CURVATURE NOTIONS ON GRAPHS LEEDS SUMMER SCHOOL, 18-19 JULY 2019

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ABSTRACT. In these lecture notes we introduce some curvature notions on graphs. After a brief discussion of Gaussian curvature of surfaces we introduce three curvature notions which can be defined in the discrete setting of graphs: combinatorial curvature of surface tessellations, Ollivier Ricci curvature based on notions of Optimal Transport Theory and, finally, Gromov hyperbolicity capturing global aspects of negative curvature. Problems inserted in the text help to become more familiar with these curvature notions and to learn more about them.

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1. INTRODUCTION

Curvature is a fundamental concept in Differential Geometry. In the case of surfaces in 3-dimensional Euclidean space, the *Gaussian* curvature at a given point of a surface is the product $\kappa_1 \kappa_2$ of the principal curvatures (with signs corresponding to a given normal vector N). These principal curvatures are determined by two (orthogonal) directions X_1, X_2 , in which the surface bends most. In other words, we take the affine plane spanned by a tangent vector X and N and intersect this plane with the surface. The result is a curve which can be approximated, up to second order, at the point of the surface by a circle. The reciprocal value of the radius of this circle is the normal curvature in direction X. Rotating this tangent direction X leads to two orthogonal directions in which this normal curvature assumes extremal values. As illustrated in Figure 1, the corresponding normal curvatures are then the principal curvatures κ_1, κ_2 at this point of the surface.

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FIGURE 1. Illustration of principal curvatures¹

The Theorema Egregium (Outstanding Theorem) of Gauss states that Gaussian curvature, even though defined orginally through the embedding of the surface in 3-dimensional Euclidean space, is indeed a local *intrinsic quantity* of the surface and does therefore not change under local isometric deformations. This is confirmed by the fact that a plane has the same constant Gaussian curvature as a rotational invariant cylinder in \mathbb{R}^3 , namely the Gaussian curvature of both surfaces is zero. The principal curvatures of a 2-dimensional sphere of radius r > 0 are both +1/r and this sphere has therefore constant Gaussian curvature $1/r^2$.

A surface has negative Gaussian curvature at points where the surface looks, locally, like a saddle (in which case the two principal curvatures κ_1, κ_2 have opposite signs). The three cases (positive curvature, negative curvature and vanishing curvature) are illustrated in Figure 2.



FIGURE 2. Surfaces of positive Gaussian curvature, negative Gaussian curvature and vanishing Gaussian curvature²

¹Picture taken from http://brickisland.net/cs177fa12/?p=214

²Picture taken from https://i1.wp.com/www.thephysicsmill.com/blog/ wp-content/uploads/comparison_of_curvatures.png. Another important illustration of positive, negative and vanishing Gaussian curvature of a surface is given via the shapes of triangles, in particular the sum of their interior angles. By triangles we mean *geodesic triangles*, that is, the three sides between their vertices are *geodesics*³. While the sum of the interior angles of any geodesic triangle in the Euclidean plane is always equal to π , this sum is strictly larger than π in the case of positive Gaussian curvature and strictly smaller than π in the case of negative Gaussian curvature. This fact is illustrated in Figure 3.



C. F. Gauss⁴ (1777-1855)



FIGURE 3. Triangles in positive Gaussian curvature, negative Gaussian curvature and vanishing Gaussian curvature 5

In fact, the *local Gauss-Bonnet Theorem* tells us that, for a geodesic triangle Δ with interior angles α, β, γ , the difference $\alpha + \beta + \gamma - \pi$ is equal to the integral of the Gaussian curvature over the interior of the triangle. The local Gauss-Bonnet Theorem leads to the following fundamental result for closed orientable surfaces (that is, compact surfaces without boundary):

³We call a curve $c: I \to X$ from an interval $I \subset \mathbb{R}$ to a metric space (X, d) a geodesic if we have for all $s, t \in I$, d(c(s), c(t)) = |t - s|.

⁴Picture taken from Wikipedia

⁵Picture taken from https://advances.sciencemag.org/content/2/5/e1501495/tab-figures-data

Theorem 1.1 (Global Gauss-Bonnet Theorem). Let $S \subset \mathbb{R}^3$ be a closed orientable surface with Gaussian curvature function $K : S \to \mathbb{R}$. Then we have

(1)
$$\int_{S} K d\text{vol} = 2\pi\chi(S).$$

where $\chi(S)$ is the Euler characteristic of S, that is, for a given triangulation of S with vertices V, edge E and faces F,

(2)
$$\chi(S) = |V| - |E| + |F|.$$

It should be noted that the Euler characteristic (2) is a purely topological invariant of the surface and does not depend on the choice of the triangulation. The formula (1) relates a geometric quantity of the surface, namely the Gaussian curvature function, which is very sensitive to deformations of the surface, to a robust combinatorial topological global invariant, the Euler characteristic.

Problem 1.2. Let $S \subset \mathbb{R}^3$ be a surface with a triangulation by geodesic triangles. Derive the equation (1) in Theorem 1.1 from the local Gauss-Bonnet Theorem.

The observation that Gaussian curvature is an *intrinsic quantity* of a surface or, more generally, a Riemannian manifold, lead to the fundamentally important *Riemannian curvature tensor*, which was introduced in Bernhard Riemann's 1827 Inaugural Lecture "Über die Hypthesen, welche der Geometrie zu Grunde liegen"⁶. The Riemannian curvature tensor is the "father" of all subsequent curvature notions like, e.g., *sectional curvature*, *Ricci curvature* and *scalar curvature*.



B. Riemann⁷ (1826-1866)

The Ricci curvature is of fundamential importance in Einstein's *The*ory of *General Relativity*. We will not discuss these curvature notions in detail but like to point out that they all coincide in the case of 2-dimensional Riemannian manifolds, that is, surfaces.

It is natural and challenging to introduce suitable curvature concepts for spaces different from smooth Riemannian manifolds. In this lecture notes, we will consider the setting of combinatorial graphs and will discuss three specific curvature concepts, namely,

⁶English translation: "On the Hypothesis which lie at the Foundation of Geometry."

⁷Picture taken from Wikipedia

- (i) Combinatorial curvature,
- (ii) Ollivier Ricci curvature,
- (iii) Gromov hyperbolicity.

A newly introduced curvature notion in a new context passes the first justification round if it exhibits one or more particular fundamental curvature properties which are known to hold the smooth setting of Riemannian manifolds. Combinational curvature is a local concept and is defined on the vertices of a surface tessellation. It is designed in such a way that it leads to a discrete version of the above mentioned global Gauss-Bonnet Theorem. Ollivier Ricci curvature is defined on pairs of vertices of a general combinatorial graph and is based on the general theory of *Optimal Transport*. This curvature notion reflects the fact that, in case of positive Ricci curvature, the average distance of corresponding points in closeby small metric balls of a surface is smaller than the distance between their centres. Finally, Gromov hyperbolicity is a global property of a metric space reflecting the fact that, in the case of negative sectional curvature, geodesic triangles are thinner and more inward bent than Euclidean triangles, a fact which can be also observed in Figure 3 above.

The emphasis in these notes is on the concept of Ollivier Ricci curvature for the simple reason that this particular discrete curvature notion is one of the author's own research fields. We refer the readers to the very recommendable survey [25] containing further information about three different curvature notions for graphs (combinatorial curvature, Bakry-Émery curvature and Ollivier Ricci curvature).

Let us finish this Introduction by presenting a model space of constant negative Gaussian curvature, the *hyperbolic plane*.

Example 1.3 (The hyperbolic plane as surface of constant negative curvature). A well-known model of constant Gaussian curvature K = -1 is the hyperbolic plane \mathbb{H}^2 , represented by the upper half plane $\mathbb{H}^2 = \{z \in \mathbb{C}^2 \mid \text{Im}(z) > 0\}$ with distance function $d_{\mathbb{H}^2}$ given by (see [26])

(3)
$$d_{\mathbb{H}^2}(z,w) = \ln \frac{|z-\bar{w}| + |z-w|}{|z-\bar{w}| - |z-w|}.$$

It is easy to see that the curve $c : \mathbb{R} \to \mathbb{H}^2$, $c(t) = x + e^t i$ is a geodesic connecting the boundary points 0 and ∞ . Note that the set of boundary points at infinity, given by $\partial \mathbb{H}^2 = \mathbb{R} \cup \{\infty\}$, do not belong to the hyperbolic plane and are infinitely far away⁸. Any two distinct

 $^{{}^{8}\}partial\mathbb{H}^{2} = \mathbb{R} \cup \{\infty\}$ carries the topology of a circle with $x_{n} \to \infty$ if and only if $|x_{n}| \to \infty$.

boundary points can be connected by a bi-infinite geodesic which assumes the shape of a Euclidean semicirle or a vertical line meeting the boundary perpendicularly (see Figure 4 for various geodesics ending in $z \in \partial \mathbb{H}^2$).



FIGURE 4. A horocycle (red) through $x, y \in \mathbb{H}^2$ and centered at $z \in \partial \mathbb{H}^2$ and asymptotic geodesics ending in z partitioning the hyperbolic plane

Moreover, for any triple $x, y, z \in \partial \mathbb{H}^2 = \mathbb{R} \cup \{\infty\}$ of distinct boundary points there exists a hyperbolic isometry $\phi : \mathbb{H}^2 \to \mathbb{H}^2$ which extends continuously to the boundary such that $\phi(x) = -1$, $\phi(y) = 1$, $\phi(z) = \infty$. These three boundary points $-1, 1, \infty \in \partial \mathbb{H}^2$ form, together with their three connecting bi-infinity geodesics, an *ideal geodesic triangle*. The local Gauss-Bonnet Theorem tells us that this triangle must have finite area π since all interior angles are equal to 0. A triangle of \mathbb{H}^2 is called *ideal* if all of its vertices lie in the boundary $\partial \mathbb{H}^2$.

It is also useful to know that hyperbolic circles in \mathbb{H}^2 have the shape of Euclidean circles (where hyperbolic and Euclidean radii are different as are the hyperbolic and Euclidean centres of these circles).

Finally, let us introduce asymptotic geodesics and horocycles: Geodesic rays ending at the same boundary point are called *asymptotic*. The set of all bi-infinite geodesics ending at a fixed boundary point $z \in \partial \mathbb{H}^2$ partition the hyperbolic plane and the curves orthogonal to them are called *horocycles centered at* $z \in \partial \mathbb{H}^2$. In the case $z \in \mathbb{R}$, the associated horocycles are Euclidean circles touching the boundary at z (see Figure 4), and in the case $z = \infty$, the associated horocycles are horizontal lines parallel to the x-axis.

Let $x, y \in \mathbb{H}^2$ be two points lying on the same horocycle centered at $z \in \partial \mathbb{H}^2$ and $c_x, c_y : [0, \infty) \to \mathbb{H}^2$ be two asymptotic geodesic rays with start- and end-points $c_x(0) = x$, $c_y(0) = y$ and $c_x(\infty) = c_y(\infty) = z$, as illustrated in Figure 4. Then it can be shown that the function

$$f(t) = d_{\mathbb{H}^2}(c_x(t), c_y(t))$$

is strictly monotone decreasing with $\lim_{t\to\infty} f(t) = 0$. In other words, the geodesic rays $c_x(t), c_y(t)$ are farthest apart at t = 0 and become closer to each other as $t \to \infty$.

Problem 1.4. Let a < b and consider the geodesics $c_1(t) = a + e^{t_i}$ and $c_2(t) = b + e^{t_i}$ in the upper half plane model of the hyperbolic plane \mathbb{H}^2 . Then c_1 and c_2 are two asymptotic geodesics with common end-point $\infty \in \partial \mathbb{H}^2$, and $c_1(t)$ and $c_2(t)$ lie on the same horocycle centered at ∞ for every $t \in \mathbb{R}$. Verify that the function

$$f(t) = d_{\mathbb{H}^2}(c_1(t), c_2(t))$$

is strictly monotone decreasing with $\lim_{t\to\infty} f(t) = 0$.

2. Combinatorial curvature

A given surface S can be tessellated by polygons such that every polygon is topologically trivial, that is, its closure is homeomorphic to a closed disc. If all polygons of such a tessellation are triangles we have a triangulation \mathcal{T} of the surface. Given such a triangulation, we can carry out the following mathematical construction: We assign to every triangle in \mathcal{T} a corresponding equilateral Euclidean triangle of side length one and glue their sides together in accordance with the combinatorial structure of the tessellation \mathcal{T} . Note that the resulting space $S_{\mathcal{T}}$ is locally Euclidean (that is every point has a neighbourhood isometric to a small disc in \mathbb{R}^2), except for the vertices of the Euclidean triangles. If less than 6 Euclidean triangles meet at such a vertex, say k < 6, then the angles of the triangles around that vertex add up to $k\frac{\pi}{3} < 2\pi$. If more than 6 Euclidean triangles meet at such a vertex, say k > 6, then the angles of the triangles around that vertex add up to $k\frac{\pi}{3} > 2\pi$. If it is precisely 6 Euclidean triangles, then their angles add up to 2π and $S_{\mathcal{T}}$ is also locally Euclidean at that vertex. From these considerations it makes sense that the discrete analogue of the "Gaussian" curvature in this space is concentrated in the vertices of $S_{\mathcal{T}}$ and is given by the angle excess $2\pi - k\frac{\pi}{3}$ (see Figure 5 for illustration).



FIGURE 5. Triangle arrangement with positive vertex curvature $2\pi - \frac{4\pi}{3} = \frac{2\pi}{3}$ and with negative vertex curvature $2\pi - \frac{8\pi}{3} = -\frac{2\pi}{3}$

These considerations give rise to the following general definition, which agrees with definitions given by various authors, amongst them Stone [37], Woess [41] and Higuchi [22].

Definition 2.1. Let \mathcal{T} be a tessellation of a surface S and G = (V, E, F) be the combinatorial representation of \mathcal{T} , that is, we think of the faces $f \in F$ as regular Euclidean polygons of side length one with interior angles equals $\frac{(|f|-2)}{|f|}\pi$, where |f| denotes the degree of the face f, that is, its number of sides. The combinatorial curvature of G is a function $K: V \to \mathbb{R}$ on the vertices and is defined by

$$K(x) = 2\pi - \sum_{f: x \in f} \frac{|f| - 2}{|f|} \pi,$$

where we mean by $x \in f$ that $x \in V$ is a vertex of the face $f \in F$.

Before we discuss interesting global consequences of this local curvature notion in the next section, we would like to mention that related curvature considerations are very useful in a specific topic of *Combinatorial Group Theory* called *Small Cancellation Theory*. This research area is based on the concept of *van Kampen diagrams* and it relies on very closely related arguments involving combinatorial curvature notions (see, for example, [31, Section V.3]). A central problem in this area is the solution of the *word problem*, that is, whether a given word in the generators of a finitely presented group coincides with the identity element of the group. 2.1. Global results about combinatorial curvature. Our first result is the following discrete version of the global Gauss-Bonnet Theorem, which is generally known as a kind of folklore result. (The special case of S equals a sphere was already proved by RENÉ DESCARTES (1596-1650)):

Theorem 2.2 (Discrete Global Gauss-Bonnet Theorem). Let G = (V, E, F) be a combinatorial representation of a surface S and K : $V \to \mathbb{R}$ be its combinatorial curvature. Then we have

$$\sum_{x \in V} K(x) = 2\pi \chi(S).$$

Problem 2.3. Show that

(4)
$$K(x) = 2\pi \left(1 - \frac{|x|}{2} + \sum_{f: x \in f} \frac{1}{|f|} \right),$$

where |x| denoted the degree of the vertex x, that is, the number of edges emanating from x, and prove the Discrete Global Gauss-Bonnet Theorem.

A fundamental result in Differential Geometry about Riemannian manifolds with strictly positive Ricci curvature is the following Theorem by Bonnet-Myers (see, e.g., [17, Theorem 9.3.1]):

Theorem 2.4 (Bonnet-Myers Theorem). Let (M, g) be a complete connected n-dimensional Riemannian manifold with Ricci curvature⁹ bounded below by $1/r^2 > 0$, that is

$$\operatorname{Ric}_p(v) \ge \frac{1}{r^2} \|v\|^2 \qquad \forall v \in T_p M.$$

Then M is a compact manifold with diameter bounded by

$$\operatorname{diam}(M) = \max\{d(x, y) \mid x, y \in M\} \le \pi r$$

where πr is the diameter of the n-dimensional round sphere of constant Ricci curvature $1/r^2$ (that is, the round sphere of radius r).

In 1976, Stone [37] investigated the possibility of a discrete analogue of this fundamental result from Differential Geometry and, similarly in spirit, Higuchi conjectured in 2001 that strictly positive combinatorial curvature of a tessellation of a surface S homeomorphic to a subset of

 $^{^{9}}$ If you are not familiar with Ricci curvature of *n*-dimensional Riemannian manifolds you may just consider the 2-dimensional case when this simplifies to Gaussian curvature of surfaces.

the sphere should imply finiteness of this tessellation (see [22, Conjecture 3.2] and also [16, Conjecture 1.6]). This conjecture was proved in 2007 by DeVos and Mohar:

Theorem 2.5 (see [16, Theorem 1.7]). Let G = (V, E, F) be a tessellation of a closed oriented surface S with strictle positive combinatorial curvature. Then S is homeomorphic to the 2-dimensional sphere and G is finite. Moreover, if G is not a prism or an antiprism then

 $(5) |V| \le 3444.$

Problem 2.6. Prisms and antiprims are finite graphs illustrated in Figure 6. The number of their vertices can be arbitrarily large. We can think of them as being tessellations of the sphere with two faces of possibly very high degree $k \ge 3$ while the others are just triangles or quadrilaterals. Calculate the combinatorial curvatures of these examples for arbitrary k.



FIGURE 6. Examples of prisms and antiprisms

The story does not end here. Various mathematicians were curious whether the upper bound $|V| \leq 3444$ in Theorem 2.5 can be improved and, if so, what upper bound will be the optimal value. This problem was finally settled by L. Ghidelli in 2017:

Theorem 2.7 (see [20, Theorem 3.1]). Let G = (V, E, F) be as in Theorem (2.5). Then the upper bound in (5) can be improved to

$$(6) |V| \le 208$$

Moreover this estimate is the optimal one.

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Remark 2.8. Optimality of (6) is guaranteed by the fact that there are planar graphs with strictly positive combinatorial curvature in all vertices and precisely 208 vertices. One such example is presented in Figure 7, which is taken from [20, Figure 18.1]. The planar graph given there can also be viewed as a tessellation of S^2 with two large faces of degrees 39 containing north and south pole and all other faces forming a belt of a fixed width around the equator. This example was discovered in 2011 by Ghidelli in private communications with J. Sneddon and later independently rediscovered by Oldridge [34].



FIGURE 7. A planar graph with |V| = 208 and strictly positive combinatorial curvature in all vertices. Its faces have the degrees 3, 5, 7, 39.

2.2. Outlook into further research and developments. A planar tessellation is a topological embedding $\varphi : (V, E) \to S$ of a simple graph into the surface S which can be either \mathbb{R}^2 or the 2-dimensional sphere, with some specific conditions on the connected components of the complement of the embedded image, the so-called faces (see, e.g., [27]). As before, F denotes the set of these faces. Let $\mathcal{P}C_{\geq 0}$ denote the class of all planar tessellations (V, E, F) with non-negative combinatorial curvature K(x) in all vertices $x \in V$. It was shown in [7, 8] that for each $G = (V, E, F) \in \mathcal{P}C_{\geq 0}$ the number of vertices with strictly positive combinatorial curvature is finite. As a consequence, the total curvature

$$K(G) = \sum_{x \in V} K(x)$$

of any such graph must be finite. B. Hua and Y. Su investigated the following two natural questions:

- 1. What is the maximal number of strictly positively curved vertices of infinite graphs in $\mathcal{P}C_{>0}$?
- 2. What are the total curvatures K(G) which can be achieved by infinite graphs G in $\mathcal{P}C_{\geq 0}$?

They addressed Question 1 in [24] and proved that the maximal number of strictly positively curved vertices is 132 and that every infinite graph in $\mathcal{P}C_{\geq 0}$ with this maximal number must contain 12 disjoint 11-gons. With regards to Question 2, they proved in [23] that the achievable total curvature values are precisely $\frac{j\pi}{6}$ with $0 \leq j \leq 12$ and they presented examples of infinite graphs in $\mathcal{P}C_{\geq 0}$ for each of these values.

With this glimpse into recent research on combinatorial curvature, we end this section and move on to the next topic: Ollivier Ricci curvature.

3. Ollivier Ricci curvature

Ollivier Ricci curvature starts from the following characterisation of positive Ricci curvature in the smooth setting of Riemannian manifolds (see von Renesse/Sturm [40]): Small spheres are closer (in transportation distance) than their centres are. Yann Ollivier explains this in his article [35] as follows: Consider two very close points x, y in a Riemannian manifold defining a tangent vector at x. Let w be another tangent vector and w' be the tangent vector at y parallel to w at x. Following the geodesics issuing from x in direction w and from y in direction w', the geodesics will get closer in the case of positive curvature. Ricci curvature along (xy) is this phenomenon, averaged in all directions w at x. This fact is illustrated in Figure 8, comparing the round 2-sphere (positive Ricci curvature) to the Euclidean plane (vanishing Ricci curvature).

Ollivier introduced a Ricci curvature in metric spaces motivated by this Ricci curvature property about small balls. These balls define probability measures (supported and equidistributed on the balls) and their distance can be measured using the Wasserstein transportation distance from Optimal Transport Theory. We present his ideas in the setting of connected graphs G = (V, E). This curvature notion for graphs features also in various contexts of applied research, for example:

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FIGURE 8. In the 2-sphere, corresponding points in small metric balls $B_{\epsilon}(x)$, $B_{\epsilon}(y)$ in parallel directions have smaller distance than d(x, y). In the Euclidean plane, they have the same distance d(x, y).

- (i) studying complex biological networks, such as cancer, brain connectivity, phylogenetic trees,
- (ii) quantifying systemic risk and fragility of financial systems,
- (iii) investigating node degree, the clustering coefficient and global measures on the internet topology,
- (iv) studying the congestion phenomenon in wireless networks under the heat-diffusion protocol,
- (v) fast approximation of 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, and
- (vi) studying the problem of quantum gravity.

These fields of applications are taken from [13].

Let us finish this introduction by mentioning that Yann Ollivier, a mathematician by training, is currently a research scientist at the Facebook Artificial Intelligence Lab in Paris, working chiefly on neural networks. You can find more information about him via his website at http://www.yann-ollivier.org/ where also his picture is taken from.



Yann Ollivier

3.1. Fundamental concepts: Transport plans, Wasserstein metric and Ollivier Ricci curvature. Let G = (V, E) be a connected graph. A *probability measure* μ on G can be understood as a function $\mu: V \to [0, 1]$ with

$$\sum_{x \in V} \mu(x) = 1.$$

The set of all probability measures on G is denoted by $\mathcal{P}_1(V)$.

Now we introduce the notion of a transport plan and its cost which leads naturally to a distance function on the space $\mathcal{P}_1(V)$ of probability measures:

Definition 3.1. Let G = (V, E) be a connected graph and $\mu, \nu \in \mathcal{P}_1(V)$ be two probability measures. A transport plan from μ to ν is a map $\pi: V \times V \to [0, 1]$ such that

$$\mu(x) = \sum_{y \in V} \pi(x, y) \qquad \forall \, x \in V$$

and

$$\nu(y) = \sum_{x \in V} \pi(x, y) \qquad \forall \, y \in V$$

The value $\pi(x, y)$ is then the mass transported from x to y along a geodesic (at cost $d(x, y)\pi(x, y)$), and the (total) cost of the transport plan π is defined as

$$\cos(\pi) := \sum_{x,y \in V} d(x,y) \pi(x,y)$$

The set of all transport plans from μ to ν is denoted by $\Pi(\mu, \nu)$ and the 1-Wasserstein distance¹⁰ between μ and ν is defined as

$$W_1(\mu,\nu) := \inf_{\pi \in \Pi(\mu,\nu)} \operatorname{cost}(\pi).$$

A transport plan $\pi \in \Pi(\mu, \nu)$ is called optimal if we have

$$W_1(\mu,\nu) = \cot(\pi).$$

(Note, however, that there might be more than one optimal transport plan for a given pair of probability measures.)

It can be checked that $W_1 : \mathcal{P}_1(V) \times \mathcal{P}_1(V) \to [0, \infty)$ is a distance function which simplifies to the combinatorial distance function on G if

¹⁰The *p*-Wasserstein distance is given by a different cost-function, namely $W_p(\mu,\nu) := \inf_{\pi \in \Pi(\mu,\nu)} \sum_{x,y \in V} d(x,y)^p \pi(x,y).$

we embed the vertex set V into $\mathcal{P}_1(V)$ via *Dirac measures*: The Dirac measure $\delta_x \in \mathcal{P}_1(V)$ of a vertex $x \in V$ is given by

$$\delta_x(y) = \delta_{xy}$$

and we obviously have

$$W_1(\delta_x, \delta_y) = d(x, y)$$

via the transport plan $\pi(z, w) = \delta_x(z)\delta_y(w)$.

Example 3.2 (A transport plan). Consider two probability measures μ and ν on a finite connected graph G = (V, E) with 8 vertices V = $\{a, b, c, d, e, f, g, h\}$ as illustrated in Figure 9.



FIGURE 9. Probability distributions μ, ν on G

We can transfer μ to ν in the following way:

- send ¹/₃ from b to f over a distance of 2,
 send ⁵/₁₂ from a to e over a distance of 2,
 send ¹/₆ from c to g over a distance of 3, and
 send ¹/₁₂ from a to g over a distance of 4.

The transport plan is then given by $\pi(b, f) = 1/3$, $\pi(a, e) = 5/12$, $\pi(c,g) = 1/6$, and $\pi(a,g) = 1/12$ with π vanishing for all other vertexcombinations. The cost of this transport plan is then given by

$$\cot(\pi) = \sum x, y \in V\pi(x, y)d(x, y) =$$

$$2\pi(b, f) + 2\pi(a, e) + 3\pi(c, g) + 4\pi(a, g)$$

$$= \frac{2}{3} + \frac{10}{12} + \frac{3}{6} + \frac{4}{12} = \frac{7}{3}.$$

Recall that we have $W_1(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \operatorname{cost}(\pi)$ and we can therefore conclude that $W_1(\mu,\nu) \leq \frac{7}{3}$. In order to conclude $W_1(\mu,\nu) = \frac{7}{3}$ we need to show that the above transport plan π is *optimal*. There is no

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obvious immediate way to prove this since there are infinitely many possibilities to transport the probability measure μ to ν . In the next section we will learn a powerful tool to show that a given transport plan is optimal, namely *duality*.

Our next aim is to introduce Ollivier Ricci curvature for a connected graph G = (V, E). For that we first need to introduce probability measures representing metric balls around vertices. These balls should be small but they should not be trivial (their radius needs to be positive). Since our distances are integers, we choose the radius 1, which means that the balls include the centre vertex $x \in V$ and all its neighbours $y \sim x$. The set of all involved vertices is then denoted by $B_1(x) = \{y \in V \mid d(x, y) \leq 1\}$. To allow some flexibility in the probability measure associated to $B_1(x)$, we do not choose equidistribution on all involved vertices, but introduce a parameter $p \in [0, 1]$, which is the probability at the centre, and the probabilities $\frac{1-p}{|x|}$ at each of the neighbours. Since these probabilities can be viewed as transition probabilities from the vertex x of a random walk, we can think of p as the probability that the random walker doesn't move. For that reason, we call the parameter p the *idleness* parameter. In conclusion, we introduce for every idleness $p \in [0,1]$ and every vertex $x \in V$ the probability measure

(7)
$$\mu_x^{\ p}(y) = \begin{cases} p & \text{if } y = x, \\ \frac{1-p}{|x|} & \text{if } y \sim x, \\ 0 & \text{otherwise.} \end{cases}$$

For any pair $x, y \in V$, $x \neq y$, the ratio $W_1(\mu_x^p, \mu_y^p)/d(x, y)$ tells us whether the optimal transport cost to move the weighted ball $B_1(x)$ to $B_1(y)$ is larger or smaller than the distance between their centres. In the former case we have $W_1(\mu_x^p, \mu_y^p)/d(x, y) > 1$, and in the latter case we have $W_1(\mu_x^p, \mu_y^p)/d(x, y) < 1$ and Ollivier Ricci curvature is then defined as follows:

Definition 3.3. Let G = (V, E) be a connected graph and $x, y \in V$. For any idleness value $p \in [0, 1]$, we define the Ollivier Ricci curvature $K_p(x, y)$ as

$$K_p(x,y) := 1 - \frac{W_1(\mu_x^p, \mu_y^p)}{d(x,y)},$$

where μ_x^p is given in (7).

Problem 3.4. Let G = (V, E) be a connected graph, $p \in [0, 1]$, and

$$x = x_0 \sim x_1 \sim \cdots \sim x_n = y$$

be a geodesic, that is, d(x, y) = n. Show the following inequality

$$K_p(x,y) \ge \min_{j \in \{0,1,\dots,n-1\}} K_p(x_j, x_{j+1})$$

using the fact that $W_1 : \mathcal{P}_1(V) \times \mathcal{P}_1(V) \times [0,\infty)$ is a distance function.

Let us mention the following useful consequence of Problem 3.4: Any lower bound of Ollivier Ricci curvature $K_p(x, y)$ for all $x, y \in V, x \neq y$, is automatically also a lower bound of Ollivier Ricci curvature on the edges, where we define the Ollivier Ricci curvature of an edge $e = \{x, y\} \in E$ as

$$K_p(e) = K_p(x, y).$$

Because of this fact, we consider often only Ollivier Ricci curvature on the edges of a graph and view it then as a local invariant of the graph.

Example 3.5 (Ollivier Ricci curvature of a k-regular tree). Let $T_k = (V, E)$ be the infinite k-regular tree, $k \ge 2$. Figure 10 illustrates the neighbourhood of an edge $b \sim c$ for the case k = 7. By choosing the idleness $p = \frac{1}{k+1}$, the probability measure μ_x^p is equidistribution on the vertices of the 1-ball $B_1(x) \subset V$ around $x \in V$. Let us calculate $W_1(\mu_b^p, \mu_c^p)$: The masses $p = \frac{1}{k+1}$ on the vertices of $B_1(b)$ need to be transported to the vertices of $B_1(c)$. One way of doing this is as follows: there are k-2 neighbours of b (the filled red ones in Figure 10), whose masses $p = \frac{1}{k+1}$ need to travel over a distance 3 to k-2 neighbours of c (the empty red ones in Figure 10). Moreover, the masses $p = \frac{1}{k+1}$ on the vertices a, b, c in Figure 10 need to be shifted over to the vertices b, c, d, and this comes always with a cost of $3p = \frac{3}{k+1}$. Any such transport plan π yields a total cost of

$$\cot(\pi) = (k-2)3p + 3p = 3\frac{k-1}{k+1}$$

It is intuitively convincing (and indeed true) that no other transport plan can do better. Assuming that the above transport strategy is optimal, we conclude

$$K_{1/(k+1)}(b,c) = 1 - W_1(\mu_b^{\ p},\mu_c^{\ p}) = 1 - 3\frac{k-1}{k+1} = \frac{4-2k}{k+1},$$

which means that T_2 has vanishing Ollivier Ricci curvature (at idleness $p = \frac{1}{3}$) and T_k has strictly negative Ollivier Ricci curvature (at idleness $p = \frac{1}{k+1}$) for all $k \ge 3$.



FIGURE 10. Neighbourhood of the edge $b \sim c$ in a k-regular tree

Remark 3.6. In the previous example it is not clear whether splitting up the masses at the vertices of $B_1(b)$ into smaller quantities and sending these smaller quantities in different directions to possibly different vertices of $B_1(c)$ might lead to a better transport plan. A transport plan which does not do that and only transfers the total masses from their original vertices to target vertices is called a *transport map*. The question about existence of optimal transport maps is the so-called Monge problem, since it was GASPARD MONGE (1746-1818) who raised this problem back in 1781. It is easy to construct examples of probability measures which do not allow transport maps at all. The more general concept of *optimal transport plans* provides a solution to overcome this problem, and this more general concept was proposed 1942 by LEONID V. KANTOROVICH (1912-1986). It is known, however, that in the case of equal masses at all original and target vertices (in our case equals $p = \frac{1}{k+1}$ there exists an optimal transport plan which is realised by a transport map. See Ambrosio's article [1] for more on this issue and its history.

3.2. Duality principle. Calculating $W_1(\mu, \nu)$ is a *Linear Optimiza*tion Problem for which a duality principle applies. To formulate this duality principle we need to introduce the notion of 1-Lipschitz functions.

Definition 3.7. A function $\phi : V \to \mathbb{R}$ on a graph G = (V, E) is called 1-Lipschitz if

$$|\phi(x) - \phi(y)| \le d(x, y) \qquad \forall x, y \in V.$$

The set of all 1-Lipschitz functions on G is denoted by 1 - Lip(G).

Theorem 3.8 (Duality principle). Let G = (V, E) be a connected graph and $\mu, \nu \in \mathcal{P}_1(V)$. Then we have (8)

$$W_{1}(\mu,\nu) = \inf_{\pi \in \Pi(\mu,\nu)} \sum_{x,y \in V} d(x,y)\pi(x,y) = \sup_{\phi \in 1-\text{Lip}(G)} \sum_{x \in V} \phi(x)(\mu(x)-\nu(x)).$$

Every function $\phi \in 1 - \text{Lip}(G)$ which assumes the supremum on the right hand side of (8) is called an optimal Kantorovich potential.

Let us show how the duality principle can be used to prove optimality of a given transport plan:

Example 3.9 (Duality principle to prove optimality). Recall the transport plan $\pi : V \times V \to [0, 1]$ from Example 3.2 which lead to a total cost of

$$\cot(\pi) = \frac{7}{3}.$$

In order to prove that this cost is optimal and that we have $W_1(\mu, \nu) = \frac{7}{3}$, we need to find a suitable 1-Lipschitz function $\phi_0 : V \to \mathbb{R}$ such that

(9)
$$\sum_{x \in V} \phi_0(x)(\mu(x) - \nu(x)) = \frac{7}{3}.$$

Then equation (8) implies that π is optimal since then

$$\frac{7}{3} = \sum_{x \in V} \phi_0(x)(\mu(x) - \nu(x)) \le \sup_{\phi \in 1 - \operatorname{Lip}(G)} \sum_{x \in V} \phi(x)(\mu(x) - \nu(x)) = W_1(\mu, \nu).$$

One the other hand we know from Example 3.2 that

$$\frac{7}{3} = \cot(\pi) \ge W_1(\mu, \nu),$$

and, putting everything together, we conclude

$$W_1(\mu,\nu) = \cot(\pi) = \frac{7}{3}.$$

A 1-Lipschitz function ϕ_0 satisfying (9) is presented in Figure 11. It is easy to check that this function is 1-Lipschitz. (By the triangle inequality, is suffices to check that the function changes its value by at most 1 along every edge!)



FIGURE 11. An optimal Kantorovich potential Φ_0

We obtain

$$\begin{split} \sum_{x \in V} \phi_0(x)(\mu(x) - \nu(x)) \\ &= \phi_0(a)\frac{1}{2} + \phi_0(b)\frac{1}{3} + \phi_0(c)\frac{1}{6} - \phi_0(f)\frac{1}{3} - \phi_0(g)\frac{1}{4} \\ &= 1 + \frac{1}{3} + \frac{1}{6} + \frac{1}{3} + \frac{2}{4} = \frac{7}{3}, \end{split}$$

which implies optimality of the transport plan π .

The strategy to calculate the Ollivier Ricci curvature $K_p(x, y)$ in an explicit example is now as follows: firstly, choose a transport plan $\pi \in \Pi(\mu_x^p, \mu_y^p)$ which seems to be a particularly good candidate for optimality and calculate its cost; secondly, find a 1-Lipschitz function which show that the chosen transport plan π is optimal; finally, use this fact to calculate $W_1(\mu_x^p, \mu_y^p)$ and $K_p(x, y) = 1 - W_1(\mu_x^p, \mu_y^p)/d(x, y)$.

Problem 3.10. A graph G = (V, E) is called strongly regular with parameters $(\nu, k, \lambda, \mu)^{11}$, if

- (i) $|V| = \nu$,
- (ii) G is k-regular, that is, |x| = k for all $x \in V$,
- (iii) each pair of adjacent vertices has precisely λ common neighbours and
- (iv) each pair of non-adjacent vertices has precisely μ common neighbours.

¹¹We always assume $(\lambda, \nu) \neq (0, 0)$ for, otherwise, the graph would have to be a set of isolated vertices or a set of isolated edges.

The girth of a graph G is the length of a shortest cycle. It is easy to see that strongly regular graph can only have girth(G) = 3 (if $\lambda > 0$) girth(G) = 4 (if $\lambda = 0$ and $\mu \ge 2$) and girth(G) = 5 (if $\lambda = 0$ and $\mu = 1$). For example, the Petersen graph in Figure 12 is strongly regular with parameters (10, 3, 0, 1).



FIGURE 12. The Petersen graph

Prove the following result for every strongly regular graph G = (V, E)of girth 5: For any pair $x, y \in V$ of adjacent vertices we have

$$K_0(x,y) = \frac{2}{k} - 1.$$

Conclude from this that a girth-5 strongly regular graph with vanishing Ollivier Ricci curvature K_0 must be the pentagon.

You can use the following fact without proof: Any 1-Lipschitz function $f_0: V_0 \to \mathbb{R}$ on a subset $V_0 \subset V$ can be extended to a 1-Lipschitz function on V, that is, there exists a 1-Lipschitz function $f: V \to \mathbb{R}$ such that $f(x) = f_0(x)$ for all $x \in V_0$.

Remark 3.11. Surprisingly, there is no complete classification of all strongly regular graphs. In not yet published joint work with D. Cushing, R. Kangaslampi and Sh. Liu [14], we showed $K_0(x, y) = 0$ for all pairs $x, y \in V$ of adjacent vertices in girth-4 strongly regular graphs G = (V, E), and we conjecture that all girth-3 strongly regular graphs have non-negative K_0 -curvature.

3.3. Global results about Ollivier Ricci curvature. Let us recall the Bonnet-Myers Theorem from the previous chapter:

Theorem 2.4 (Bonnet-Myers Theorem). Let (M, g) be a complete connected *n*-dimensional Riemannian manifold with Ricci curvature bounded below by $1/r^2 > 0$, that is

$$\operatorname{Ric}_p(v) \ge \frac{1}{r^2} \|v\|^2 \qquad \forall v \in T_p M.$$

Then M is a compact manifold with diameter bounded by

(10) $\operatorname{diam}(M) = \max\{d(x, y) \mid x, y \in M\} \le \pi r$

where πr is the diameter of the *n*-dimensional round sphere of constant Ricci curvature $1/r^2$ (that is, the round sphere of radius r).

Interestingly, this theorem has a very natural discrete counterpart for k-regular graphs using Ollivier Ricci curvature with idleness $p = \frac{1}{k+1}$. Before we discuss this analogue, we want to mention the following rigidity result in the smooth setting of Riemannian manifolds due to Cheng [9]:

Theorem 3.12 (Cheng's Rigidity Theorem). Let (M, g) be a complete connected n-dimensional Riemannian manifold with Ricci curvature bounded below by $1/r^2 > 0$, that is

$$\operatorname{Ric}_p(v) \ge \frac{1}{r^2} \|v\|^2 \qquad \forall v \in T_p M.$$

If we have

$$\operatorname{diam}(M) = \pi r$$

then (M, g) is isometric to the n-dimensional round sphere of radius r.

This result tells us that equality in the Bonnet-Myers diameter estimate (10) necessarily implies that the Riemannian manifold is the round sphere. This statement is called a *rigidity result* since it is a full classification of all objects satisfying a relatively weak condition.

It is natural to ask for a discrete counterpart of this rigidity result. The first problem to solve is to find a discrete analogue of the n-dimensional round sphere. A natural candidate is the k-dimensional hypercube:

Definition 3.13. The k-dimensional hypercube $Q^k = (V, E)$ is the following graph: The vertex set of Q^k consists of all k-tuples in $\{0, 1\}^k$. As a consequence, we have $|V| = 2^k$. Two vertices $x, y \in \{0, 1\}^k$ are adjacent iff their Hamming distance is 1, that is, these k-tuples differ in precisely one entry.

We may think of the k-tuples representing vertices x of the hypercube Q^k as a set of coordinates of the vertex x in \mathbb{R}^k , and two vertices are then connected by an edge if they differ in just one coordinate.

The Ollivier Ricci curvature $K_{1/(k+1)}(x, y)$ of every edge $x \sim y$ of a k-dimensional hypercube is known to be (see [29])

(11)
$$K_{1/(k+1)}(x,y) = \frac{2}{k+1}.$$

This formula is also derived in Section 2.1 of [36] by Ollivier and Villani. They discuss suitable curvature notions and a *Brunn-Minkowski Inequality* for the hypercube in this article.

Problem 3.14. Derive the formula (11) for the curvature of the hypercube Q^k via the following steps:

- (i) Check that $K_{1/2}(x, y) = 1$ for the edge $x \sim y$ in Q^1 .
- (ii) Let $G = (V_g, E_G)$ and $H = (V_H, E_H)$ be two regular graphs with vertex degrees d_G and d_H , respectively. Let $x_1 \sim x_2$ be an edge in G and $y \in V_H$. Use the formula

(12)
$$K_{1/(d_G+d_H+1)}^{G\times H}((x_1,y),(x_2,y)) = \frac{d_G+1}{d_G+d_H+1}K_{1/(d_G+1)}^G(x_1,x_2)$$

(from [3, Corollary 1.3]) without proof and the fact that $Q^{k+1} = Q^k \times Q^1$ to give an induction proof of (11).

Let us now present the following discrete version of the Bonnet-Myers Theorem:

Theorem 3.15 (Discrete Bonnet-Myers Theorem for Ollivier Ricci curvature). Let G = (V, E) be a connected k-regular graph with Ollivier Ricci curvature bounded below by $K_0 > 0$, that is

$$K_{1/(k+1)}(x,y) \ge K_0 \qquad \forall x \sim y.$$

Then G is finite with diameter bounded by

(13)
$$\operatorname{diam}(G) = \max\{d(x,y) \mid x, y \in V\} \le \frac{2k}{(k+1)K_0}.$$

Note that in the case of the k-dimensional hypercube Q^k we have $K_0 = 2/(k+1)$ and $(2k)/((k+1)K_0) = k$ is the diameter of C^k . This shows that the inequality (13) cannot be improved.

Problem 3.16. Prove the discrete Bonnet-Myers Theorem for Ollivier Ricci curvature, using the following fact for Dirac δ -measures of any pair of vertices $x, y \in V$:

$$W_1(\delta_x, \delta_y) \le W_1(\delta_x, \mu_x^p) + W_1(\mu_x^p, \mu_y^p) + W_1(\mu_y^p, \delta_y),$$

since W_1 is a distance function on \mathcal{P}_1 , and the statement in Problem 3.4.

Note that the statement in Theorem 3.15 for connected k-regular graphs G with strictly positive Ollivier Ricci curvature can be reformulated as the inequality

(14)
$$\operatorname{diam}(G) \le \frac{2k}{(k+1)\inf_{x \sim y} K_{1/(k+1)}(x,y)}$$

We also know that (14) holds with equality in the case of the kdimensional hypercube Q^k . It is natural to ask whether there is also a discrete analogue of the Cheng Rigidity Theorem. The first guess would be the following conjecture:

Conjecture (First try!). If (14) holds with equality for a connected k-regular graph G with strictly positive Ollivier Ricci curvature then this graph must be isomorphic to Q^k .

It turns out that this conjecture is false. Indeed, there are other families of graphs satisfying (14) with equality. One such example are the cocktail party graphs CP(k) with 2k vertices $u_1, \ldots, u_k, v_1, \ldots, v_k$ where all vertices are adjacent unless they share the same index. The name cocktail party graph stems from the following interpretation: the vertices correspond to guests of a cocktail party; the participants are kcouples and, at arrival, they shake hands (hand-shaking is represented by edges between the corresponding vertices); now, each guest shakes hands with all other guests except for their own spouse. Another way of describing cocktail party graphs CP(k) is as follows: we start with a complete graph K_{2k} of 2k vertices, that is, there is an edge between each pair of vertices; then we remove from this graph a perfect matching, that is a set of k edges which do not share any vertices with each other (these edges describe the couples in the party). In particular, the cocktail party graph CP(4) with 8 edges is the one-skeleton of the octahedron, where opposite vertices correspond to couples.

It is natural to ask whether it is possible to completely classify all regular connected graphs with strictly positive Ollivier Ricci curvature satisfying (14) with equality. In [12], we call these graphs *Bonnet-Myers* sharp graphs and prove the following result:

Theorem 3.17 (see [12]). Let G be a connected k-regular self-centered¹² graph with strictly positive Ollivier Ricci curvature such that (14) holds with equality. Then G is one of the following:

- 1. hypercubes Q^k , $k \ge 1$,
- 2. cocktail party graphs $CP(k), k \geq 3$,

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¹²A graph G = (V, E) is called *self-centered* if, for every vertex $x \in V$, there exists a vertex $\overline{x} \in V$ such that $d(x, \overline{x}) = \text{diam}(G)$.

- 3. the Johnson graphs $J(2k, k), k \geq 3$,
- 4. even-dimensional demi-cubes $Q_{(2)}^{\overline{2k}}, \ k \ge 3$,
- 5. the Gosset graph,

and Cartesian product $G_1 \times G_2 \times \cdots \times G - k$ of 1.-5. satisfying

$$\frac{d_1}{\operatorname{diam}(G_1)} = \frac{d_2}{\operatorname{diam}(G_2)} = \dots = \frac{d_k}{\operatorname{diam}(G_k)},$$

where d_i is the vertex degree of the graph G_i .

The Johnson graph J(6,3) and the Gosset graph are illustrated in Figure 13. We conjecture that the self-centeredness assumption is not necessary and can be removed but this seems to be a very challenging problem.



FIGURE 13. The Johnson graph J(6,3) and the Gosset graph¹³

Challenge. Let G = (V, E) be a finite connected k-regular graph. The (normalized) Laplacian Δ_G is a linear operator defined on functions $f: V \to \mathbb{R}$ as follows:

$$\Delta_G f(x) := f(x) - \frac{1}{k} \sum_{y \sim x} f(y).$$

This operator has real eigenvalues which can be ordered with their multiplicities as

 $0 = \lambda_1 < \lambda_2 \le \lambda_3 \le \dots \le \lambda_N \le 2,$

where N = |V| and the eigenvalue $\lambda_1 = 0$ is simple and the corresponding eigenfunctions are precisely the non-trivial constant functions.

¹³Picture taken from https://en.wikipedia.org/wiki/Gosset_graph# /media/File:E7_graph.svg

(You don't need to prove this fact!) Show the following fact: If the Ollivier Ricci curvature of G = (V, E) is bounded below by $K_0 > 0$, that is,

$$K_{1/(k+1)}(x,y) \ge K_0 \qquad \forall x \sim y,$$

(we know then from Theorem 3.15 that G is finite), then the first positive eigenvalue of Δ_G satisfies

$$\lambda_2 \ge \frac{k+1}{k} K_0$$

3.4. Outlook into further research and developments. The appeal of Ollivier Ricci curvature for graphs is that this curvature notion can be calculated reasonably well in concrete examples while, at the same time, there are striking analogies with curvature phenomena in the smooth setting of Riemannian manifolds. A natural question is, for given pair of distinct vertices x, y, the dependence of the curvature $K_p(x, y)$ on the idleness parameter $p \in [0, 1]$. This was investigated for edges $x \sim y$ in [3] and for arbitrary pairs x, y of vertices with $d(x, y) \geq 2$ in [11]: in fact, the function $[0, 1] \ni p \mapsto K_p(x, y)$ is concave and piecewise linear with at most three linear parts (and at most two linear parts in the case of adjacent vertices in regular graphs). A slight modification of Ollivier Ricci curvature measuring the slope near p = 1 was introduced by Lin/Lu/Yau in [29].

A very useful interactive web-tool (see Figure 14) to calculate various kinds of graph curvatures has been developed by G. Stagg and D. Cushing. This tool is ideal to test conjectures and to obtain deeper insights into various curvature notions. Details about this tool can be found in [13]. This tool is freely accessible through

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

Ollivier Ricci curvature is not the only successful utilisation of Optimal Transport Theory to introduce a Ricci curvature notion in new settings. Sturm [38] and Lott/Villani [30] (see Figure 15 below, pictures taken from Wikipedia) used Optimal Transport Theory to generalise Ricci curvature from the smooth setting of Riemannian manifolds to general metric measure spaces. This approach is based on the observation, proved in [40], that a global lower Ricci curvature bound of a Riemannian manifold (M, g) by a constant K is equivalent to K-convexity of the Boltzmann-Shannon entropy functional on the space of probability measures on M along geodesics with respect to the W_2 -Wasserstein distance. The K-convexity property in the space of probability measures can be defined for general metric measure spaces which are geodesic and is used in [38, 30] to introduce a general synthetic notion of Ricci curvature which is stable under Gromov-Hausdorff convergence. CURVATURE NOTIONS ON GRAPHS



FIGURE 14. Graph curvature calculator by G. Stagg and D. Cushing

This new approach to curvature opened the door to a currently highly active and exciting research field.



FIGURE 15. Karl-Theodor Sturm, John W. Lott and Cédric Villani

As mentioned before, the generalisation to metric measure spaces due to Sturm and Lott/Villani requires them to be *geodesic spaces*¹⁴. On the other hand, graphs equipped with the combinatorial distance

¹⁴A metric space (X, d) is called *geodesic* if any pair $x, y \in X$ can be joined by a geodesic $c: I \to X$ with $I = [a, b] \subset \mathbb{R}$ a closed interval and x = c(a) and y = c(b), that is, d(c(s), c(t)) = |t - s| for all $s, t \in I$.

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are discrete spaces and fail to be geodesic. A discrete curvature notion for finite Markov chains (and therefore combinatorial graphs as particular examples) in the spirit of Sturm and Lott/Villani was given by Erbar/Maas in [19]. Their global discrete curvature notion is called *en*tropic curvature and is based on a modification of the W_2 -Wasserstein distance. This curvature notion behaves well under taking Cartesian products but it is very difficult to explicitly calculate entropic curvature in concrete examples (even in the simplest case if the underlying space is just two points).

These comments conclude the section on Ollivier Ricci curvature and we move on into the last curvature notion, which is non-local in nature: Gromov hyperbolicity.

4. Gromov hyperbolicity

Cayley graphs and Gromov hyperbolicity play a central role in a highly research active area called *Geometric Group Theory*. We will introduce these concepts and will see that Gromov hyperbolicity is a kind of a *global negative curvature notion* for unbounded connected graphs or, more generally, for geodesic metric spaces.

4.1. Cayley graphs and δ -hyperbolic graphs. Let us start with the definition of Cayley graphs.

Definition 4.1. Let Γ be a group with a finite set S of generators such that $e \notin S$ and if $s \in S$ then also $s^{-1} \in S$. The Cayley graph $\operatorname{Cay}(\Gamma, S) = (V, E)$ of Γ with respect to S is the graph with $V = \Gamma$ and two vertices $\gamma_1, \gamma_2 \in \Gamma$ are connected by an edge if and only if there exists $s \in S$ such that $\gamma_2 = \gamma_1 s$.

Cayley graphs can be viewed as realisations of a group Γ as a metric space with the combinatorial distance function $d: \Gamma \times \Gamma \to \mathbb{N} \cup \{0\}$ on the vertex set of $\operatorname{Cay}(\Gamma, S) = (V, E)$. They form a very interesting class of graphs since there is another tool besides combinatorics available to work with them, namely algebra and, in particular, group theory and representation theory.

Note that every edge of a Cayley graph corresponds to an element s of S and can therefore be labelled by s. Moreover, if $\operatorname{ord}(s) \geq 3$, then the edge corresponding to $\gamma \sim \gamma s$ can be understood as being directed from γ to γs . In the case $\operatorname{ord}(s) = 2$ we have $s = s^{-1}$ and the Cayley graph $\operatorname{Cay}(\Gamma, S)$ has then precisely one undirected edge between γ and γs .

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FIGURE 16. $Cay(S_4, \{(12), (23), (34)\})$

Example 4.2. The Cayley graph of the symmetric group S_4 with generator set $S = \{(12), (23), (34)\}$ is illustrated in Figure 16. Since all generators have order 2, the edges, labelled by a = (12), b = (23) and c = (34), are undirected.

Proposition 4.3. All Cayley graphs are vertex transitive and connected.

Proof. Let $Cay(\Gamma, S) = (V, E)$. For $\gamma_1, \gamma_2 \in V = \Gamma$ let

$$\phi: V \to V, \qquad \phi(\gamma) = \gamma_2 \gamma_1^{-1} \gamma.$$

It is easy to see that ϕ is a graph automorphism and that we have $\phi(\gamma_1) = \gamma_2$. This shows vertex transitivity.

By vertex transitivity, it suffices to show that $e \in \Gamma = V$ can be connected to any other vertex $\gamma \in \Gamma = V$. By the definition of generators, we can write γ in the form

$$\gamma = s_1 s_2 \cdots s_N$$

with $s_1, s_2, \ldots, s_N \in S$. Then the path

$$e \sim s_1 \sim s_1 s_2 \sim s_1 s_2 s_3 \sim \dots \sim s_1 s_2 \cdots s_N = \gamma$$

connects e with γ . This proves that a Cayley graph is connected. \Box

Problem 4.4. Construct the Cayley graph $Cay(D_{12}, S)$ where D_{2n} is the dihedral group given by

$$D_{2n} = \{s, r \mid s^2 = r^n = e, r^i s = sr^{n-i} \text{ for } 1 \le i \le n-1\},\$$

and

$$S = \{s, sr, sr^2, sr^4\}.$$

Check also that S is a symmetric set of generators of D_{12} .

Now we introduce the notion of *Gromov hyper*bolicity. It is a fundamental concept which was introduced by M. Gromov in his seminal paper [21] and which turned out to have profound consequences. While we need this notion in the setting of combinatorial graphs, we start with its definition in the context of a *geodesic* metric space¹⁵ (X, d).



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In short, Gromov hyperbolicity is the property that there exists a constant $\delta \geq 0$ such that any geodesic triangle is δ -thin, that is, every side of the triangle is contained in the δ -neighbourhodds of the other two sides. This property is illustrated in Figure 17 below.

Definition 4.5 (Gromov hyperbolicity for geodesic metric spaces). A geodesic metric space (X, d) is called δ -hyperbolic if we have the following for any geodesic triangle $\Delta = c_1 \cup c_2 \cup c_3$: The side c_i are completely contained in the union of the δ -tubes around the sides c_j and c_k , where $\{i, j, k\} = \{1, 2, 3\}$. In other words, we have

$$c_i \subset T_{\delta}(c_j) \cup T_{\delta}(c_k)$$

where

$$T_{\delta}(c) = \{ x \in X \mid \exists x_0 \in c : d(x_0, x) \le \delta \}.$$

A geodesic metric space (X, d) is called Gromov hyperbolic if it is δ -hyperbolic for some $\delta \geq 0$.

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¹⁵Recall that a metric space (X, d) is called *geodesic* if any pair $x, y \in X$ can be joined by a geodesic $c : I \to X$ with $I = [a, b] \subset \mathbb{R}$ a closed interval and x = c(a) and y = c(b), that is, d(c(s), c(t)) = |t - s| for all $s, t \in I$.

¹⁶Picture taken from https://en.wikipedia.org/wiki/Mikhail_ Leonidovich_Gromov#/media/File:Gromov_Mikhail_Leonidovich.jpg



FIGURE 17. Illustration of Gromov hyperbolicity¹⁷

Before we provide two examples of Gromov hyperbolic spaces, we first like to address the issue that combinatorial graphs G = (V, E) are discrete objects and, therefore, as metric spaces with the integer valued combinatorial distance function they are not geodesic. One way to overcome this problem is to view G as a metric graph with all its edges realised as line segments of length 1 and to extend the combinatorial distance function to arbitray points on these edges in a natural way. Another way to solve this problem is to stick with the combinatorial nature of G = (V, E) and to define geodesics in G as maps $c : \{k, k + 1, \ldots, l\} \rightarrow V$ such that d(c(i), c(j)) = |j - i| for all $i, j \in \{k, \ldots, l\}$. We denote the set of vertices contained in c by V(c), that is, V(c) = $\{c(i) \mid i \in \{k, \ldots, l\}$. We then modify Definition 4.5 in this context the following way:

Definition 4.6 (Gromov hyperbolicity for combinatorial graphs). A connected graph G = (V, E) is called δ -hyperbolic if we have the following for any geodesic triangle $\Delta = c_1 \cup c_2 \cup c_3$: The vertices of the side c_i are completely contained in the union of the δ -tubes around the sides c_j and c_k , where $\{i, j, k\} = \{1, 2, 3\}$. In other words, we have

$$V(c_i) \subset T_{\delta}(c_j) \cup T_{\delta}(c_k)$$

where

$$T_{\delta}(c) = \{ x \in V \mid \exists x_0 \in V(c) : d(x_0, x) \le \delta \}.$$

A connected graph G = (V, E) is called Gromov hyperbolic if it is δ -hyperbolic for some $\delta \geq 0$.

¹⁷Picture taken from https://commons.wikimedia.org/wiki/File:Delta_thin_triangle_condition.svg.



FIGURE 18. 0-hyperbolicity of a tree

Let us now discuss two important examples:

Example 4.7 (Trees as Gromov hyperbolic spaces). Let T = (V, E) be a tree. Then any triangle $\Delta = c_1 \cup c_2 \cup c_3$ with vertices $x, y, z \in V$ is a Y-shaped structure – as illustrated in Figure 18 – with uniquely defined mid point $o \in V$ such that Δ consists of three paths p_{xo}, p_{yo}, p_{zo} (with p_{uv} the unique path in T from $u \in V$ to $v \in V$) such that

$$\begin{array}{rcl} c_1 &=& p_{xo} \cup p_{yo}, \\ c_2 &=& p_{yo} \cup p_{zo}, \\ c_3 &=& p_{zo} \cup p_{xo}. \end{array}$$

Therefore, we have $c_i \subset c_j \cup c_k$ for any choice $\{i, j, k\} = \{1, 2, 3\}$ and T is 0-hyperbolic.

Example 4.8 (The hyperbolic plane as Gromov hyperbolic space). Let us consider \mathbb{R}^2 with the Euclidean distance (the *Euclidean plane*) and the *hyperbolic plane* \mathbb{H}^2 , represented by the upper half plane $\mathbb{H}^2 = \{z \in \mathbb{C}^2 \mid \text{Im}(z) > 0\}$ with hyperbolic metric $d_{\mathbb{H}^2}$ given by (see [26])

$$d_{\mathbb{H}^2}(z,w) = \ln \frac{|z-\bar{w}| + |z-w|}{|z-\bar{w}| - |z-w|}.$$

Both spaces are geodesic metric spaces. The Euclidean plane \mathbb{R}^2 is obviously not Gromov hyperbolic: Choose the right-angled Euclidean triangle with vertices x = (0,0), y = (c,0) and z = (0,c), c > 0. Then the point (c/2, c/2) lies on the side connecting y and z and this point has obviously Euclidean distance c/2 to the other two sides of



FIGURE 19. Gromov hyperbolicity of the hyperbolic plane

this triangle (which are parts of the x- and y-axis). Since c > 0 can be arbitrary large, the Euclidean plane is not Gromov hyperbolic.

We show now, in contrast, that the hyperbolic plane is Gromov hyperbolic. As in the Euclidean case, it is true that any (geodesic) triangle in $(\mathbb{H}^2, d_{\mathbb{H}^2})$ contains a unique (hyperbolic) incircle touching all three sides if the triangle.

We first show that the radius of this incircle is bounded by $\frac{1}{2} \ln 3$ for any triangle in $(\mathbb{H}^2, d_{\mathbb{H}^2})$: Every triangle Δ sits completely inside an ideal triangle Δ_{∞} with all its vertices in $\partial \mathbb{H}^2$. Obviously, the radius of the incircle of Δ_{∞} is greater or equal to the radius of the incircle of Δ and we only need to show the upper bound of the inradius for ideal triangles. On the other hand, any ideal triangle is isometric to the ideal triangle Δ_0 with its vertices at -1, 1, and ∞ . Recall that hyperbolic circles in \mathbb{H}^2 have the shape of Euclidean circles. The hyperbolic incircle of the ideal triangle Δ_0 is the blue circle in Figure 19. Note that this blue circle is invariant under Euclidean reflection along the imaginary axis which happens to be a hyperbolic isometry. Therefore, the hyperbolic centre of this incircle lies on the imaginary axis and the vertical Euclidean line segment rfom u = i to 3i is a geodesic diameter of the incircle. We have

$$d_{\mathbb{H}^2}(i,3i) = \ln \frac{4+2}{4-2} = \ln 3,$$

and the hyperbolic radius of this incircle is, therefore, $r = \frac{1}{2} \ln 3$.

Now we use this fact to prove that $(\mathbb{H}^2, d_{\mathbb{H}^2})$ is Gromov-hyperbolic. As a consequence of $= \frac{1}{2} \ln 3$, we have

$$d_{\mathbb{H}^2}(u,v) = 2r = \ln 3$$

for the points $u, v \in \mathbb{H}^2$ in Figure 19. Note that the bi-infinite sides of the triangle Δ_0 containing u and v are asymptotic with common end-point $1 \in \partial \mathbb{H}^2$ and since u, v both lie on a horocycle centered at 1, the distance between the geodesic rays from u = i to $1 \in \partial \mathbb{H}^2$ and from v = 1 + 2i to $1 \in \partial \mathbb{H}^2$ is bounded above by $d_{\mathbb{H}^2}(u, v) = \ln 3$. This shows that the side of the triangle Δ_0 with end-points -1, 1 is contained in the union of the δ -tubes around the other two sides of Δ_0 for $\delta = \ln 3$. This shows that \mathbb{H}^2 is $(\ln 3)$ -hyperbolic. In fact, it can be shown with more work that the optimal δ -value for \mathbb{H}^2 is $\ln(1 + \sqrt{2})$.

The main difference between \mathbb{R}^2 with Euclidean metric and $(\mathbb{H}^2, d_{\mathbb{H}^2})$ is that the first space has curvature zero and the second one has constant curvature -1. Therefore, we can consider δ -hyperbolicity as a kind of a *global negative curvature property* with the understanding that the smaller the constant $\delta > 0$ the more negatively curved is the given metric space.

Note, however, that every bounded metric space (X, d) is Gromov hyperbolic. This means that Gromov hyperbolicity is an asymptotic property of the whole space and not a *local curvature concept*.

4.2. Quasi-geodesics and quasi-isometries.

Definition 4.9. Let (X_1, d_1) and (X_2, d_2) be two metric spaces and $\lambda \geq 1$ and $K \geq 0$. A map $f : X_1 \to X_2$ is called a (λ, K) -quasiisometry if we have for any pair $x, y \in X_1$,

(15)
$$\frac{1}{\lambda}d_1(x,y) - K \le d_2(f(x), f(y)) \le \lambda d_1(x,y) + K.$$

We call a map $f: X_1 \to X_2$ a quasi-isometry if there exist λ, K such that f is a (λ, K) -quasi-isometry. If $f: X_1 \to X_2$ is a $(\lambda, 0)$ -quasi-isometry for some λ , then we call f a quasi-isometry in the strong sense.

Note that there are no further conditions on f other than (15) to be a quasi-isometry. In particular, we do not require f to be continuous or surjective or almost surjective in some specific sense. Moreover, a map $f: X_1 \to X_2$ is quasi-isometric in the strong sense if and only if f is globally bi-Lipschitz.

Problem 4.10. Let Γ be a group with a two different finite sets S_1, S_2 of generators such that $e \notin S_i$ and if $s \in S_i$ then also $s^{-1} \in S_i$ for $i \in \{1, 2\}$. Show that the map

$$\phi_0 : \operatorname{Cay}(\Gamma, S_1) \to \operatorname{Cay}(\Gamma, S_2), \quad \phi_0(\gamma) = \gamma \quad \forall \gamma \in \Gamma$$

is a quasi-isometry in the strong sense.

Definition 4.11. Let G = (V, E) be a connected graph with combinatorial distance function $d: V \times V \to \mathbb{N} \cup \{0\}$. Let $a \leq b$ be two integers. We call a map

$$c: \mathbb{Z} \cap [a, b] \to V$$

a quasi-geodesic if it is a quasi-isometry between $(\mathbb{Z} \cap [a, b], d(n, m) = |n - m|)$ and (V, d), that is, we have

$$\frac{1}{\lambda}|m-n| - K \le d(c(n), c(m)) \le \lambda|m-n| + K$$

for suitable fixed parameters λ, K and all $n, m \in \mathbb{Z} \cap [a, b]$.

The following fundamental result on quasi-ismetries is also called the *Morse Lemma* (see [18, Theorem 11.40]). Its proof is more involved and beyond these lecture notes. Interested readers can consult [6, Theorem 1.3.2] or [10, Théorème 3.1.3] or [4, Theorem III.H.1.7]:

Theorem 4.12 (Stability of quasi-geodesics). Let G = (V, E) be a δ -hyperbolic graph and $\lambda \geq 1$ and K > 0. Then there exists a constant R > 0, only depending on δ, λ, K , such that we have the following: any (λ, K) -quasi-geodesic $c : \mathbb{Z} \cap [a, b] \to V$ with x = c(a) and y = c(b) stays in the R-neighbourhood of any geodesic

$$c_0: \{0, 1, \dots, d(x, y)\} \to V$$

with $c_0(0) = x$ and $c_0(d(x, y)) = y$, that is, for every $k \in \mathbb{Z} \cap [a, b]$ there exists $k' \in \{0, 1, \ldots, d(x, y)\}$ with

$$d(c(k), c_0(k')) \le R.$$

The next problem is the main goal of this chapter, namely, that Gromov hyperbolicity of a finitely generated group does not depend on the choice of generators. **Problem 4.13.** Let Γ , S_1 , S_2 be as in Exercise 4.10. Show the following: If $Cay(\Gamma, S_1)$ is Gromov hyperbolic then $Cay(\Gamma, S_2)$ is also Gromov hyperbolic. You can use Theorem 4.12 without proof in your arguments.

4.3. **Outlook: The Gromov boundary.** An important concept associated to a non-compact Gromov space (X, d) is the *Gromov bound*ary ∂X . Recall that the boundary of the hyperbolic plane \mathbb{H}^2 , represented by the upper half space $\mathbb{H}^2 = \{z \in \mathbb{C}^2 \mid \text{Im}(z) > 0\}$ with the distance function (3), was given by $\partial \mathbb{H}^2 = \mathbb{R} \cup \{\infty\}$. In the case of ideal triangles in \mathbb{H}^2 , their vertices could be understood as points of $\partial \mathbb{H}^2$. The Gromov boundary can be viewed as a generalization of this boundary of the hyperbolic plane to general Gromov hyperbolic spaces. The first step towards the Gromov boundary of (X, d) is to choose a reference point $o \in X$ and to introduce the so-called *Gromov product*

$$(x \mid y)_o = \frac{1}{2}(d(x, o) + d(y, o) - d(x, y)).$$

We then say that a sequence (x_n) converges to infinity if

$$\lim_{k,l\to\infty} (x_k \mid x_l)_o = \infty.$$

In the case of a bounded Gromov hyperbolic space there are no sequences converging to infinity.

There is an equivalence relation on the sequences converging to infinity, given as follows: $(x_n) \sim (y_n)$ if

$$\lim_{k \to \infty} (x_k \mid y_k)_o = \infty.$$

The Gromov boundary ∂X is then defined as the space of equivalence classes of sequences converging to infinity. It turns out that this construction is independent of the reference point $o \in X$.

In the case of a proper¹⁸ geodesic Gromov hyperbolic space, one can introduce natural topologies on X, ∂X and on the disjoint union $\overline{X} := X \cup \partial X$ such that the topologies of X, ∂X are relative topologies of \overline{X} and that \overline{X} is compact. In the case of the above-mentioned hyperbolic plane \mathbb{H}^2 , viewed as a Gromov hyperbolic space, the Gromov compactification $\overline{\mathbb{H}^2} = \mathbb{H}^2 \cup (\mathbb{R} \cup \{0\})$ carries a topology which is homeomorphic to a closed unit disk (which coincides with the standard compactification of the *Poincaré unit disk model* of the hyperbolic plane, which we did not introduce). An important result is that the Gromov boundary is "topologically stable" under quasi-isometries in the following sense:

¹⁸A metric space (X, d) is called proper if for all $x \in X$, $R \ge 0$, the closed metric balls $\overline{B_R(x)} := \{y \in X \mid d(x, y) \le R\}$ are compact.

Theorem 4.14 (see, e.g., Théorème 3.2.2 in [10]). Let (X_1, d_1) and (X_2, d_2) be two geodesic metric spaces and $f : X_1 \to X_2$ be a quasiisometry. If (X_2, d_2) is Gromov hyperbolic, then (X_1, d_1) is also Gromov hyperbolic and the map f induces a natural map

$$\partial f: \partial X_1 \to \partial X_2.$$

In the particular case that 19

$$\sup\{d_2(x, f(X_1)) \mid x \in X_2\} < \infty,$$

then ∂f is a homeomorphism.

These boundary structures turn out to be of crucial importance in the study of asymptotic properties of metric spaces (see, e.g., [6]). With this brief glimpse into the Gromov boundary, we finish this section on Gromov hyperbolicity.

5. Summary

The seemingly simple question

"What is curvature?"

gave rise to intensive research over the centuries going far beyond the boundaries of theoretical mathematics: In the 1820's, Gauss measured angles between three mountains (Hohenhagen, Brocken und Inselberg) using his newly invented heliotrope (see Figure 20 below) in order to investigate and capture the curvedness of a particular part of Germany through triangulations. From 1907 to 1915, Einstein developed his Theory of General Relativity which is based on the fact that the curvature of our universe is directly related to the energy and momentum of heavy objects like stars and black holes and radiation.

In recent decades it became apparent that curvature notions like Gaussian (or sectional) curvature and Ricci curvature can be generalised to singular spaces and metric measure spaces. This lead to new curvature notions, some of which were even of non-local nature. In the particular case of graphs (with combinatorial distance function) these new curvature concepts are not only of theoretical interest: for example, they are relevant to measure connectivity and robustness of complex and dynamical networks like the human brain or the World Wide Web.

¹⁹In a metric space (X, d) we define d(x, A) for $x \in X$ and a subset $A \subset X$ by $d(x, A) := \inf \{ d(x, y) \mid y \in A \}.$



FIGURE 20. The Heliotrope of Gauss²⁰

The aim of these lecture notes was to provide some basic insights into three particular curvature notions on graphs (combinatorial curvature, Ollivier Ricci curvature and Gromov hyperbolicity) with connections to various research areas of modern mathematics like Combinatorial or Geometric Group Theory or the Theory of Optimal Transport.

While curvature has been studied over the centuries, it is fair to say that the above question with all its ramifications is still far from being conclusively settled.

We recommend the book [32] to all readers whose interest is raised and who want to continue studying further aspects of the first two curvature notions, namely combinatorial curvature and Ollivier Ricci curvature. In particular, the survey articles [2] and [28] in that book should be understandable with the background provided by these lecture notes. Recommendable books providing a wealth of information on metric spaces are, for example, [4] or [5]. Readers interested to learn more about Geometric Group Theory are encouraged to consult, e.g., [15] or the more recent monograph [18]. Special focus on hyperbolic groups is given the in lecture notes [10], written in French. Readers who want to learn more about the Sturm and Lott/Villani definition of Ricci curvature via Optimal Transport Theory might benefit from looking into the classical monograph [39] or the survey [33].

²⁰Picture taken from https://en.wikipedia.org/wiki/Heliotrope_ (instrument)#/media/File:Gauss'_Heliotrope.jpg

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