Coarse Ricci curvature and flow in graph problems

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Abstract

We survey a recently developed geometric approach to complex network analysis. As a generalization of the Ricci curvature on Riemannian manifolds, the coarse Ollivier-Ricci curvature describes local shape of graphs by their local connectivity. This is quantified by optimal transport distance of transition probabilities of a random walk on the graph. Novel graph embeddings via the coarse curvature have been proposed and applications have been found in network robustness analysis, community detection and noisy graph alignment.

1 Introduction

Much of real-world data comes naturally in the form of graphs. Graphs are nodes connected by edges which can furthermore be equipped with numerical weights and both numerical and non-numerical attributes. Practical examples where the data consists of a collection of individuals with some connectivity structure include social networks, internet traffic, and protein-protein interaction networks.

Network structure has been investigated in the past by statistical and graph-theoretical tools, using notions such as edge betweenness centrality, farness centrality, node degree distribution. From a geometric perspective, on the other hand, an efficiently computable and interpretable "coarse" Ricci curvature for general metric spaces (and hence weighted graphs) offers a fresh perspective on computational graph problems.

The coarse notion of curvature discussed here was introduced by Y.Ollivier in [Oll09], along with proofs that the coarse curvature agrees with smooth Ricci curvature on Riemannian manifolds and carries over many (though not all) properties from the smooth to the coarse case. An informal visual introduction to what is presented in this section can be found in [Oll10]. For elementary definitions and results in Riemannian geometry, see for example J. Jost's textbook [Jos17].

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2 Ollivier-Ricci coarse curvature

We lay out a notion of coarse curvature that is inspired by properties of parallel transport of spheres and balls on Riemannian manifolds. The coarse Ricci curvature, sometimes called Ollivier-Ricci curvature in the literature, uses for its definition larger scale properties of the space instead of the infinitesimal property of differentiation of functions near a point as in the case of common notions of curvature on Riemannian manifolds. In particular, the key insight of Ollivier [Oll09] is that curvature is related to transport distance of balls on the manifold in the limit as the centers of the two balls get arbitrarily close.

In the following, let (M, g) be a complete Riemannian manifold. Let $x \in M$ and $v, w_x \in T_xM$ and define $y := \exp_x v$ the endpoint of the geodesic starting from x in the direction of the tangent vector v. The tangent vector $w_y \in T_yM$ is one which is obtained by transporting $w_x \in T_xM$ along the geodesic between x and y to T_yM.

An observation about local behaviour of geodesics is that if the sectional curvature $K(v, w_x)$ is positive and y is close to x, the two geodesics emanating from x in the direction w_x and from y in the direction w_y will come closer to each other in the neighbourhood of x and y. Similarly, if $K(v, w_x)$ is negative then the two geodesics will drift apart locally.

Quantitatively, the sectional curvature $K(v, w)$ can be characterized by the following asymptotic relationship.

Lemma 1. *[Oll09] Let $x \in M$ and $v, w_x \in T_xM$ unit tangent vectors. Let $\delta, \epsilon > 0$, $y := \exp_x \delta v$ and $w_y \in T_yM$ the unit tangent vector obtained by parallel transport of w_x from x along v to y. Then*

$$d\left(\exp_x \varepsilon w_x, \exp_y \varepsilon w_y\right) = \delta\left(1 - \frac{\varepsilon^2}{2}K(v, w) + O\left(\varepsilon^3 + \varepsilon^2\delta\right)\right)$$

as $(\delta, \epsilon) \to 0$.

The Ricci curvature $Ric(v, v)$ is the average of the sectional curvature $K(v, w)$ over w on the unit circle in the tangent space T_xM. One can then show the following analogous result for the Ricci curvature.

Lemma 2. *[Oll09] Let $B_\epsilon(x), B_\epsilon(y)$ be balls of radius ϵ in T_xM and T_yM respectively. The average distance between points of $B_\epsilon(x)$ and their parallel transport images in $B_\epsilon(y)$ is*

$$\delta\left(1 - \frac{\varepsilon^2}{2(N+2)}\operatorname{Ric}(v, v) + O\left(\varepsilon^3 + \varepsilon^2\delta\right)\right)$$

as $(\delta, \epsilon) \to 0$.

The intuition to support this result is that on Riemannian manifolds with positive curvature (that is, locally sphere-like surfaces), the transportation distance of two balls with centers that are close to each other is on average smaller than the distance of the centers.

In general metric spaces, there is no notion of either a tangent space or parallel transport. Nonetheless, Lemma motivates a definition of curvature that does not rely on a smooth structure of the space. The balls $B_\epsilon(x)$ and $B_\epsilon(y)$ can be substituted with probability measures m_x, m_y with finite first moments and optimal transport distance (Wasserstein distance) W_1 can be used in place of parallel transport. This yields

Definition 1. [Oll09] Let $(X.d, m)$ be a metric space equipped with a Markov transition kernel $m = (m_x)_{x \in X}$. The coarse curvature between two points x and y is defined as

$$K(x, y) = 1 - \frac{W_1(m_x, m_y)}{d(x, y)}$$

It was shown in [Oll09] that this definition indeed coincides with Ricci curvature $\mathrm{Ric}(v, v)$ in the limit as $y \to x$.

3 Applications

We follow a line of work by C.-C. Ni et al. [Ni+15] [Ni+18] [Ni+19] which investigates properties of real-world networks as well as generative models for networks from the perspective of Ollivier-Ricci curvature and the associated curvature flow. Another related prominent line of work on discrete curvature in the complex network setting is [WSJ17] [Sau+18] [Sam+18] [Sre+16] which will nonetheless be omitted in this article.

For a basic setup, we consider the metric space generated by an undirected graph $G = (V, E)$ with edge weights $w : E \to \mathbb{R}_+$, associated metric

$$d(x, y) := \inf_{J \in \mathbb{N}} \left\{ \sum_{j=0}^{J-1} w_{x_j x_{j+1}} : x_0 = x, x_J = y, (x_j, x_{j+1}) \in E \right\}, \quad x, y \in V$$

and equipped with a nearest neighbour random walk defined by the transition probabilities

$$m_x^{\alpha,p}(y) = \begin{cases} \alpha, & y = x \\ \frac{1-\alpha}{C} \exp(-d(x, y)^p), & (x, y) \in E \\ 0 & \text{otherwise} \end{cases}$$

where $C := \sum_{y:(x,y) \in E} \exp(-d(x, y)^p)$ is a normalising constant.

3.1 Computing the curvature

Let $(x, y) \in E$ and let $\{x_i\}, \{y_j\}$ be vertices adjacent to x and y respectively. Computing the optimal transport distance $W_1(m_x, m_y)$, and hence the coarse curvature $\kappa(x, y)$ of the edge (x, y), corresponds to solving the linear program

$$\text{minimize} \sum_{i,j} d(x_i, y_j) M(x_i, y_j)$$

$$\text{with constraints} \begin{cases} \sum_j M(x_i, y_j) = m_x(x_i) & \forall i \\ \sum_i M(x_i, y_j) = m_y(y_j) & \forall j \end{cases}$$

minimizing over all stochastic matrices $M : V \times V \to [0, 1]$. These matrices are called transfer plans from m_x to m_y.

It is known that this can be computed for all edges in polynomial time with respect to the number of edges. Nonetheless, finding the *optimal* transport becomes costly for large networks. Ni et al. [Ni+18] propose a computational workaround by choosing a *sub-optimal* transfer plan, namely one which transports equal mass from each neighbour x_i of x to every neighbour y_j of y. Denoting the corresponding distance between x, y as $A(m_x, m_y)$, this yields the alternative definition

$$\kappa^a(x, y) := 1 - \frac{A(m_x, m_y)}{d(x, y)}$$

The approximate curvature κ^a can then be computed in linear time with respect to total number of edges. Empirical results show that this curvature exhibits properties similar to the original curvature κ.

3.2 Empirical properties of curvature

The authors in [Ni+15] conducted an empirical study of the distribution of the coarse Ricci curvature in common generative graph models as well as in several real-world networks related to the Internet. The authors found negative correlation of the curvature and edge betweenness centrality measure, and substantial positive correlation between curvature and both of the measures of clustering coefficient and farness centrality.

Moreover, important bridging edges tend to have negative curvature. The authors show that removing such edges quickly leads to dividing the graph into multiple connected components. This supports the intuitive thesis that edges with high negative curvature contribute to global network connectivity.

3.3 Community detection

Inspired by Hamilton's Ricci flow, the Ricci flow deforming the metric can be defined similarly for coarse spaces. In the same way that the Ricci flow on smooth manifolds separates geometric components, the authors in [Ni+19] proposed that the coarse analogy may separate communities in a network. Moreover, depending on how many steps the Ricci flow is left running, communities on multiple scales may be discovered.

Definition 2. [Ni+19] The metric $d(x, y)$ is said to follow the Ollivier-Ricci curvature flow if it satisfies

$$\frac{d}{dt}d(x, y) = -\kappa(x, y)d(x, y)$$

In their applications, the authors [Ni+19] approximate the solution numerically by the scheme

$$\begin{aligned} w^{(0)}(x, y) &:= w(x, y) \\ w^{(i+1)}(x, y) &:= d^{(i)}(x, y)(1 - \kappa^{(i)}(x, y)) \\ d^{(i+1)}(x, y) &:= \inf \left\{ \sum_{j=0}^{n} w^{(i)}(x_j, x_{j+1}) : x_0 = x, x_{n+1} = y, (x_j, x_{j+1}) \in E \right\} \end{aligned}$$

The Ollivier-Ricci flow increases the weights of edges with negative curvature and these edges usually connect communities. Hence, if edges with weights above a certain threshold are removed, one can isolate connected components of the graph as communities. This heuristic is applied in [Ni+19] to real-world networks as well as generative models. For example, the authors test this on a sample Facebook social network of 792 vertices and 14025 edges, detecting all 24 ground truth communities.

The clustering ability of the coarse Ricci flow algorithm is compared in [Ni+19] based on the Adjusted Rand Index clustering measure with other algorithms that are prevalent in the literature, such as the spinglass model, an edge betweenness based algorithm, and the infomap algorithm. The comparison is performed with respect to the stochastic block model (a generative model for graphs with communities) and various ratios of intra- and interconnectedness of communities, $\frac{p_{inter}}{p_{intra}}$. The authors conlude that the Ricci curvature algorithm is very robust to this ratio and performs on par with the spinglass model and performs better than the other algorithms mentioned above.

Moreover, along the progression of the Ricci flow and upon subsequent removals of the detected backbone edges, several scales of modular structure can be detected in networks. This is demonstrated on the GNet generative model as well as the aforementioned Facebook network example.

3.4 Noisy graph alignment

Ni et al. [Ni+18] address the following problem. Suppose $G_1 = (V_1, E_1)$ is an undirected graph and $G_2 = (V_2, E_2)$ is a subgraph of G_1 that is obtained by randomly removing some nodes and edges from graph G_1. Assume now that the vertex and edge labels are hidden. The graph alignment problem is to match the nodes of G_1 with those of G_2 with minimal misalignment, the measure of which is to be defined.

A graph embedding is a representation of graph vertices as vectors in a Euclidean space. The authors use the discrete Ricci flow to define a graph embedding which they found to be efficient in solving this noisy graph alignment problem.

Let $G = (V, E, w)$ be an undirected weighted graph and reference vertices $v_1, \ldots, v_k \in V$. Run the discrete Ricci flow until convergence and obtain a new metric d_R on G, called the Ricci flow metric. Define the coordinates of a vertex v with respect to the reference points in $\mathbb{R}^k$ as

$$v_L := [d_R(v, v_1), \ldots, d_R(v, v_k)] \in \mathbb{R}^k$$

For every pair $u \in V_1, v \in V_2$ and any metric d on $\mathbb{R}^k$, define the alignment cost $C_{uv} := \|u - v\|_2 = \sqrt{\sum_{i=1}^{k}(d(u, v_i) - d(v, v_i))^2}$. Several $\mathbb{R}^k$ embeddings (and their corresponding metrics) existing in the literature are compared with respect to recovery accuracy that they yield. The alignment algorithms based on these embeddings are optimized with respect to total alignment cost of G_1 to G_2, that is

$$\sum_{u \in V_1, v \in V_2} C_{uv}$$

using the Hungarian algorithm, which is an alternative to the greedy algorithm. This cost is a summary of recovery accuracy upon graph alignment.

The authors demonstrate superior performance of the Ricci metric as compared with a spectral and spring embeddings, IsoRank and Network Similarity Decomposition algorithms, in generative model networks as well as several real-world networks.

4 Conclusion

The works mentioned in this article demonstrate that the coarse Ricci curvature and flow offer innovative tools for the study of complex network properties which differ substantially from existing tools of complex systems theory and unsupervised learning. Although some empirical studies have been conducted, many of the mentioned concepts remain largely unexplored from the perspective of discrete geometry, for example the convergence of the space along the Ricci flow in the Gromov-Hausdorff-Prokhorov topology or the sensitivity of the curvature and flow to the choice of the Markov transition kernel.

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