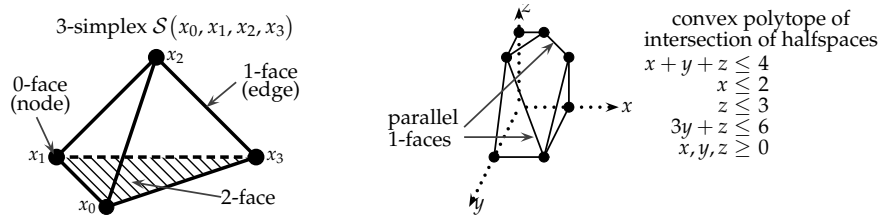


Fig. 2 (modified from [54]) Illustrations of some topological concepts discussed in Section 3.1 over \mathbb{R}^3 .

3.2 Topological association of networks with a complex

Informally, a *complex* is “glued” from nodes, edges, cycles and other sub-graphs of the given graph via topological identification. There are many alternate ways such topological associations can be performed. Here we describe a simple association as used in [21]; for other possible alternative associations the reader is referred to papers such as [11, 25, 63, 64].

To begin our topological association, we (topologically) associate a q -simplex with a $(q + 1)$ -clique \mathcal{K}_{q+1} ; for example, 0-simplexes, 1-simplexes, 2-simplexes and 3-simplexes are associated with nodes, edges, 3-cycles (triangles) and 4-cliques, respectively. Next, we would also need the concept of an “order” of a simplex for more non-trivial topological association. Consider a p -face f^p of a q -simplex. An order d association of such a face, which we will denote by the notation f_d^p with the additional subscript d , is associated with a sub-graph of *at most* d nodes that is obtained by starting with \mathcal{K}_{p+1} and then *optionally* replacing each edge by a path between the two nodes. For example,

- ▷ f_d^0 is a node of G for all $d \geq 1$.
- ▷ f_2^1 is an edge, and f_d^1 for $d > 2$ is a path having at most d nodes between two nodes adjacent in G .
- ▷ f_3^2 is a triangle (cycle of 3 nodes or a 3-cycle), and f_d^2 for $d > 3$ is obtained from 3 nodes by connecting every pair of nodes by a path such that the total number of nodes in the sub-graph is at most d .

Naturally, the higher the values of p and q are, the more complex are the topological associations.

3.3 Defining geometric curvatures for elementary components of given graph

By elementary components of a graph, we mean sub-graphs of small size such as edges, triangles, 4-cycles and so forth. In this section, we discuss the case when the elementary components are edges; the other cases can be found in the previously cited references. As discussed in Section 3.2, geometric curvatures are defined by “extrapolating” graphs to higher-dimensional complexes via topological association. For these associations, it is often useful to assign a positive “weight” from the interval $[0, 1]$ to every pair of nodes (1-simplexes) and to every node (0-simplexes) of the graph $G = (V, E)$. If G comes with its own node or edge weights, we may use them directly after normalizing them such that all weights lie between 0 and 1. Otherwise, some choices for these weights that may be appropriate are the following:

- (a) For every pair of nodes $e_{i,j} = \{v_i, v_j\}$, a natural choice for the weight would be $w_{\text{edge}}(e_{i,j}) = 1$ (*resp.*, $w_{\text{edge}}(e_{i,j}) = 0$) if $\{v_i, v_j\} \in E$ (*resp.*, $\{v_i, v_j\} \notin E$). One may also consider more refined choices, *e.g.*, $w_{\text{edge}}(e_{i,j}) = 1/\text{dist}_G(v_i, v_j)$ or a

“distance-thresholded” version of it, that may be useful in the study of social networks of the “small world” type [63].

- (b) A natural choice for the weight of a node v_i would be $w_{\text{node}}(v_i) = 1$. A more sophisticated choice that one may consider is

$$w_{\text{node}}(v_i) = \frac{\sum_{v_j: w_{\text{edge}}(\{v_i, v_j\}) \geq \gamma} w_{\text{edge}}(\{v_i, v_j\})}{|\{w_{\text{edge}}(e) \mid e \in E \text{ and } w_{\text{edge}}(e) \geq \gamma\}|}$$

that provides more weight to nodes with higher weighted-degree [63].

Once we have fixed a weighting scheme for 0-simplexes and 1-simplexes, we can assign weights to *higher-dimensional* objects such as k -faces as follows:

- 2-faces:** For a triangle, say $\mathcal{S}(v_1, v_2, v_3)$ with $e_{i,j} = \{v_i, v_j\}$ for $i, j \in \{1, 2, 3\}$, we may assign its weight based on the area of the triangle [64]:

$$w(\mathcal{S}(v_1, v_2, v_3)) = \left[s \left(\prod_{\substack{i,j \in \{1,2,3\} \\ i \neq j}} (s - w_{\text{edge}}(e_{i,j})) \right) \right]^{1/2} \text{ where } s = \frac{\sum_{\substack{i,j \in \{1,2,3\} \\ i \neq j}} w_{\text{edge}}(e_{i,j})}{2}$$

For a polygon of p sides with $p > 3$, we can first do a triangulation of the polygon and then add the weights of these triangles to get the weight for the entire polygon.

- k -faces for $k > 2$:** We can compute the weight by adding the weights of the $(k - 1)$ -subfaces of this face (for the degenerate case, we will consider subfaces of dimensions lower than $k - 1$ also). Alternately, for some cases, we may also use direct combinatorial formulae for the volume.

Let $w(f)$ denote the weight of an arbitrary face f .

1-complex-based geometric curvature for a pair of nodes

A graph is naturally defined by 1-simplexes (edges) and 0-simplexes (nodes). Thus, without further topological association, a 1-complex-based Forman’s combinatorial Ricci curvature for a pair of nodes $\{v_i, v_j\}$ is given by [25, 63]:

$$\mathfrak{C}_{i,j}^1 = \begin{cases} 0, & \text{if } w_{\text{edge}}(e_{i,j}) = 0 \\ w_{\text{edge}}(e_{i,j}) \left[\frac{w_{\text{node}}(v_i)}{w_{\text{edge}}(e_{i,j})} + \frac{w_{\text{node}}(v_j)}{w_{\text{edge}}(e_{i,j})} - \sum_{\substack{e_{i,j_1}, e_{i_1,j} \\ w_{\text{edge}}(e_{i,j_1}) \neq 0 \\ w_{\text{edge}}(e_{i_1,j}) \neq 0}} \left(\frac{w_{\text{node}}(v_i)}{\sqrt{(w_{\text{edge}}(e_{i,j})w_{\text{edge}}(e_{i,j_1}))}} + \frac{w_{\text{node}}(v_j)}{\sqrt{(w_{\text{edge}}(e_{i,j})w_{\text{edge}}(e_{i_1,j}))}} \right) \right], & \text{otherwise} \end{cases} \quad (1)$$

2-complex-based geometric curvature for a pair of nodes

For 2-complex-based geometric curvatures, we also include topological associations with 2-simplexes (cycles of 3 nodes). Let $\mathcal{C}(v_i, v_j, v_k)$ denote a cycle of length 3 consisting of the edges $\{v_i, v_j\}$, $\{v_j, v_k\}$ and $\{v_i, v_k\}$. Note that in Equation (1) the edges e_{i,j_1} and $e_{i_1,j}$ in the summation actually satisfy $e_{i,j_1} \parallel e_{i,j}$ and $e_{i_1,j} \parallel e_{i,j}$. This observation helps us to lead to Forman's combinatorial Ricci curvature for 2-complexes [64]:

$$\mathfrak{C}_{i,j}^2 = \begin{cases} 0, & \text{if } w_{\text{edge}}(e_{i,j}) = 0 \\ w_{\text{edge}}(e_{i,j}) \left[\left(\sum_{v_k \neq v_i, v_j} \frac{w(\mathcal{C}(v_i, v_j, v_k))}{w_{\text{edge}}(e_{i,j})} \right) + \frac{w_{\text{node}}(v_i)}{w_{\text{edge}}(e_{i,j})} + \frac{w_{\text{node}}(v_j)}{w_{\text{edge}}(e_{i,j})} \right. \\ \left. - \sum_{\substack{e_{i_1,j_1}: e_{i_1,j_1} \parallel e_{i,j} \\ w_{\text{edge}}(e_{i_1,j_1}) \neq 0}} \left| \sum_{\substack{v_k \neq v_i, v_j \\ w(\mathcal{C}(v_i, v_j, v_k)) \neq 0}} \frac{\sqrt{w_{\text{edge}}(e_{i,j}) w_{\text{edge}}(e_{i_1,j_1})}}{w(\mathcal{C}(v_i, v_j, v_k))} + \sum_{v \in \{v_i, v_j\} \cap \{v_i, v_{j_1}\}} \frac{w_{\text{node}}(v)}{\sqrt{(w_{\text{edge}}(e_{i,j}) w_{\text{edge}}(e_{i_1,j_1}))}} \right| \right], & \text{otherwise} \end{cases} \quad (2)$$

Higher-dimensional geometric curvature for a pair of nodes

k -complex-based curvature $\mathfrak{C}_{i,j}^k$ for $k > 2$ can be defined in a similar manner (e.g., a clique of $k + 1$ nodes correspond to a k -simplex).

3.4 Overall (scalar) curvature value for a network

One can compute a single scalar value \mathfrak{C} of geometric curvature based on the values of $\mathfrak{C}_{i,j}^k$ values using curvature functions defined by Bloch [11], by using *Euler characteristics* [21] or similar other methods. We discuss the simplest unweighted Euler characteristics based scalar graph curvature as used by DasGupta *et al.* in [21]. Let \mathcal{F}_d^k be the set of all f_d^k 's that are topologically associated as described in Section 3.2. With such associations via p -faces of order d , the Euler characteristics of the graph $G = (V, E)$ and consequently the curvature can be defined as

$$\mathfrak{C}_d^p(G) \stackrel{\text{def}}{=} \sum_{k=0}^p (-1)^k |\mathcal{F}_d^k|$$

It is easy to see that both $\mathfrak{C}_d^0(G)$ and $\mathfrak{C}_d^1(G)$ are too simplistic to be of use in practice. Considering the next higher value of p , namely $p = 2$, and letting $\mathcal{C}(G)$ denote the number of cycles of at most $d + 1$ nodes in G , we get the following scalar curvature measure for a given graph $G = (V, E)$:

$$\mathfrak{C}_d^2(G) = |V| - |E| + |\mathcal{C}(G)| \quad (3)$$

3.5 Computation of geometric curvatures

Let $G = (V, E)$ be the given connected graph with n nodes and m edges. Using Equations (1) and (2) and appropriate data structures, $\mathfrak{C}_{i,j}^1$ and $\mathfrak{C}_{i,j}^2$ can be computed roughly in $O(m^2)$ and $O(m^3)$ times, respectively. More generally, $\mathfrak{C}_{i,j}^k$ can be computed in $O(m^{O(k)})$ time and $\mathfrak{C}_d^2(G)$ in Equation (3) can be computed in $O(m^d)$ time.

3.6 Real-world networks and geometric curvatures

The usefulness of geometric curvatures for real-world networks was demonstrated in publications such as [59, 63, 64]. Some of these results are as follows.

- ▷ Samal *et al.* in [59] empirically compared geometric curvatures of the type discussed in this chapter with another notion of network curvature, namely the Ollivier's discretization of Ricci curvature [53]. Although the Ollivier-Ricci curvature measures were developed based on quite different properties of the classical smooth notion as compared to the geometric curvatures discussed in this chapter, somewhat surprisingly they found that these two measures are correlated for many real networks. However, as the authors themselves cautioned in [53], their results should not be construed as implying that one of these curvature measures can be used as a *universal substitute* for the other measure, but merely that for many real networks using one of these that allow faster implementation may suffice.
- ▷ Weber, Saucan and Jost in [64] computed a specific version of the geometric curvatures discussed in this chapter (the ‘‘Euler characteristics’’ with only up to 2-faces of degree 3) for several real-world networks, such as Zachary's karate club, social interactions of dolphins and *E. coli* transcription networks, and showed that networks with a high number of high-degree faces have positive Euler characteristics whereas low numbers of high-degree faces might hint on negative Euler characteristics.

3.7 Statistical validations for all curvature measures

We may test the statistical significance of any curvature measure $\mathfrak{C}(G)$ by computing its statistical significance value (commonly called *p-value*) with respect to a *null hypothesis model* of the network. For this purpose, we may use a method as described below that is similar to that used by many other researchers in the network science literature (*e.g.*, see [2, 60]). For each graph G , we will generate a large number q of random graphs G_1, \dots, G_q of the *same* type as G . There are many methods for generating such random graphs. Two such methods are as follows.

Generative null-hypothesis models: One most frequently reported topological characteristics of graphs is the distribution of degrees of nodes. We may select appropriate degree distributions for our given class of graphs that is consistent with the findings in prior literature. For example, based on the known topological characterizations for biological *transcriptional* and *signaling* networks we may use the following degree distributions [1, 30, 43]: (**a**) the in-degree distribution is *exponential*, and (**b**) the out-degree distribution is governed by a *power-law*. Random networks with prescribed degree distributions can be generated using the method by Newman *et al.* [52].

Non-generative null-hypothesis models: For graphs where a consensus degree distribution may be difficult to ascertain, we can use the following methods:

- ▷ We may generate random networks using a *Markov-chain algorithm* [38] by repeatedly swapping randomly chosen compatible pairs of connections in G .
- ▷ We may generate random networks from the degree-distribution of G using the method pioneered by Newman and others in [31, 42, 48, 49, 51] that preserves *in expectation* the degree distribution of each node.

Once the random graphs G_1, \dots, G_q have been generated, we first compute the values of $\mathfrak{C}(G_1), \dots, \mathfrak{C}(G_q)$, and next use a suitable statistical test to determine the probability that $\mathfrak{C}(G)$ belongs to the same distribution as $\mathfrak{C}(G_1), \dots, \mathfrak{C}(G_q)$.

4 Two applications of curvature analysis of graphs

In this section, we discuss two applications for curvature measures in graphs, namely in finding *critical* elementary components and in detecting *change-points*.

4.1 Detecting critical elementary components of networks

Often real-world networks may have so-called *critical* elementary components (or simply critical components) whose absence alter some significant *non-trivial global* property of these networks. For example, there is a rich history in finding various types of critical components of a networks dating back to quantifications of *fault-tolerances* or *redundancies* in electronic circuits or routing networks. Recent examples of practical application of determining critical components in the context of systems biology include quantifying redundancies in biological networks [2, 40, 61] and confirming the existence of central influential neighborhoods in biological networks [3]. Network curvatures can be applied to these kinds of problems by using the curvature measure as the non-trivial global property of a network. We discuss below a simple formalization of these types of problems as used in [21] where edges are elementary components and they can only be added or deleted but *not* both.

Thus, in this setting, the basic question is to find a subset (optionally among a set of prescribed edges) whose deletion may change the network curvature significantly. This question was formalized as the *extremal anomaly detection problem* in [21] in the following manner.

Definition 5 (Extremal Anomaly Detection Problem (EADP)). [21] Given a connected graph $G = (V, E)$, a curvature measure $\mathcal{C} : G \mapsto \mathbb{R}$, an edge subset $\tilde{E} \subseteq E$ such that $G \setminus \tilde{E}$ is connected, and a real number $\gamma < \mathcal{C}(G)$ (resp., $\gamma > \mathcal{C}(G)$) find an edge subset $\hat{E} \subseteq \tilde{E}$ of minimum cardinality such that $\mathcal{C}(G \setminus \hat{E}) \leq \gamma$ (resp., $\mathcal{C}(G \setminus \hat{E}) \geq \gamma$).

4.2 Detecting change points in dynamic networks

Another application similar to that in Section 4.1 is related to change point detection in dynamic (*i.e.*, time-evolving) networks. Dynamic networks are networks whose elementary components (such as nodes or edges) are added or removed as the network evolves over time. Examples of such networks include biological signal transduction networks with node dynamics, biochemical reaction networks and dynamic social networks. The *anomaly detection* or *change-point detection* problem for such networks involve finding elementary components whose addition and/or removal alters a significant topological property of the network between two *successive* time steps. There is an extensive history of research works dealing with change point detection problems over the last several decades in the “non-network” context of time series data [4, 39] with applications to areas such as medical condition monitoring [12, 65], weather change detection [24, 56] and speech recognition [15]. Again using edges as elementary components and the assumption that edges can only be added or deleted but *not* both, a simple formalization of these type of problems under the name “Targeted Anomaly Detection Problem” appeared in [21]. The formalization is as follows.

Definition 6 (Targeted Anomaly Detection Problem (TADP)). [21] Given two connected graphs $G_1 = (V, E_1)$ and $G_2 = (V, E_2)$ with $E_2 \subset E_1$ and a curvature measure $\mathcal{C} : G \mapsto \mathbb{R}$, an edge subset $E_3 \subseteq E_1 \setminus E_2$ of minimum cardinality such that $\mathcal{C}(G_1 \setminus E_3) = \mathcal{C}(G_2)$.

For both these applications (*i.e.*, for both the problems EADP and TADP stated in the previous two sub-sections), the authors in [21] prove several algorithmic results for both the cases when \mathcal{C} is the Gromov curvature and when \mathcal{C} is the geometric curvature given by Equation (3) with fixed d . Informally, some of the results proved in [21] are as follows:

- ▷ When \mathcal{C} is the Gromov curvature, it is NP-hard to design a polynomial-time algorithm to approximate both EADP and TADP within a factor of cn for some constants $c > 0$, where n is the number of nodes (the hardness result for EADP holds only for the case when $\gamma > \mathcal{C}$).
- ▷ The following results hold when \mathcal{C} is the geometric curvature:

- ▷ EADP is NP-hard but admits a non-trivial approximation algorithm when either γ is sufficient larger than \mathfrak{C} or γ is not too far below \mathfrak{C} .
- ▷ Polynomial time approximation of TADP within a factor of 2 is hard.

5 Conclusion

Notions of curvatures play a fundamental role in physics and mathematics for visualizing higher-dimensional geometric shapes and topological spaces. However, usage of curvature measures for networks is *not* yet very common due to several reasons such as lack of preferred geometric interpretation of networks and lack of experimental evidences that may lead to specific desired curvature properties. In this chapter we have reviewed two curvature measures for networks, namely the Gromov-hyperbolic and the geometric curvature measures, and two motivating applications of these curvature measures, and we hope that this review will act as a stimulator and motivator of further theoretical or empirical research on the exciting interplay between notions of curvatures from network and non-network domains.

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