Ricci curvature on Graphs

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Theory

We will first present the theoretical framework. Subsequently we will discuss about our implementation and design details and then the experimentation and its applications.

Lemma 1 : A temporally changing network can be thought of a discrete Riemannian manifold, equipped with a probability measure, dynamically changing w.r.t. time.

Definition 2 : Curvature of a geometric surface is defined as the deviation from being flat in this context whereas, intrinsic curvature, is defined at each point on a Riemannian manifold, independent on the embedding, i.e. how the manifold is realized in an ambient euclidean space.
For instance, for a surface M in R^3, a point $p : p \in M$, the plane containing the tangent vector T and surface normal N, cut out a curve of surface M through p. The normal curvature of M is defined to be the curvature of this curve. The principal curvature k_1 and k_2 are defined to be the maximum and minimum of the normal curvatures. The Gaussian curvature is defined to be $k_1 k_2$. It is positive for spheres, negative for one-sheet hyperboloid and zero for planes. It also has the character of being locally saddle (-ve) or locally convex (+ve).

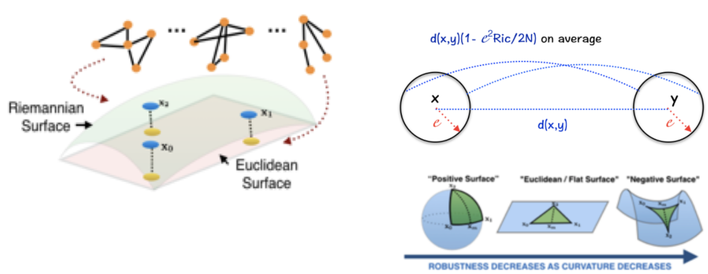

Figure 1: [Left] Visualisation of the manifold; [Top Right] Definition of curvature; [Bottom Right] Positive, zero and negative curvature

Definition 3 : Let M be a n-dimensional Riemannian manifold, $x \varepsilon M$ and $T_x M$ is the tangent space at x and $u_1, u_2 \varepsilon T_x M$ are orthonormal vectors. For geodesics $\gamma_i = exp(t\mu_i) : i = 1, 2$, sectional curvature, deviation of geodesics w.r.t. euclidean geometry, $K(u_1, u_2)$ is defined as

$$d(\gamma_1(t), \gamma_2(t)) = \sqrt(2)t(1 - \frac{K(u_1, u_2)}{12}t^2 + O(t^4))$$

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The Ricci-curvature is defined to be the average sectional curvature. For a given unit vector $u\varepsilon T_x M$,

$$Ric(u) = \frac{1}{n-1}\sum_{2}^{n} K(u, u_i)$$

Corollary 4 : As we mentioned, in the previous formal definition, if point x and y are on surface M, and v is a tangent vector from x to y, let's take another tangent vector w_x and transport it along v till y, to become a tangent vector w_y. if x' and y' are the other end points of w_x and w_y,

$$\text{the surface is flat} \iff xx'y'y \text{ is a triangle}$$

Otherwise, $x'y' \neq |\overline{v}|$, and this difference is used to define sectional curvature. Ricci curvature is the average sectional curvature over all directions of w, it only depends on v.

Definition 5 : Monge's Problem defined in 1781, where it is defined as: some mass has to be transferred from one space X with Borel probability measure μ to another space Y equipped with ν, where the cost of transporting a unit mass from x to y is $c(x, y)$ where $c : X \times Y \rightarrow R$, where $R \geq 0$ assuming the cost of transportation per unit distance is constant. The solution should look for an optimal transport plan $T : X \rightarrow Y$ with $inf \int_X c(x, T(x))d\mu(x)$ | T : transportation

Definition 6 : Let X be a metric measure space equipped with distance d where μ_1 and μ_2 are two measures of same mass. Now, $\mu : \mu_1 \rightarrow \mu_2$ is a $X \times X$ coupling or a mass preserving transportation plan, $\mu\varepsilon\Pi(\mu_1, \mu_2)$ such that,

$$\int_y d\mu(x, y) = d\mu_1(x)$$

$$\int_x d\mu(x, y) = d\mu_2(y)$$

Wasserstein/ Earth Mover/ Kantorovich-Rubenstein distance between x and y is defined as

$$W_p(\mu_1, \mu_2) = [\inf_{\mu\varepsilon\Pi(\mu_1,\mu_2)} \int\int d(x, y)^p d\mu(x, y)]^{1/p}$$

Definition 7 : According to analytical definition of convexity, if a function $f : R^n \rightarrow R$ is C^2, the convexity can be characterized by $\nabla^2 f(x) \geq 0$. On the other hand, according to synthetic definition of convexity, f is convex if $f((1-t)x + ty) \leq (1-t)f(x) + tf(y)\ \forall x, y\varepsilon R^n$ and $t\varepsilon[0, 1]$

Lemma 8 : In a Riemannian manifold setting M, if P(M) is a probability measure equipped with a Wasserstein-2 distance metric, and μ_t is the geodesic curve on P(M),

$$Ric \geq 0 \iff t \rightarrow \int \mu_t \log \mu_t \text{ curve is convex in t}$$

Hence, the lower bound of Ricci curvature is related to entropy.

Definition 9 : If (X, d, m) is a geodesic space, a probability measure P can be set as,

$$P(X, d, m) = \mu \geq 0 : \int_x \mu dm = 1$$

$$P^*(X, d, m) = \mu\varepsilon P(X, d, m) : \overline{\lim}_{\varepsilon\rightarrow 0^+} \int_{\mu\geq\varepsilon} \mu \log \mu dm < \infty$$

Hence it can be defined,

$$H(\mu) = \overline{\lim}_{\varepsilon \to 0^+} \int_{\mu \geq \varepsilon} \mu \log \mu dm \ , \forall \mu \varepsilon P^*(X, d, m)$$

It can be noted, that Boltzmann's Entropy $S(\mu) = -H(\mu)$ and hence, if $H(\mu)$ is convex, $S(\mu)$ is concave.

Theorem 10 : If for the geodesic space, X's ricci curvature is bounded from below by $k \ \forall \mu_0, \mu_1 \ \varepsilon P(X) \ \exists$ a constant speed geodesic μ_t w.r.t. Wasserstein metric connecting μ_0 and μ_1 such that,

$$S(\mu_t) \geq tS(\mu_0) + (1-t)S(\mu_1) + \frac{kt(1-t)}{2} W(\mu_0, \mu_1)^2 : 0 < t < 1$$

$$\implies \Delta S \times \Delta Ric \geq 0$$

Theorem 11 : The fluctuation theorem for networks consider random fluctuation of a given network that result in perturbation of some observed variable. If $p_\varepsilon(t)$ is the probability that the mean of the observed variable deviates more than ε from the unperturbed value at time t. Hence, $p_\varepsilon(t) \to 0$ at $t \to \infty$. The relative rate function is defined as $R = \lim_{t \to \infty}(-\frac{1}{t} \log p_\varepsilon(t))$. It is worth noting that R is negatively correlated with the amount of deviation. And,

$$\Delta S \times \Delta R \geq 0$$

Corollary 12 : From Theorem 6 and Theorem 7, it can be safely extended to claim $\Delta R \times \Delta Ric \geq 0$.

Definition 13 : Let's say (X, d) is a metric space equipped with a probability measure $\mu_x : x \in X$. Ollivier-Ricci curvature $\kappa(x, y)$, in a discrete setting such as a graph, along the geodesic connecting x and y is defined as

$$W_1(\mu_x, \mu_y) = (1 - \kappa(x, y))d(x, y)$$

where d is geodesic distance on the graph and it is measured as $d_x = \sum_y w_{xy}$ and w_{xy} is the weight of the edge connecting x and y, (it is zero when there is no such edge), hence one step random walk from x in the graph is measured as $\mu_x(y) = \frac{w_{xy}}{d_x}$.

Lemma 14 : As have been suggested by past researchers, in a discrete graphical setting G, for a vertex $X \in G$ with degree of freedom $k = |\Gamma(x)|$, let the neighbors be $\Gamma(x) = x_1, x_2, ...x_k$. The probability measure μ_x is defined as.

$$\begin{aligned} \mu_x^\alpha &= \alpha : x_i = x \\ &= (1-\alpha)/k : x_i \in \Gamma(x) \\ &= 0 : otherwise \end{aligned}$$

Lemma 15 : With linear programming (LP) model, the Wasserstein distance can be formulated between two nodes in a graph, only with the local knowledge. The LP model for $W(\mu_x^\alpha, \mu_y^\alpha)$ is represented as a $m \times n$ matrix, where $\rho_{ij} \geq 0$ refers to the mass transported from vertex x_i to y_j.

We try to find:

$$W(\mu_x^\alpha, \mu_y^\alpha) = inf[\sum_j \sum_i d(x_i, y_j)\rho_{ij}\mu_x^\alpha(x_i)] : \sum_j \rho_{ij} = 1 \ \forall i, \rho_{ij}\varepsilon[0, 1] \ \forall i, j,$$

$$\sum \rho_{ij}\mu_x^\alpha(x_i) = \mu_y^\alpha(y_j) \ \forall j$$

Definition 16 : The discrete Ricci flow on a network is defined as an evolving process, where in each iteration, we update the edge weights by the following formula:

$$w_{xy}^{i+1} = d^i(x,y) - k_{xy}^i \times d^i(x,y)$$

Definition 17 : The scalar curvature in general is defined as $S(x) = \sum_y \kappa(x,y)$. So, in discrete setting it can be defined as $\overline{S}(x) = \sum_y \kappa(x,y)\mu_x(y)$. We keep on repeating this until $|k_{xy}^i - k_{xy}^{i-1}| < \varepsilon$

Definition 18 : Entropy in a discrete setting is defined as $\overline{S}_x = -\frac{1}{\log \overline{d}_x} \sum_y \mu_x(y) \log \mu_x(y)$

Implementation:

The algorithm to get Ricci curvature for the edges of a weighted undirected graph can be presented as follows. The complete implementation is available at `https://github.com/srkaysh/Graph-Ricci-Curvature.git`.

1. we take an adjacency matrix as an input
2. V = number of vertices, we ensure that number of edges, $E \geq 0.8\binom{V}{2}$, so that the graph is connected
3. we get the all pairs shortest path using Dijkstra's algorithm
4. for each pair of adjacent nodes we do the following:

   we calculate the neighbors of the source node and target node and keep them in two arrays, $source - neighbors$ and $target - neighbors$, let's say their size is m and n.

   $d_x = \sum$ weight(source-neighbors) and $d_y = \sum$ weight(target-neighbors)

   $\mu_x = \frac{source-neighbors}{d_x}$ and $\mu_y = \frac{target-neighbors}{d_y}$

   we define $d_{m \times n}$, such that d_{ij} = weight-shortest-path(node i, node j)

   we define ρ, a transportation plan, of the size $n \times m$.

   objective: $min(\mu_x d_{m \times n} \rho_{n \times m})$

   constraints: $\rho_{n \times m}(\mu_x)_{m \times 1} = (\mu_y)_{n \times 1}$ [mass preservation law], $\sum \rho_{\text{row-wise}} =$ [1, 1, ... m terms] and $0 \leq \rho_{i,j} \leq 1$ $\forall$ i,j

   m being the solution, Ricci-curvature = $1 - \frac{m}{\text{hop-distance(source, target)}}$

Results:

Experiment 1:

The graph is shown in picture and the edge weights taken are as follows:

1. source node = 1, target node = 2, weight = 6
2. source node = 1, target node = 5, weight = 3
3. source node = 1, target node = 6, weight = 3
4. source node = 2, target node = 3, weight = 20

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('number of nodes', 7)
('number of edges', 9)
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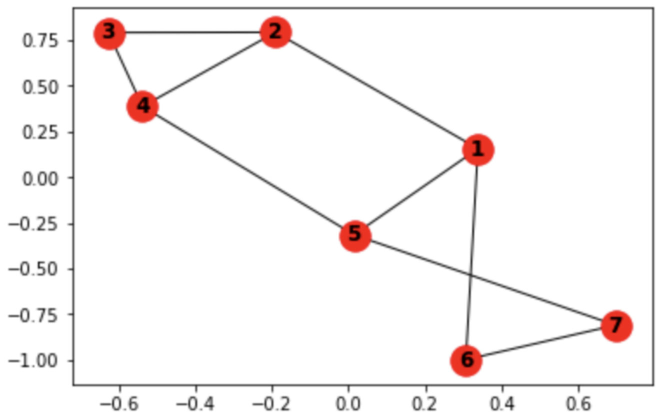

Figure 2: A synthetic graph to have the experiments

5. source node = 2, target node = 4, weight = 6
6. source node = 3, target node = 4, weight = 25
7. source node = 4, target node = 5, weight = 6
8. source node = 5, target node = 7, weight = 6
9. source node = 6, target node = 7, weight = 6

For all the pairs of nodes, the discrete Ricci curvatures are as follows.

1. source node = 1, target node = 2, 'Olivier-Ricci curvature: ', -1.5520833334097541
2. source node = 1, target node = 5, 'Olivier-Ricci curvature: ', -0.9000000000675072
3. source node = 1, target node = 6, 'Olivier-Ricci curvature: ', -1.5000000000529874
4. source node = 2, target node = 3, 'Olivier-Ricci curvature: ', 0.24548611091372918
5. source node = 2, target node = 4, 'Olivier-Ricci curvature: ', 0.5456081080504109
6. source node = 3, target node = 4, 'Olivier-Ricci curvature: ', 0.341861861836402
7. source node = 4, target node = 5, 'Olivier-Ricci curvature: ', -2.542342343262393
8. source node = 5, target node = 7, 'Olivier-Ricci curvature: ', 0.0999999996485249
9. source node = 6, target node = 7, 'Olivier-Ricci curvature: ', 0.16666666666666696

Experiment 2:

Later we devised a random graph generation protocol, that will create a connected graph and measure the Ricci and scalar curvature. Please take a look in out Github link provided. The adjacency matrix is given as:

$$\begin{matrix} 0. & 0. & 3. & 5. & 0. & 0. & 0. & 4. \\ 0. & 0. & 7. & 0. & 0. & 0. & 1. & 0. \\ 3. & 7. & 0. & 0. & 0. & 7. & 0. & 6. \\ 5. & 0. & 0. & 0. & 6. & 2. & 4. & 0. \\ 0. & 0. & 0. & 6. & 0. & 8. & 1. & 0. \\ 0. & 0. & 7. & 2. & 8. & 0. & 0. & 0. \\ 0. & 1. & 0. & 4. & 1. & 0. & 0. & 0. \\ 4. & 0. & 6. & 0. & 0. & 0. & 0. & 0. \end{matrix}$$

The result that we had is as follows:

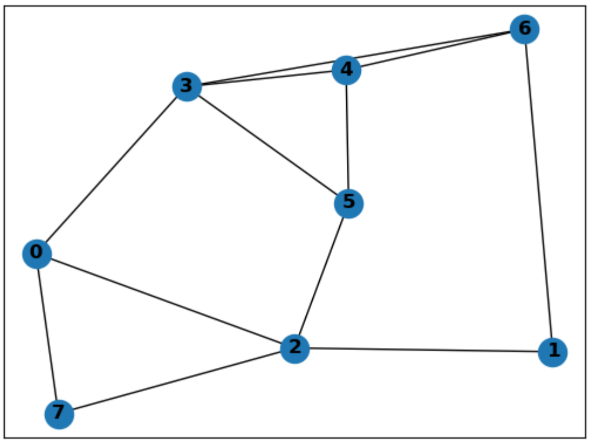

Figure 3: A randomly generated graph to generate Ricci and scalar curvature

1. source: 0, target: 2, Olivier-Ricci curvature: 0.007246375949974571
2. source: 0, target: 3, Olivier-Ricci curvature: -0.050000000043875836
3. source: 0, target: 7, Olivier-Ricci curvature: -0.03333333418645945
4. source: 1, target: 2, Olivier-Ricci curvature: 0.21894409913674573
5. source: 1, target: 6, Olivier-Ricci curvature: -6.00000000054448
6. source: 2, target: 5, Olivier-Ricci curvature: 0.4184782598317718
7. source: 2, target: 7, Olivier-Ricci curvature: 0.11594202540880472
8. source: 3, target: 4, Olivier-Ricci curvature: 0.0711538459805473
9. source: 3, target: 5, Olivier-Ricci curvature: -0.15625000005265233
10. source: 3, target: 6, Olivier-Ricci curvature: 0.23958333330425508
11. source: 4, target: 5, Olivier-Ricci curvature: 0.26510988913964584
12. source: 4, target: 6, Olivier-Ricci curvature: -1.4358974359231937
13. The scalar curvature is: -6.339022941998916

Future Work:

We want to extend this work to calculate discrete Ricci flow on networks in a C++ implementation and apply it on different networks (like social network, internet, cancer network) to design an experimental framework for the mathematical advancement made in these genre.

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