Introduction to discrete curvatures

and Graph curvature calculator

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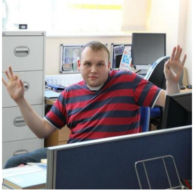
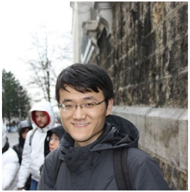
Our research group

In collaboration with

- David Cushing (Newcastle University)
- Shiping Liu (USTC, Hefei)
- Florentin Münch (MPI Leipzig)
- Norbert Peyerimhoff (Durham University)

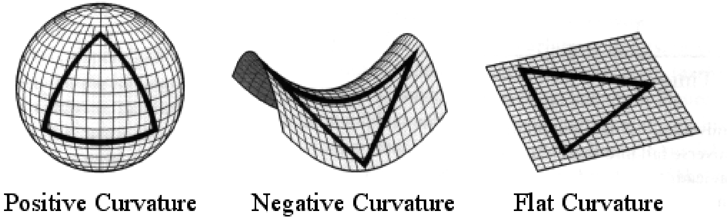
Classical curvature notions

C. F. Gauss (1777-1855)

[1]

[1] https://www.banknoteworld.com/germany-federal-republic-10-deutsche-mark-banknote-1999-p-38dz-unc-replacement.html

Classical curvature notions



[1]

[1] http://abyss.uoregon.edu/~js/cosmo/lectures/lec15.html

Classical curvature notions

B. Riemann[1]
1826-1866

- Riemannian Curvature Tensor

$$R(X,Y)Z = \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X,Y]} Z$$

- Sectional Curvature

$$K(\text{span}\{X,Y\}) = \frac{\langle R(X,Y)Y, X\rangle}{|X|^2|Y|^2 - \langle X,Y\rangle^2}$$

- Ricci Curvature

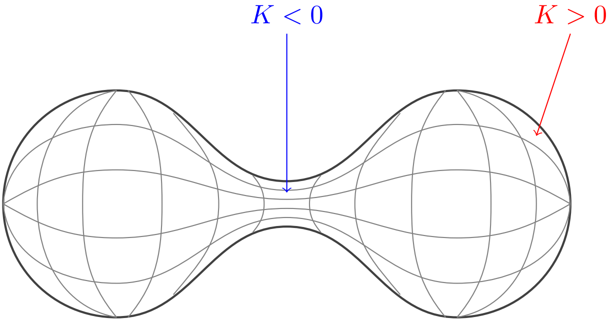
$$Ric(X,Y) = \frac{1}{n-1}\text{trace}(Z \mapsto R(Z,X)Y)$$

- Scalar Curvature

$$S(p) = \frac{1}{n}\text{trace}\,\text{Ric}$$

[1] https://www.sil.si.edu/DigitalCollections/hst/scientific-identity/explore.htm

Curvature is a local property

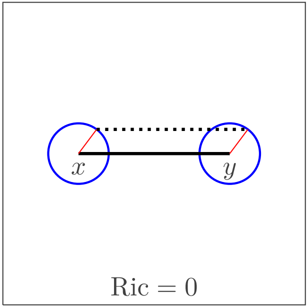


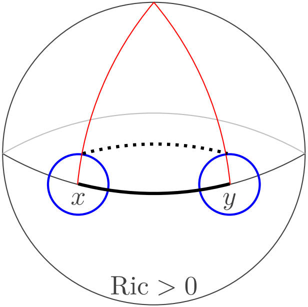
Curvatures via Optimal Transport

Relations to Optimal Transport Theory

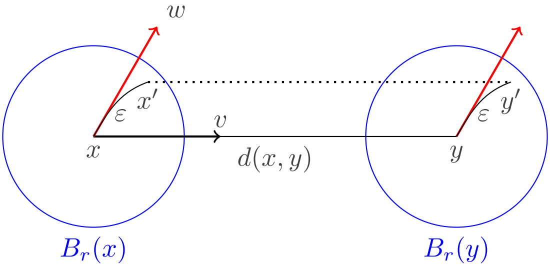
(M^n, g) complete, connected Riemannian manifold

von Renesse and Sturm (2005): If $\mathrm{Ric} > 0$, the average distance of corresponding points in nearby balls of small radius $r > 0$ is smaller than the distance between their centres.





Relations to Optimal Transportation Theory

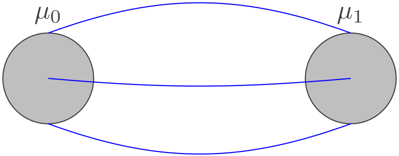


Average distance is

$$d(x, y)\left(1 - \frac{r^2}{N+2}\,\mathrm{Ric}\right)$$

Relations to Optimal Transport Theory

μ_0, μ_1 probability measures on (X, d, m)



- Minimal-cost distance

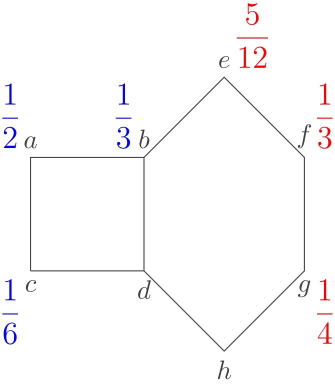
$$W_n(\mu_0, \mu_1) := \inf_{\pi} \int_{X \times X} c(x, y) \mathrm{d}\pi(x, y)$$

- $\pi \in \mathcal{P}(X \times X)$ is a transport plan from μ_0 to μ_1:

$$\pi(A \times X) = \mu_0(A)$$
$$\pi(X \times B) = \mu_1(B)$$

- cost function $c(x, y) = d^n(x, y)$. L^n-Wasserstein distance

Transport plan: Example



Transport plan π:

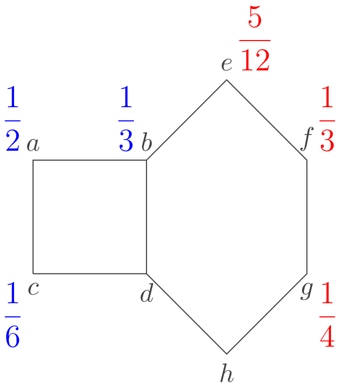
$$\pi(b,f) = \frac{1}{3}$$
$$\pi(a,e) = \frac{5}{12}$$
$$\pi(a,g) = \frac{1}{12}$$
$$\pi(c,g) = \frac{1}{6}$$

Cost($\propto$ distance):

$$\frac{1}{3}\cdot(2)$$
$$\frac{5}{12}\cdot(2)$$
$$\frac{1}{12}\cdot(4)$$
$$\frac{1}{6}\cdot(3)$$

$$\text{Total cost} = \frac{7}{3}.$$

Transport plan: Example



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Cost($\propto$ distance):

$$\frac{1}{3} \cdot (2)$$
$$\frac{5}{12} \cdot (2)$$
$$\frac{1}{12} \cdot (4)$$
$$\frac{1}{6} \cdot (3)$$

Total cost $= \frac{7}{3}$.

This cost is minimized:

$$W_1(Blue, Red) = \frac{7}{3}.$$

Relations to Optimal Transport Theory

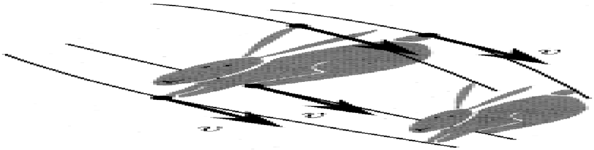
Another famous approach by Lott–Villani–Sturm (2009). Idea from Cordero-Erausquin, McCann, and Schmuckenschläger in 2001

Theorem

(M^n, g) has lower Ricci curvature bound $\mathrm{Ric}(M) \geq K$ iff Entropy functional along Wasserstein geodesics is K-convex:

$$\mathrm{Ent}(\mu_t) \leq (1-t)\mathrm{Ent}(\mu_0) + t\mathrm{Ent}(\mu_1) - \frac{K}{2}t(1-t)W_2(\mu_0, \mu_1)$$

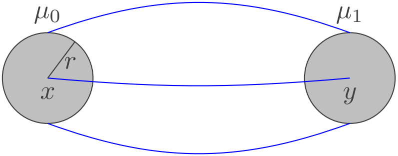
$\mathrm{Ent}(\mu) := \int \rho \log \rho d\mathrm{vol}$
$\rho = d\mu / d\mathrm{vol}$



[1] Y. Ollivier, *A survey of Ricci curvature for metric spaces and Markov chains*

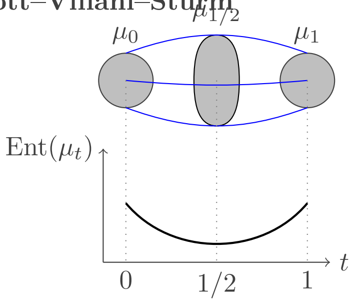
Two curvatures via Optimal Transport

Ollivier



$$K_{x,y,r} := 1 - \frac{W_1(\mu_0,\mu_1)}{d(x,y)}$$

Lott–Villani–Sturm



$$\mathrm{Ent}(\mu_t) \leq (1-t)\mathrm{Ent}(\mu_0) + t\mathrm{Ent}(\mu_1) - \frac{K}{2}t(1-t)W_2(\mu_0,\mu_1)$$

$\mathrm{Ent}(\mu) := \int \rho \log \rho d\mathrm{vol}$; $\rho = d\mu/d\mathrm{vol}$

Ollivier Ricci curvature on graphs

On graphs/networks:

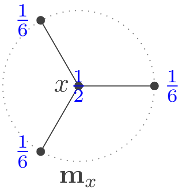
Definition (Ollivier Ricci curvature)

Given two points x, y,

$$\kappa(x,y) := 1 - \frac{W_1(\mathbf{m}_x, \mathbf{m}_y)}{d(x,y)}.$$

This is the modified definition by Lin-Lu-Yau (2011).

Y. Ollivier[1]
Facebook AI Research,
Paris (2017-)



[1] http://www.yann-ollivier.org/

Curvature via analytic approach

Analytic approach to curvature

Bakry-Émery (1985):

Bochner's formula:

$$\frac{1}{2}\Delta|\nabla f|^2 = \|\operatorname{Hess} f\|^2 + \langle \nabla f, \nabla \Delta f\rangle + \operatorname{Ric}(\nabla f, \nabla f).$$

With $\operatorname{Ric}_x(v,v) \geq K_x |v|^2$:

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

$$\Updownarrow$$

$$\Gamma_2(f,f) \;\geq\; K\Gamma(f,f).$$

where *carré du champ*
$2\Gamma(f,g) := \Delta(f \cdot g) - f \cdot \Delta g - g \cdot \Delta f. = 2\langle \nabla f, \nabla g\rangle$
$2\Gamma_2(f,g) := \Delta(\Gamma(f,g)) - \Gamma(f,\Delta g) - \Gamma(g,\Delta f).$

Bakry-Émery curvature

In fact, $\mathrm{Ric}(M) \geq K$ iff $\Gamma_2(f,f)(x) \geq K\Gamma(f,f)(x)$ for all x, f.

Also, iff $\Gamma(P_t f, P_t f)(x) \leq e^{-2Kt} P_t \Gamma(f,f)(x)$.
$P_t := e^{t\Delta}$. Heat diffusion: $u = P_t f$ solves $\partial_t u = \Delta u$.

Definition (Elworthy('89), Schmuckenschläger('98), Lin–Yau(2010))

The *Bakry-Émery curvature* at $x \in X$ to be

$$K_x := \sup \{ \, k \in \mathbb{R} \; : \; \Gamma_2(f,f)(x) \geq k\Gamma(f,f)(x) \text{ for all f } \}.$$

Graph Laplacian Δ

$$\Delta f(x) := \sum_{y \in N(x)} p_{xy}(f(y) - f(x))$$

Bakry-Émery curvature

Quadratic form: $A(f,g) = \sum_{i,j} a_{ij} f(v_i) g(v_j) = \underline{f}\mathbf{A}\underline{g}^T$

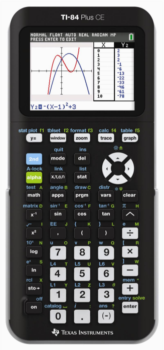
Here $\mathbf{A}$ is a matrix, and $\underline{f}, \underline{g}$ are vector representations.

$\Gamma_2(f,f)(x) \geq K\Gamma(f,f)(x)$ for all $f \iff \Gamma_2(x) - K\Gamma(x) \succeq 0$

Compare curvature notions

Curvature notions	**Where is it defined?**	**Computation**
Bakry-Émery	vertices	SDP
Ollivier	edges	LP
Entropic	global	not known

Graph Curvature Calculator



Nothing to do with Graphic calculator[1]

[1] https://www.tech-line-inc.com/shop/ti-84-plus-ce-graphing-calculator/

Curvature calculator tool by Cushing–Stagg

Graph curvature calculator v0.8.0
If you have found this software useful, please cite the following article:
The Graph Curvature Calculator and the curvatures of cubic graphs, Experimental Mathematics, 2019
(arXiv:1712.03033 [math.CO])

[Show Help]

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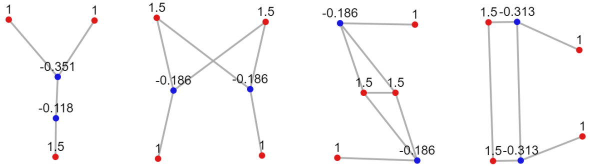
Autolayout: Circle



Non-normalised Curvature

Adjacency Matrix [Hide]

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[0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,1,0,0,0],[0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,1,0,1,0],[0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0],[0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0],[0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0]]

[Undo] [Load]

Web Link

This tool is freely available at

http://www.mas.ncl.ac.uk/graph-curvature/

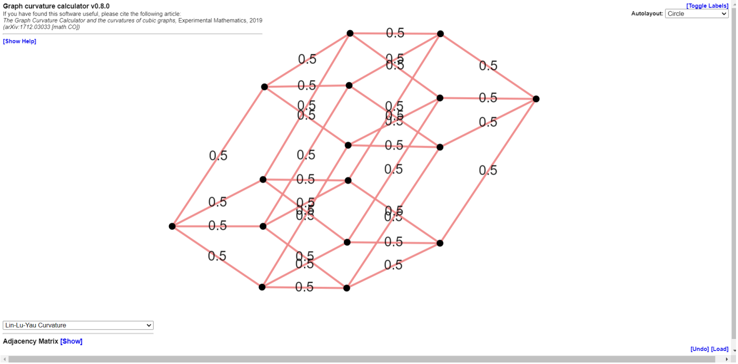
Easy to use and very helpful to make lots of discoveries!!

Alternatively, it can also be installed locally on your computer. For installation details, see

https://mas-gitlab.ncl.ac.uk/graph-curvature

Examples of graphs(1)

Discrete hypercube $Q^n = \{0,1\}^n$



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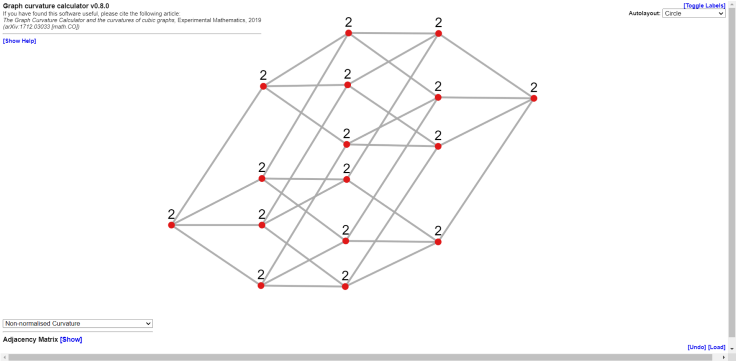
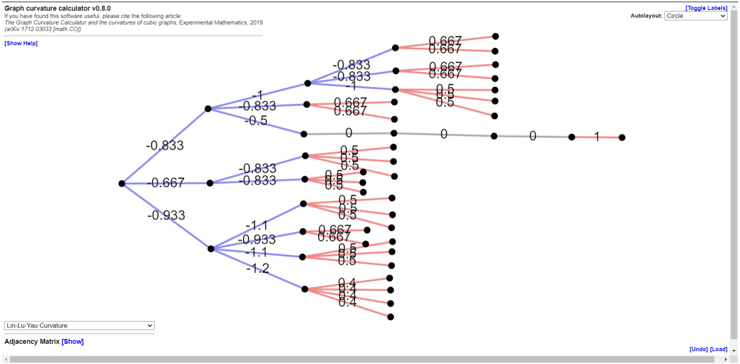


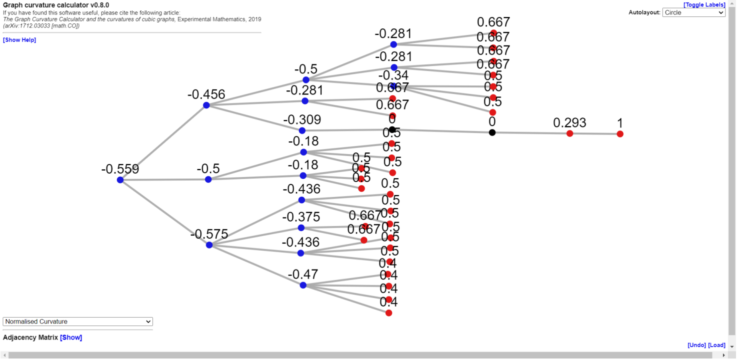
Examples of graphs(2)

Tree



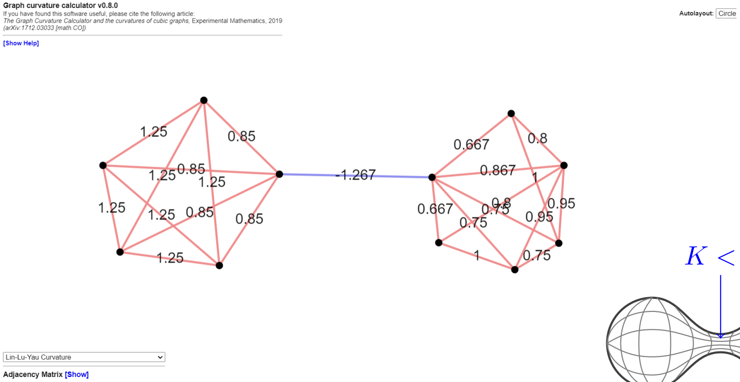
Examples of graphs(2)

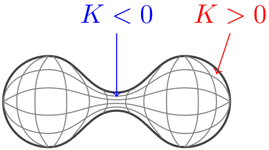
Tree



Examples of graphs(3)

Dumbbell graph



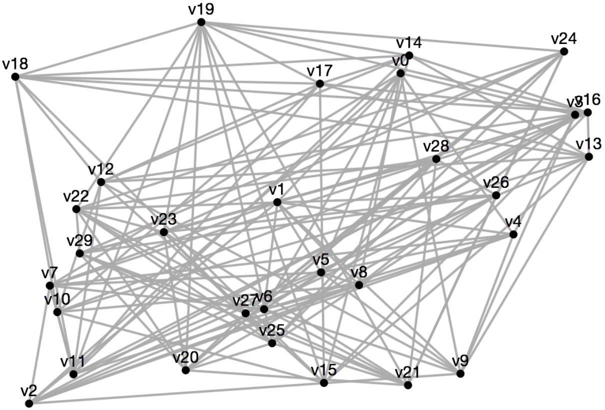


Applications

- **Connectivity:** clusters and bridges.
- **Dynamics.**
- **Discoveries:** Which graphs look like spheres?

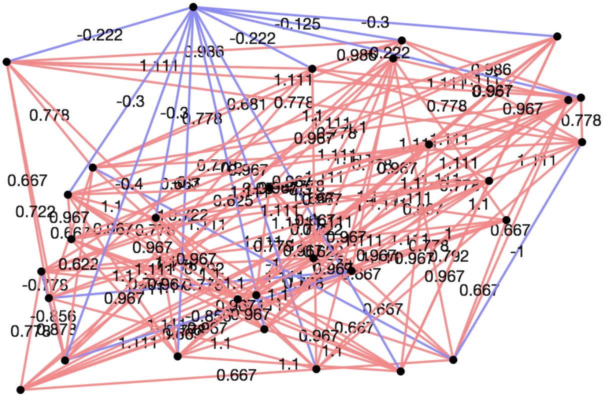
Connectivity

Looking for clusters and bridges...

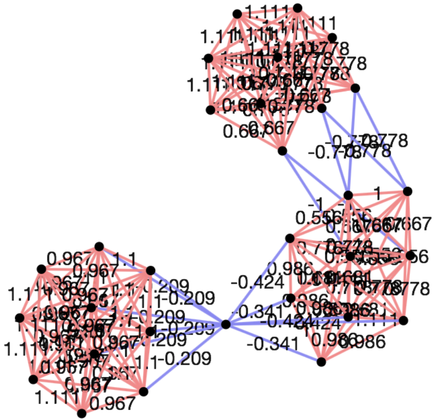


Connectivity

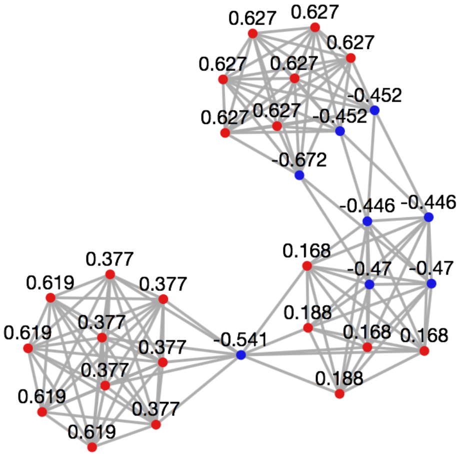
Looking for clusters and bridges



Connectivity



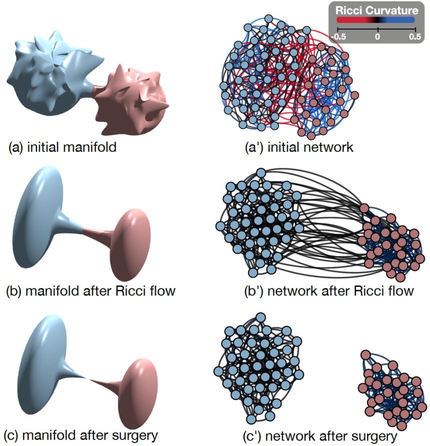
Connectivity



Dynamics

Community Detection on Networks with Ricci Flow

C.-C. Ni, Y.-Y. Lin, F. Luo, J. Gao, 2019



Dynamics

Ollivier Ricci curvature in applied fields...

- Complex biological networks: cancer, brain connectivity, phylogenetic tree
- Quantifying the systemic risk and fragility of financial systems
- Investigating node degree, the clustering coefficient and global measures on the in- ternet topology
- “Congestion” phenomenon in Wireless network under heat diffusion protocol
- Fast approximating to the tree-width of a graph and applications to determining whether a Quadratic Unconstrained Binary Optimization problem is solvable on the D-Wave quantum computer
- the problem of quantum grativity

Bonnet-Myers Diameter bound: $K = \inf \mathrm{Ric} > 0$

Bonnet-Myers:

$$\mathrm{diam}(M) \leq \pi\sqrt{\frac{n-1}{K}}.$$

Cheng's Rigidity:

$$\text{equality} \Leftrightarrow M \text{ is } n\text{-sphere}.$$

Discrete Bonnet-Myers:

$$\mathrm{diam}(G) \leq \frac{2}{K}.$$

Rigidity:

$$\text{equality} \Leftrightarrow G = ???$$

i.e., which graphs look like

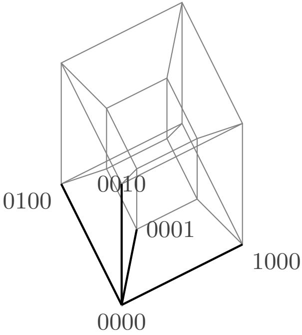
spheres?

Call G **Bonnet-Myers sharp**. Hypercubes Q^n are Bonnet-Myers sharp. Are there others?

Hypercube Q^n and Demi-cube $Q^{2n}_{(2)}$

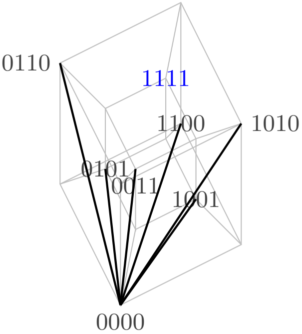
Hypercube Q^n

$V = \{n\text{-bit strings}\}$
$x \sim y$ if Hamming distance $= 1$



Demi-cube $Q^{2n}_{(2)}$

$V = \{2n\text{-bit strings with even 0's}\}$
$x \sim y$ if Hamming distance $= 2$



Cocktail party graph $CP(n)$

Cocktail party graph $CP(n)$

$V = \{n \text{ couples}\}$, that is, $|V| = 2n$
Everyone shakes hands with everyone else except for their partner.

vertex degree $= 2n - 2$;   diam $= 2$

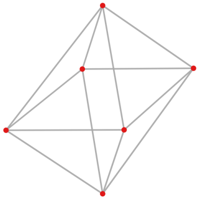


Figure: $CP(3)$ a.k.a. Octahedron

Johnson graph $J(2n, n)$

Johnson graph $J(2n, n)$

$V = \{x \subset [2n] : \ |x| = n\}$ where $[2n] = \{1, 2, ..., 2n\}$
$x \sim y$ if $|x \cap y| = n - 1$

vertex degree $= n^2$; $\quad$ diam $= n$

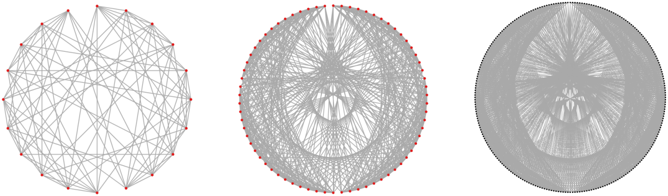


Figure: Johnson graphs $J(6, 3)$, $J(8, 4)$, and $J(10, 5)$

The Gosset graph

The Gosset graph

$$|V| = 56 \qquad \text{vertex deg} = 27 \qquad \text{diam} = 3.$$

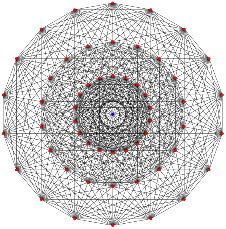


Figure: the Gosset graph [1]

[1] https://en.wikipedia.org/wiki/Gosset_graph

Surprising relation to strongly spherical graphs

Available at
www.ElsevierMathematics.com
POWERED BY SCIENCE DIRECT®
European Journal of Combinatorics 25 (2004) 299–310

European Journal of Combinatorics
www.elsevier.com/locate/ejc

The structure of spherical graphs

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Dedicated to the memory of Prof. J.J. Seidel

Abstract

A spherical graph is a graph in which every interval is antipodal. Spherical graphs are an interesting generalization of hypercubes (a graph G is a hypercube if and only if G is spherical and bipartite). Besides hypercubes, there are many interesting examples of spherical graphs that appear in design theory, coding theory and geometry e.g., the Johnson graphs, the Gewirtz graph, the coset graph of the binary Golay code, the Gosset graph, and the Schläfli graph, to name a few. In this paper we study the structure of spherical graphs. In particular, we classify a subclass of these graphs consisting of what we call the strongly spherical graphs. This allows us to prove that if G is a triangle-free spherical graph then any interval in G must induce a hypercube, thus providing a proof for a conjecture due to Berrachedi, Havel and Mulder.

A more complete answer...

Theorem (Cushing, K., Koolen, Liu, Münch, Peyerimhoff, 2018)

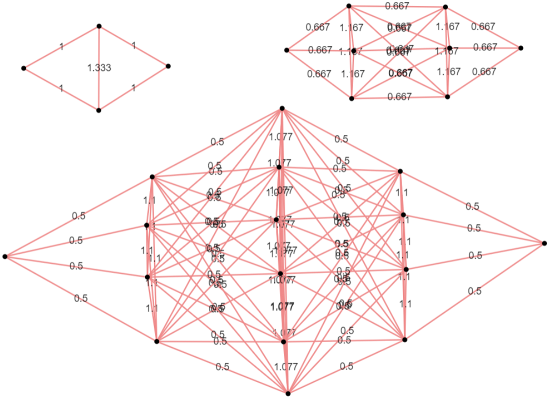
*A regular self-centered graph G which is **Bonnet-Myers sharp** must be one of the following:*

- *a hypercube Q^n, $n \geq 2$,*
- *a cocktail party graph $CP(n)$, $n \geq 2$,*
- *a demi-cube $Q^{2n}_{(2)}$, $n \geq 2$,*
- *a Johnson graph $J(2n, n)$, $n \geq 2$,*
- *the Gosset graph,*
- *a Cartesian product $G = G_1 \times G_2 \times ... \times G_m$ of the above graphs with the condition*

$$\frac{\deg(G_1)}{\mathrm{diam}(G_1)} = \frac{\deg(G_2)}{\mathrm{diam}(G_2)} ... = \frac{\deg(G_m)}{\mathrm{diam}(G_m)}.$$

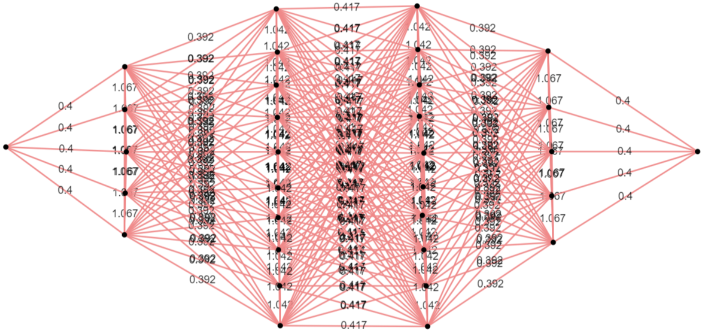
Non-regular Bonnet-Myers sharp

- $K = 2/\operatorname{diam}(G)$
- antitrees: $\mathcal{AT}(1,2,1)$, $\mathcal{AT}(1,3,3,1)$, $\mathcal{AT}(1,4,6,4,1)$



Non-regular Bonnet-Myers sharp

- $\mathcal{AT}(1, 5, 10, 10, 5, 1)$ is NOT.
- $\mathcal{AT}(1, 6, 15, 19, 15, 6, 1)$ is.



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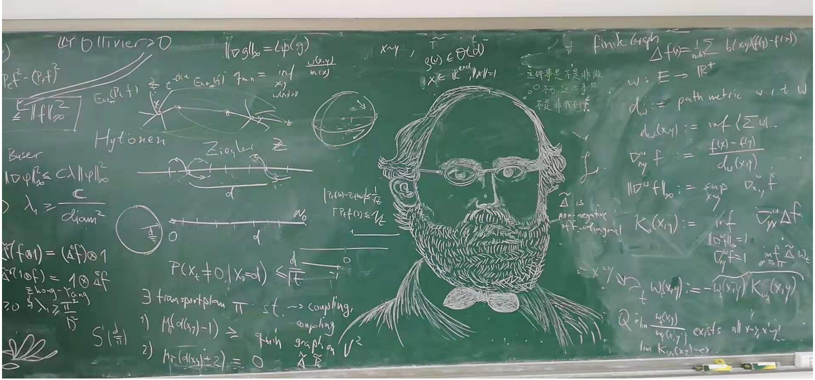
Thank you for your attention!



Graphs with positive curvature

Bonnet-Myers (or discrete B.-M.) requires $\mathrm{Ric} \geq K > 0$. Can we drop the $\geq K$ condition, i.e. is it still true that a manifold is compact (or a graph is finite), assuming that $\mathrm{Ric} > 0$ but $\inf \mathrm{Ric} = 0$?

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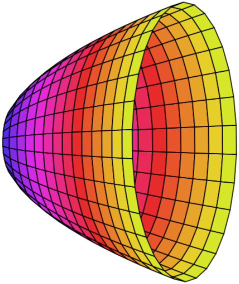
Answer: No. **Counterexample:** Paraboloid[1]



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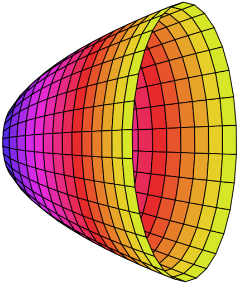
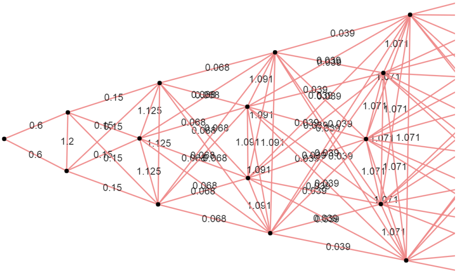
Answer: No. **Counterexample:** Paraboloid[1] and Anti-tree $\mathcal{AT}$





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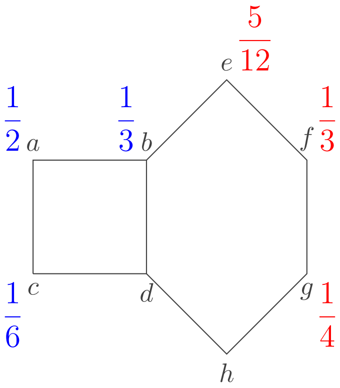
Transport plan: Example



Transport plan π:

$$\pi(b,f) = \frac{1}{3}$$
$$\pi(a,e) = \frac{5}{12}$$
$$\pi(a,g) = \frac{1}{12}$$
$$\pi(c,g) = \frac{1}{6}$$

Cost($\propto$ distance):

$$\frac{1}{3} \cdot (2)$$
$$\frac{5}{12} \cdot (2)$$
$$\frac{1}{12} \cdot (4)$$
$$\frac{1}{6} \cdot (3)$$

Total cost $= \frac{7}{3}$.

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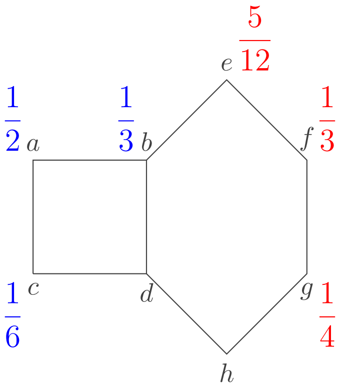

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Total cost $= \frac{7}{3}$.

This cost is minimized:

$$W_1(\textit{Blue}, \textit{Red}) = \frac{7}{3}.$$

Transport plan: Definition

Definition (probability measure on graph)

A **probability measure** μ on V (written as $\mu \in P(V)$) is a function $\mu : V \to [0,\infty)$ such that $\sum_{x\in V} \mu(x) = 1$, and $\mathrm{supp}(\mu) < \infty$.

Definition (transport plan)

A **transport plan** π from μ_1 to μ_2 (written as $\pi \in \prod(\mu_1,\mu_2)$) is a function $\pi : V \times V \to [0,\infty)$ such that

$$\sum_{w\in V} \pi(z,w) = \mu_1(z) \quad \text{and} \quad \sum_{z\in V} \pi(z,w) = \mu_2(w).$$

(i.e. $\pi(z,w)$ is amount of mass transported from z to w).
The **(total) cost** of π is $\sum_{z,w\in V} \pi(z,w)c(z,w)$, where $c(z,w) = d^1(z,w)$.

Wasserstein distance

Definition (1-Wasserstein distance)

For $\mu_1, \mu_2 \in P(V)$,

$$W_1(\mu_1, \mu_2) := \inf_{\pi \in \Pi(\mu_1, \mu_2)} \sum_{z,w \in V} \pi(z,w) d^1(z,w).$$

Any π realizing the infimum is called an ***optimal transport plan***.

Bakry-Émery curvature $CD(K,n)$

Bochner's formula:

$$\frac{1}{2}\Delta|\nabla f|^2 = \|\operatorname{Hess} f\|^2 + \langle \nabla f, \nabla \Delta f \rangle + \operatorname{Ric}(\nabla f, \nabla f).$$

$$\Downarrow$$

With $\operatorname{Ric}_x(v,v) \geq K_x|v|^2$:

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

$$\Updownarrow$$

$$\Gamma_2(f,f) \quad \geq \quad \tfrac{1}{n}(\Delta f)^2 \ + \ K\Gamma(f,f).$$

where *carré du champ*
$2\Gamma(f,g) := \Delta(f \cdot g) - f \cdot \Delta g - g \cdot \Delta f. = 2\langle \nabla f, \nabla g \rangle$
$2\Gamma_2(f,g) := \Delta(\Gamma(f,g)) - \Gamma(f, \Delta g) - \Gamma(g, \Delta f).$