Ricci curvature and local clustering of graphs

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Outline

- Ollivier's Ricci curvature ←----→ Local clustering
- Curvture dimension inequality ←----→ Local clustering
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Many estimates are also obtained on weighted graphs, and even graphs with self-loops. For simplicity, we constraint ourself on unweighted simple graphs.

Ricci curvature

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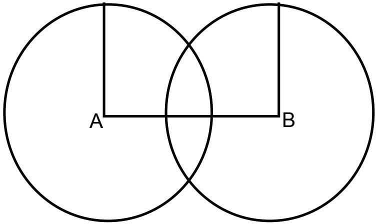
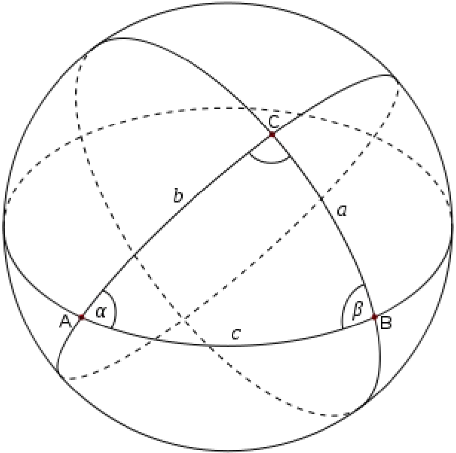
- It controls how fast geodesics starting at the same point diverge on average. Equivalently, it controls how fast the volume of distance balls grows as a function of the radius.
- It also controls the amount of overlap of two distance balls in terms of their radii and the distance between their centers. In fact, such upper bounds follow from a lower bound on the Ricci curvature.



Geodesics on a sphere



from:www.johndcook.com

Generalized Ricci curvature on metric measure space

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Definition (Ollivier)

On (X, d, m), for any two distinct points $x, y \in X$, the (Ollivier-) Ricci curvature of (X, d, m) along (xy) is defined as

$$\kappa(x, y) := 1 - \frac{W_1(m_x, m_y)}{d(x, y)}. \tag{1}$$

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i.e.

$$W_1(m_x, m_y) = (1 - \kappa(x, y))d(x, y)$$

We understand a locally finite graph as a structure (V, d, m), where d is the graph distance, m is the family of probability measures $\{m_x\}$.

$$m_x(y) = \begin{cases} \frac{1}{d_x}, & \text{if } y \sim x; \\ 0, & \text{otherwise.} \end{cases} \tag{2}$$

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Definition (Transportation distance)

For two probability measures μ_1, μ_2 on a metric space (X, d), the transportation distance between them is defined as

$$W_1(\mu_1, \mu_2) := \inf_{\xi \in \prod(\mu_1, \mu_2)} \int_{X \times X} d(x, y) d\xi(x, y), \tag{3}$$

where $\prod(\mu_1, \mu_2)$ is the set of probability measures on $X \times X$ projecting to μ_1 and μ_2.

In other words, ξ satisfies

$$\xi(A \times X) = \mu_1(A), \;\; \xi(X \times B) = \mu_2(B), \;\forall A, B \subset X.$$

Local clustering

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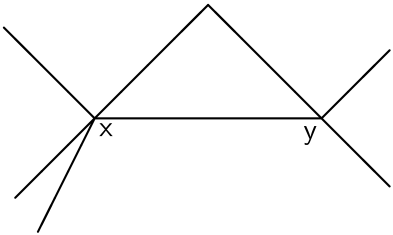
- Ricci curvature ←----→ relative abundance of triangles



$$c(x) = \frac{1}{10}$$

Watts-Strogatz clustering coefficient

For any pair of neighboring vertices x, y, we denote the number of triangles which include x, y as vertices by

$$\sharp(x, y) := \sum_{x_1, x_1 \sim x, x_1 \sim y} 1.$$

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The local clustering coefficient introduced by Watts-Strogatz is

$$c(x) := \frac{\text{number of edges between neighbors of } x}{\text{number of possible existing edges between neighbors of } x},$$

which measures the extent to which neighbors of x are directly connected, i.e.,

$$c(x) = \frac{1}{d_x(d_x - 1)} \sum_{y, y \sim x} \sharp(x, y). \tag{4}$$

Main result

Theorem

For any neighbors x and y, we have a sharp estimate

$$k(x,y) \le \kappa(x,y) \le \frac{\sharp(x,y)}{d_x \vee d_y},$$

where

$$k(x,y) = -\left(1 - \frac{1}{d_x} - \frac{1}{d_y} - \frac{\sharp(x,y)}{d_x \wedge d_y}\right)_+ - \left(1 - \frac{1}{d_x} - \frac{1}{d_y} - \frac{\sharp(x,y)}{d_x \vee d_y}\right)_+ + \frac{\sharp(x,y)}{d_x \vee d_y}.$$

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- Without the term $\sharp(x,y)$, the lower bound estimate is due to Lin-Yau.
- Both bounds are sharp on a complete graph, where $\kappa(x,y) = \frac{n-2}{n-1}$.

Relation with local clustering

We might also introduce some kind of scalar curvature (suggested in Problem Q of Ollivier) as

$$\kappa(x) := \frac{1}{d_x} \sum_{y, y \sim x} \kappa(x, y). \tag{5}$$

For simplicity of exposition, let our graph be d-regular, that is, $d_z = d$ for all vertices z. When $1 \geq \frac{2}{d} - \frac{\sharp(x,y)}{d}$ for all $y \sim x$, we would then get

$$-2 + \frac{4}{d} + \frac{3(d-1)}{d} c(x) \leq \kappa(x) \leq \frac{d-1}{d} c(x). \tag{6}$$

This example nicely illustrates the relation between Ollivier's curvature and the Watts-Strogatz clustering coefficient.

Remarks on lower bound

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- Trees attain the lower bound of κ.

Proposition

On a tree $T = (V, E)$, for any neighboring x, y, we have

$$\kappa(x, y) = -2\left(1 - \frac{1}{d_x} - \frac{1}{d_y}\right)_+ . \tag{7}$$

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Trees have the fastest volume growth rate.

Remarks on upper bound

- Geometric intuition of positive Ollivier's Ricci curvature: If $\kappa(x, y) > 0$, then $\sharp(x, y)$ is at least 1.

- Proposition

  If $\kappa(x, y) \geq k > 0$*, we have*

  $$\sharp(x, y) \geq \lceil k d_x \vee d_y \rceil, \tag{8}$$

  where $\lceil a \rceil := \min\{A \in \boldsymbol{Z} | A \geq a\}$*, for* $a \in R$*.*

Analytic respects of Ricci curvature

In the Riemannian case, the following well-known Bochner formula characterize the fact $Ric \geq K$,

$$\frac{1}{2}\Delta(|\nabla f|^2) \geq \frac{\Delta f^2}{m} + \langle \nabla(\Delta f), \nabla f \rangle + K|\nabla f|^2.$$

- Spectral gap inequalities
- Sobolev inequalities
- Logarithmic Sobolev inequalites

Bakry-Émery's calculus

Definition

The Laplace operator on (X, d, m) is defined as follows

$$\Delta f(x) = \int_X f(y) dm_x(y) - f(x), \text{ for functions } f : X \longrightarrow R. \quad (9)$$

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Starting from an operator Δ, define iteratively,

$$\Gamma(f,g) = \frac{1}{2}\{\Delta(fg) - (f\Delta g) - (\Delta f g)\},$$
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Curvature dimension inequality $CD(m, K)$:

$$\Gamma_2(f, f)(x) \geq \frac{1}{m}(\Delta f(x))^2 + K(x)\Gamma(f, f)(x), \ \forall x \in X, \ \forall f \quad (10)$$

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$$\Gamma(f, g) \sim \nabla f \cdot \nabla g,$$
$$\Gamma_2(f, g) \sim \frac{1}{2}\Delta|\nabla f|^2 - \langle \nabla(\Delta f), \nabla f \rangle\}.$$

Curvature dimension inequality $CD(m, K)$:

$$\frac{1}{2}\Delta(|\nabla f|^2)(x) - \langle \nabla(\Delta f), \nabla f \rangle(x) \geq \frac{\Delta f^2}{m}(x) + K(x)|\nabla f|^2(x), \ \forall x \ \forall f \quad (12)$$

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This construction has been studied on locally finite graphs by Lin-Yau.

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In fact this CD inequality is also related to the local clustering in graph setting.

Theorem

On a locally finite graph $G = (V, E)$, the Laplace operator satisfies

$$\Gamma_2(f,f)(x) \geq \frac{1}{2}(\Delta f(x))^2 + \left(\frac{1}{2}t(x) - 1\right)\Gamma(f,f)(x), \qquad (13)$$

where

$$t(x) := \min_{y, y \sim x}\left(\frac{4}{d_y} + \frac{1}{D(x)}\sharp(x,y)\right).$$

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$\kappa(x, y) \Rightarrow CD(m, K)$

Corollary

On a locally finite graph $G = (V, E)$, if $\kappa(x, y) \geq k > 0$, then we have

$$\Gamma_2(f, f)(x) \geq \frac{1}{2}(\Delta f(x))^2 + \left(\frac{2}{D(x)} + \frac{kd_x}{2D(x)} - 1\right)\Gamma(f, f)(x).$$

- $D(x) := \max_{y, y \sim x} d_y$
- Positive κ increase the curvature term in the CD inequality.

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Example: A complete graph satisfies $\kappa(x, y) = \frac{n-2}{n-1}$ and $CD(2, \frac{4-n}{2(n-1)})$. But as $n \to +\infty$,

$$\frac{4-n}{2(n-1)} \searrow -\frac{1}{2} \text{ whereas } \kappa \nearrow 1.$$

A discussion about the dimension of graphs

Proposition

On a complete graph $\mathcal{K}_n$ $(n \geq 2)$ with n vertices, the Laplace operator Δ satisfies for $m \in [1, +\infty]$,

$$\Gamma_2(f, f)(x) \geq \frac{1}{m}(\Delta f(x))^2 + \left(\frac{4-n}{2(n-1)} + \frac{m-2}{m}\right)\Gamma(f, f)(x).$$

Moreover, for every fixed dimension parameter m, the curvature term is optimal.

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Moreover, for every fixed dimension parameter m, the curvature term is optimal.

Interesting point: choose m as $n-1$. Then we have

$$\Gamma_2(f,f) \geq \frac{1}{n-1}(\Delta f)^2 + \frac{1}{2}\frac{n-2}{n-1}\Gamma(f,f),$$

where the curvature term is exactly $\frac{1}{2}\kappa$.

What is the proper dimension for graphs?

- $\mathcal{K}_n$ could be considered as the boundary of a $(n-1)$ dimensional simplex
- Erdös-Harary-Tutte: the dimension of a graph $G =$ the minimum number n such that G can be embedded into a n dimensional Euclidean space with every edge of G having length 1

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- Erdös-Harary-Tutte: the dimension of a graph $G =$ the minimum number n such that G can be embedded into a n dimensional Euclidean space with every edge of G having length 1
- It seems natural to expect stronger relations between the lower bound of κ and the curvature term in the curvature dimension inequality if one chooses proper dimension parameters.

J. Jost and S. Liu, *Ollivier's Ricci curvature, local clustering and curvature dimension inequalities on graphs*, http://arxiv.org/pdf/1103.4037v2.

Thank you for your attention!