Metric Curvatures and Applications

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Since considering triangulations (of surfaces), one is faced with *finite graphs*, or, in many cases – when given just the vertices of the triangulation (e.g. Clouds of Points) – only with finite – thus discrete – metric spaces. Therefore, the following natural questions arise:

(A) Is one fully justified in employing discrete metric spaces when evaluating numerical invariants of continuous surfaces?

and the following more general one:

(B) Can one find discrete, metric equivalents of the differentiable notions, notions that are intrinsically more apt to describe the properties of finite spaces under investigations?

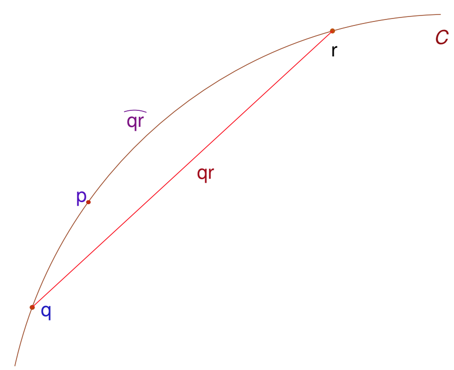
First let's try and define *metric curvature* for *curves*:

Since it We choose the (not so well known) Haantjes curvature since it:

- **Does not impose** an Euclidian structure upon the given metric space*;
- Is extremely versatile.

*Like the Menger and Alt curvatures

Definition Let (M,d) be a metric space, let $c : I = [0,1] \overset{\simeq}{\to} M$ be a homeomorphism, and let $p, q, r \in c(I)$, $q, r \neq p$. Denote by $\widehat{qr}$ the arc of $c(I)$ between q and r, and by qr segment from q to r.



Then c has *Haantjes Curvature** $\kappa_H(p)$ at the point p iff:

$$\kappa_H^2(p) = 24 \lim_{q,r \to p} \frac{l(\widehat{qr}) - d(q,r)}{\left(l(\widehat{qr})\right)^3};$$

where "$l(\widehat{qr})$" denotes the length†

*1947

† given by the intrinsic metric induced by d of $\widehat{qr}$.

Of course, this definition would represent nothing but a nice exercise in esoteric pass-time, where it not for the following result:

Theorem 1 *Let* $\gamma \in \mathcal{C}^1$ *be smooth curve in* $\mathbb{R}^3$ *and let* $p \in \gamma$ *be a regular point. Then the Haantjes curvature of* γ *at* p $K_H(p)$ *exists and equals the classical curvature of* γ *at* p*.*

Remark 2 *The Haantjes Curvature is a notion restricted only to rectifiable curves.**

*For fractals one should use the Menger curvature.

And now for some (possible) applications...

We start with the **most obvious** (at least in this "milieux"):

- In the view of the Theorem 1 above, it is clear that one can use $K_H(p)$ as an approximation of sectional curvatures for triangulated surfaces. But one can expect **obvious errors** (since one uses an approximation of a classical notion on an approximation of a smooth curve.) But this curvature is ideally fitted for the intelligence of PL-curves (and surfaces).

Since Haantjes curvature – as an analogue of sectional curvature – does not convey an intrinsic measure of surface curvature, a proper notion is to be searched for... Once again, Gauss' idea of comparing the given surface to a model one provides the answer!...

However, we can't restrict ourselves to the unit sphere $\mathbb{S}^2$ as a *gauge* surface, but we shall compare the given surface S to any of the *the complete, simply connected surface of constant curvature* κ, i.e.

$$\boxed{S_\kappa \equiv \mathbb{R}^2, \text{ if } \kappa = 0}$$

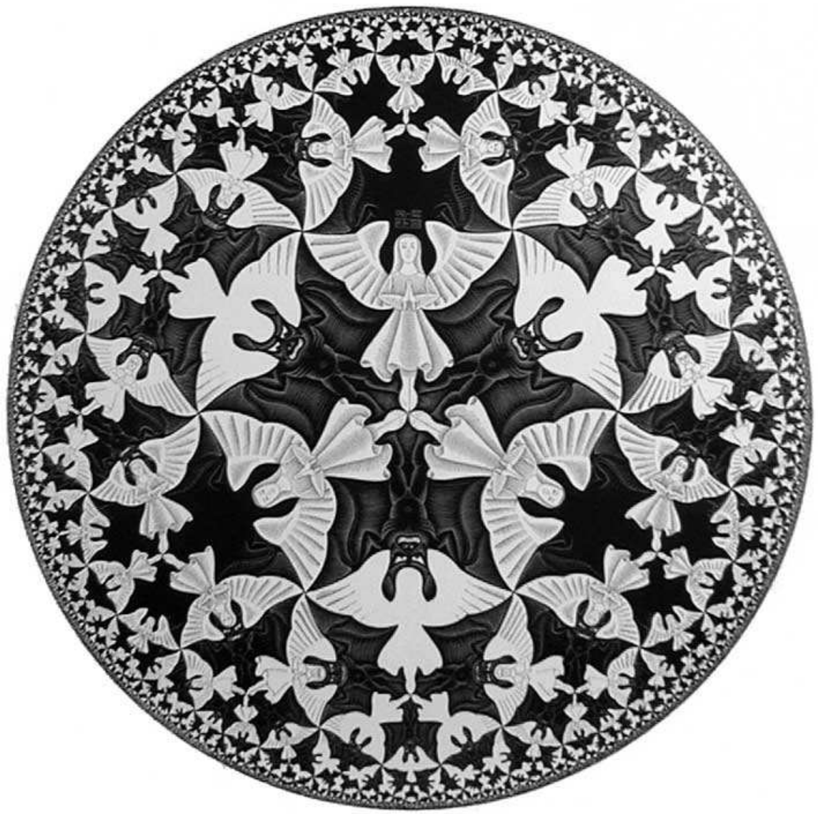
$$\boxed{S_\kappa \equiv \mathbb{S}^2_{\sqrt{\kappa}}, \text{ if } \kappa > 0}$$

$$\boxed{S_\kappa \equiv \mathbb{H}^2_{\sqrt{-\kappa}}, \text{ if } \kappa < 0}$$

Here $S_\kappa \equiv \mathbb{S}^2_{\sqrt{\kappa}}$ denotes the Sphere of radius $R = 1/\sqrt{\kappa}$,

and

$S_\kappa \equiv \mathbb{H}^2_{\sqrt{-\kappa}}$ stands for the *Hyperbolic Plane* of curvature $\sqrt{-\kappa}$, as represented by the *Poincare Model* of the plane disk of radius $R = 1/\sqrt{-\kappa}$.



We can now start towards our goal of defining an intrinsic metric curvature for surfaces.

We do this by comparing quadruples on the given metric space, to those in a gauge surface. It is, in fact, a natural idea, since quadruples are classically* the "minimal" geometric figures that allow the differentiation between metric spaces.

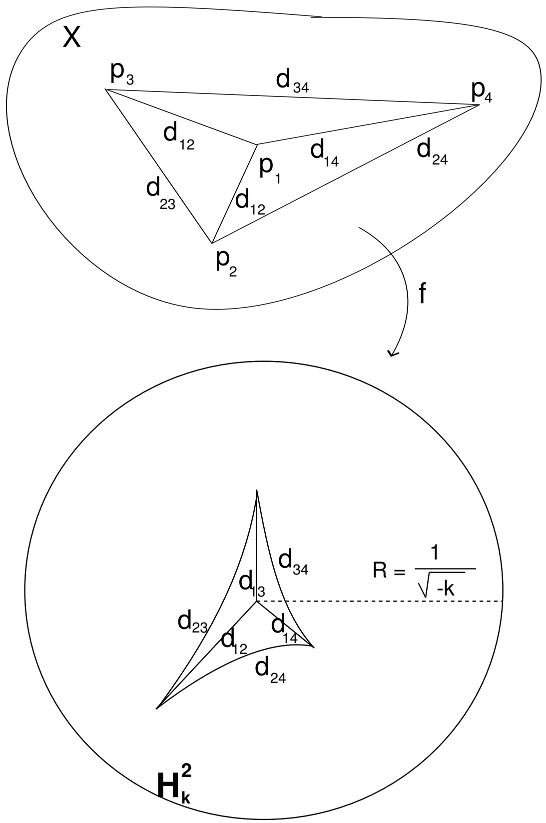
*as illustrated by the time-honored principles of Projective Geometry...

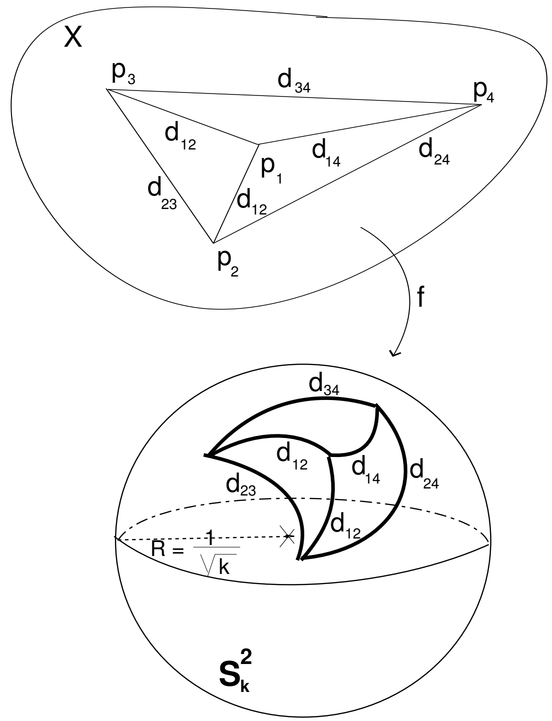
Definition 3 *Let* (M,d) *be a metric space, and let* $Q = \{p_1,...,p_4\} \subset M$*, together with the mutual distances:* $d_{ij} = d_{ji} = d(p_i,p_j)$; $1 \leq i,j \leq 4$*. The set* Q *together with the set of distances* $\{d_{ij}\}_{1\leq i,j\leq 4}$ *is called a* metric quadruple*.*

Remark 4 *One can define metric quadruples in slightly more abstract manner, without the aid of the ambient space: a metric quadruple being a* 4 *point metric space; i.e.* $Q = \Big(\{p_1,...,p_4\},\{d_{ij}\}\Big)$*, where the distances* d_{ij} *verify the axioms for a metric.*

The following definition is almost obvious:

Definition 5 *The* embedding curvature $\kappa(Q)$ *of the metric quadruple* Q *is defined be the curvature* κ *of* S_κ *into which* Q *can be isometrically embedded.*





We can now define the embedding curvature at a point in a natural way by passing to the limit (but without neglecting the existence conditions), more precisely:

Definition 6 *Let* (M, d) *be a metric space, and let* $p \in M$ *be an accumulation point. Then* M *is said to have* Wald curvature $\kappa_W(p)$ *at* p *iff*

1. $\nexists\, N \in \mathcal{N}(p), N$ *linear** ;

2. $\forall\, \varepsilon > 0,\ \exists\, \delta > 0$ *s.t.* $Q = \{p_1, ..., p_4\} \subset M$, *and s.t.* $d(p, p_i) < \delta\, (i = 1, ..., 4) \Longrightarrow |\kappa(Q) - \kappa_W(p)| < \varepsilon$.

*The neighborhood N of p is called linear iff N is contained in a geodesic.

Remark 7 *If one uses the second (abstract) definition of the metric curvature of quadruples, then the very existence of $\kappa(Q)$ is not assured, as it is shown by the following*

Counterexample 8 *The metric quadruple of lengths*

$$d_{12} = d_{13} = d_{14} = 1;\ d_{23} = d_{24} = d_{34} = 2$$

admits no embedding curvature.

Remark 9 *Even if a quadruple has an embedding curvature, it still may be not unique (even if Q is not linear), indeed, one can study the following examples:*

Counterexample 10 *The quadruple Q of distances $d_{ij} = \pi/2,\ 1 \leq i < j \leq 4$ is isometrically embeddable both in $S_0 = \mathbb{R}^2$ and in $S_1 = \mathbb{S}^2$.*

Counterexample 11 *The quadruple Q of distances $d_{13} = d_{14} = d_{23} = d_{24} = \pi$, $d_{12} = d_{34} = 3\pi/2$ admits exactly two embedding curvatures: $\kappa_1 \in (1.5, 2)$ and $\kappa_2 = 3$.*

So the notion of *Embedding Curvature*, however interesting, may prove to be either ambiguous or even – in some cases – empty!...

However, for "good" metric spaces* the embedding curvature **exists and it is unique**. And, what is even more relevant for us, this embedding curvature coincides with the classical Gaussian curvature.

Indeed, the discussion above would be nothing more than a nice intellectual exercise where it not for the fact that the **metric (Wald)** and the **classical (Gauss)** curvatures coincide whenever the second notion makes sense, that is for smooth† surfaces in $\mathbb{R}^3$.

*i.e. spaces that are locally "plane like"

†i.e. of class $\geq \mathcal{C}^2$

More precisely the following Theorem holds:

Theorem 12 (Wald) *Let $S \subset \mathbb{R}^3$, be a smooth surface.*[*]*. Then $\kappa_W(p)$ exists, for all $p \in S$, and $\kappa_W(p) = \kappa_G(p), \forall\, p \in M$.*

Moreover, Wald also proved that a partial reciprocal theorem holds, more precisely he proved the following:

Theorem 13 (Wald) *Let M be a compact and convex metric space. If $\kappa_W(p)$ exists, for all $p \in M$, then M is a smooth surface and $\kappa_W(p) = \kappa_G(p), \forall\, p \in M$.*

[*] i.e. $S \in \mathcal{C}^m$, $m \geq 2$

Unfortunately, the proof of these beautiful results is far beyond our scope.

Even proving that that a compact, convex metric space locally mimics $\mathbb{R}^2$, that is that the following Proposition holds:

Proposition 14 *Any convex, compact metric space is locally homeomorphic to the real plane.*

is far beyond our scope...

However we can **compute** the Embedding Curvature, this being not only an interesting quandary in itself, but an absolute minimum if we want to employ Wald Curvature in any practical implementation...

We follow first the classical approach of **Wald-Blumenthal** that employs the so-called *Cayley-Menger determinants*:

Given a general metric quadruple $Q = Q(p_1, p_2, p_3, p_4)$, of distances $d_{ij} = dist(p_i, p_j)$, $i = 1, ..., 4$, we denote by $D(Q) = D(p_1, p_2, p_3, p_4)$ the following determinant:

$$D(p_1, p_2, p_3, p_4) = \begin{vmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 \\ 1 & d_{12}^2 & 0 & d_{23}^2 & d_{24}^2 \\ 1 & d_{13}^2 & d_{23}^2 & 0 & d_{34}^2 \\ 1 & d_{14}^2 & d_{24}^2 & d_{34}^2 & 0 \end{vmatrix}$$

Then the *embedding curvature* $\kappa(Q)$ of Q is given – depending upon the embedding space (i.e. upon the sign of the curvature) – by the following formulae:

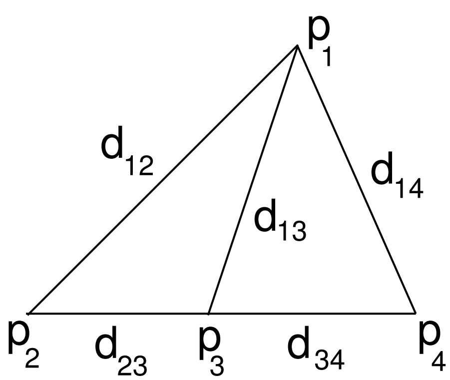
$$(\circledast)\ \kappa(Q) = \begin{cases} 0 & \text{if } D(Q) = 0\,; \\ \kappa,\ \kappa < 0 & \text{if } det(\cosh\sqrt{-\kappa}\cdot d_{ij}) = 0\,; \\ \kappa,\ \kappa > 0 & \text{if } det(\cos\sqrt{\kappa}\cdot d_{ij}) \text{ and } \sqrt{\kappa}\cdot d_{ij} \leq \pi \\ & \text{and all the principal minors} \\ & \text{of order 3 are } \geq 0. \end{cases}$$

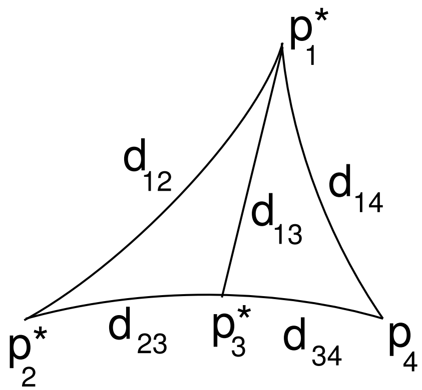
We sincerely admit that this formulae ”per se” can only mystify... Moreover, however nice and elegant(?!...) these formulae may be, they have a HUGE drawback from both the Theoretical and the Practical points of view:

They are Transcendental!... ...and, even more tragically, a given quadruple may have *two different emebedding curvatures!...*

However, it turns out that if one restrict himself to precisely those quadruples that admit a unique embedding curvature, a simple *approximation* of their embedding curvature may be computed! Note here that every “nice” neighbouhoods of “locally plane-like spaces“ contains “good” quadruples.

Definition 15 *A metric quadruple* $Q = Q(p_1, p_2, p_3, p_4)$, *of distances* $d_{ij} = dist(p_i, p_j),\ i = 1, ..., 4$, *is called* semi-dependent *(a* sd-quad*, for brevity), iff 3 of its points are on a common geodesic, i.e. there exist 3 indices – e.g. 1,2,3 – s.t.:* $d_{12} + d_{23} = d_{13}$.*





*Thus one is reduced two the study of "augmented" triangles.

As wished for, one has the following:

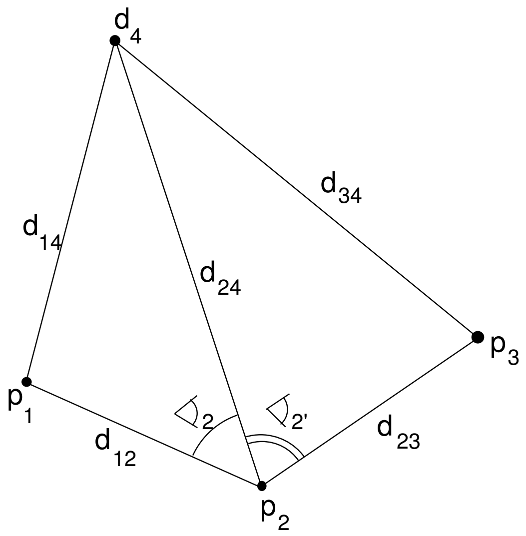
Proposition 16 *An sd-quad admits at most one embedding curvature.*

Now we can safely state the promised approximation result:

Proposition 17 (Robinson, 1944) *Given the metric quadruple* $Q = Q(p_1, p_2, p_3, p_4)$, *of distances* $d_{ij} = dist(p_i, p_j),\ i = 1, \ldots, 4$, *the embedding curvature* $\kappa(Q)$ *is well approximated by:*

$$(\star) \qquad \boxed{K(Q) = \frac{6(\cos\angle_0 2 + \cos\angle_0 2')}{d_{24}(d_{12}\sin^2(\angle_0 2) + d_{23}\sin^2(\angle_0 2'))}\,;}$$

where: $\angle_0 2 = \angle(p_1 p_2 p_4)$, $\angle_0 2' = \angle(p_3 p_2 p_4)$ *represent the angles of the Euclidean triangles of sides* d_{12}, d_{14}, d_{24} *and* d_{23}, d_{24}, d_{34}, *respectively.*



The *error* R can be estimated by using the following inequality:

$$(\odot)\ \ |R| = |R(Q)| = |\kappa(Q) - K(Q)| < 4\kappa^2(Q) diam^2(Q)/\lambda(Q)\,;$$

$$\lambda(Q) = d_{24}(d_{12} \sin \angle_0 2 + d_{23} \sin \angle_0 2')/S^2;$$

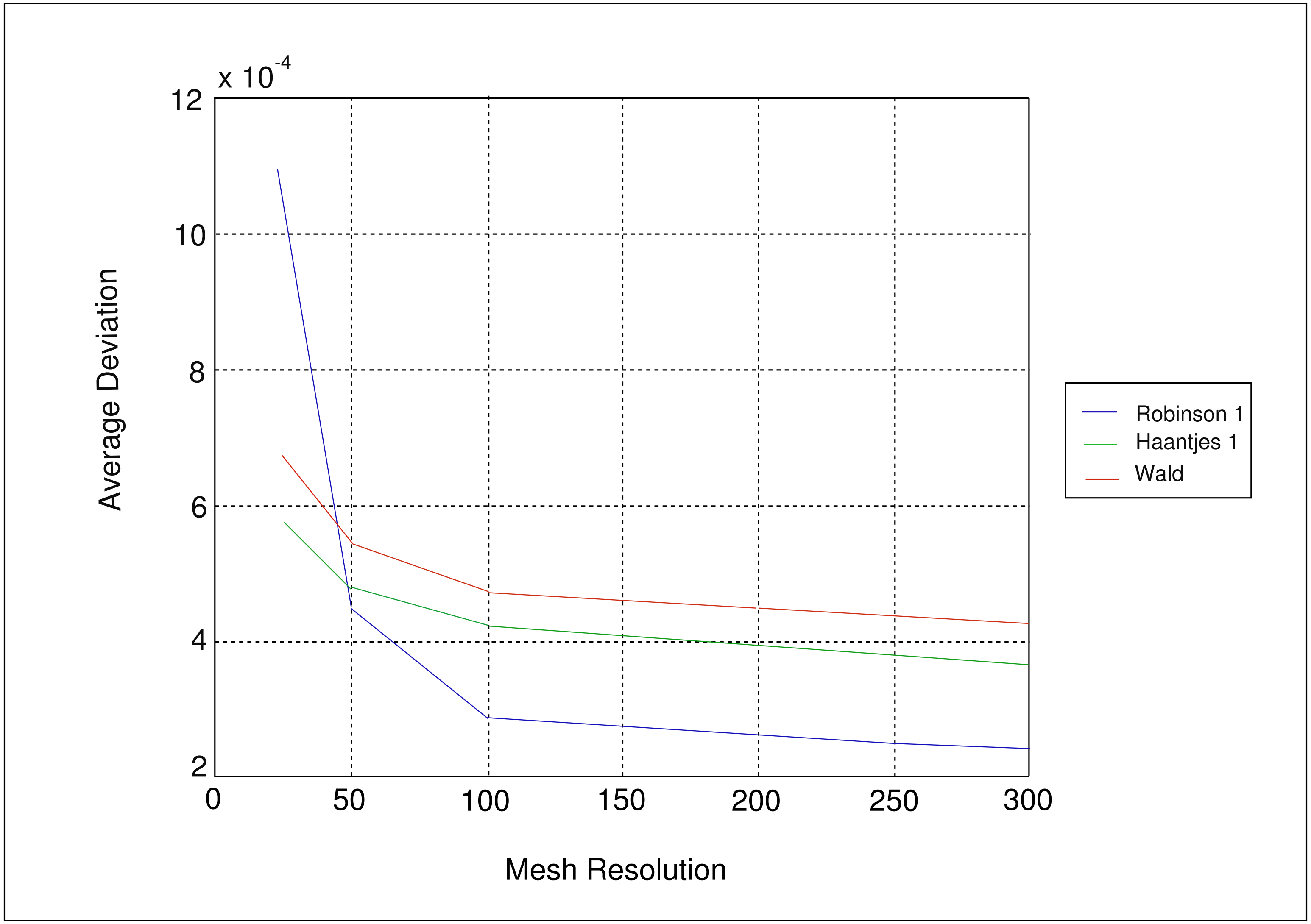
$$S = Max\{p, p'\};\ 2p = d_{12} + d_{14} + d_{24}\,,\ 2p' = d_{32} + d_{34} + d_{24}.$$

While the full details of the proof would be tedious* and arborescent, we can still give

The basic idea of the proof: that is to recreate, in a general metric setting, the Gauss Map – in this case one measures the curvature by the amount of "bending" one has to apply to a general planar quadruple so that it may be "straightened" (i.e. isometrically embedded as a *sd-quad*) in some S_κ.

*based upon Taylor expansion of "$sinh$" and some clever trigonometric manipulations.

We bring some (very preliminary) results obtained on a torus:



...And now, to some applications (in a non-graphics context) of the Haantjes curvature in

- DNA Microarraay Data Analysis;
- Communication Network Analysis;
- Geodesics in Network/Holes in Networks.

Application to DNA Microarraay Data Analysis*

We start by adapting Haantjes curvature to *vertex weighted graphs*:

Definition 18 *Let (G, E, μ) be a connected vertex weighted graph. Define (for all $v \sim u$):*

$$d(v,w) = \begin{cases} \frac{|\mu(v)|+|\mu(w)|}{|\mu(v)\mu(w)|} & v \neq w\,,\ \mu(v), \mu(w) \neq 0; \\ 1 & v \neq w\,,\ \mu(v) = 0 \text{ or } \mu(w) = 0; \\ 0 & v = w\,. \end{cases}$$

Curvature Based Clustering for DNA Microarray Data Analysis*, Lecture Notes in Computer Science, IbPRIA 200, **3523, pp. 405-412, Springer-Verlag, 2005.

Remark 19 *In our context is natural to choose positive, integer weights.*

Remark 20 *The metric just defined may appear arbitrary but in fact it is rather general, because of the following reasons:*

- *One can easily "jiggle" the given metric to obtain an equivalent one by applying a function with certain properties (s.a.* $\sqrt{d}$, $|\ln d|$*)*

- *Any family of (bounded) metric spaces* $\left\{(M_i, d_i)_i\right\}$ *admits an isometric embedding in some (bounded) metric space* (M, d)*.*

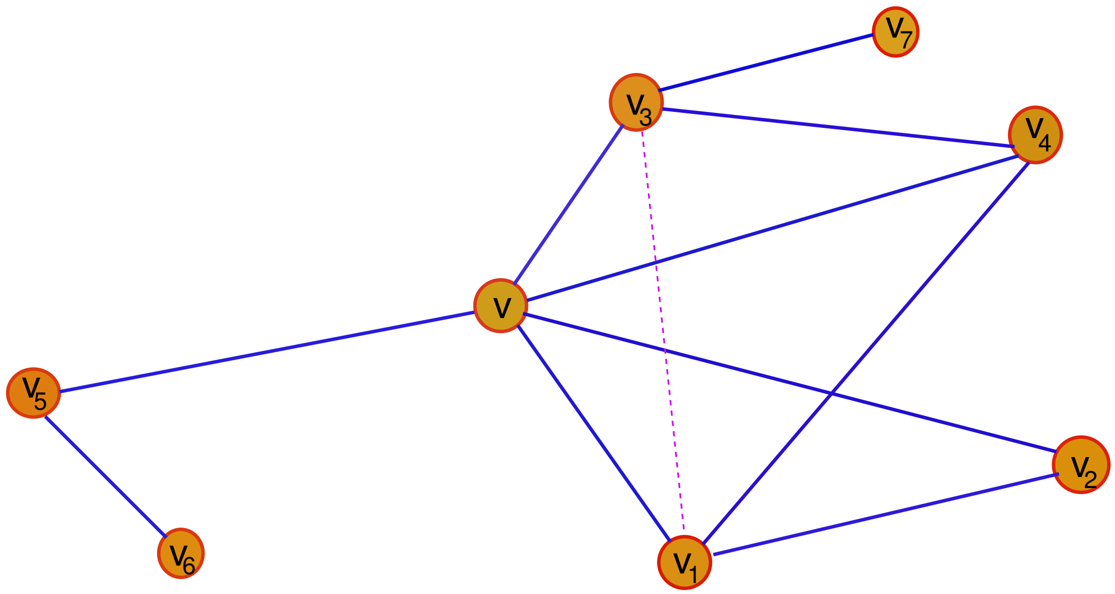
- *The metrics of any finite family of metric spaces are Lipschitz equivalent.*

Definition 21 *Let $G = (V, E, \mu)$ be as before, let d be the metric on G defined above, and let $v \in V$. Let $\pi = v_1 v v_2$ be a path through v. First we define the* curvature of triangles *with vertex v as being:*

$$\kappa'_H(\triangle v_1 v v_2) = \begin{cases} \sqrt{24 \frac{|d(v_1,v)+d(v,v_2)-d(v_1,v_2)|}{\left(d(v_1,v)+d(v,v_2)\right)^3}} & e = (v_1, v_2) \in E; \\ 0 & e = (v_1, v_2) \notin E. \end{cases}$$

Then the *modified* Haantjes curvature $\kappa'_{H,\pi} = \kappa'_H(v)$ of π at v is defined to be the arithmetic mean of the curvatures of all the triangles with apex v:

$$\kappa'_H(p) = \frac{\sum_{v_i \sim v,\, v_{ij} \sim v,\, v_{ij} \neq v_i} \kappa'_H(\triangle v_i v v_{ij})}{|\{\triangle v_i v v_{ij} \mid v_i \sim v, v_{ij} \sim v, v_{ij} \neq v_i\}|}$$



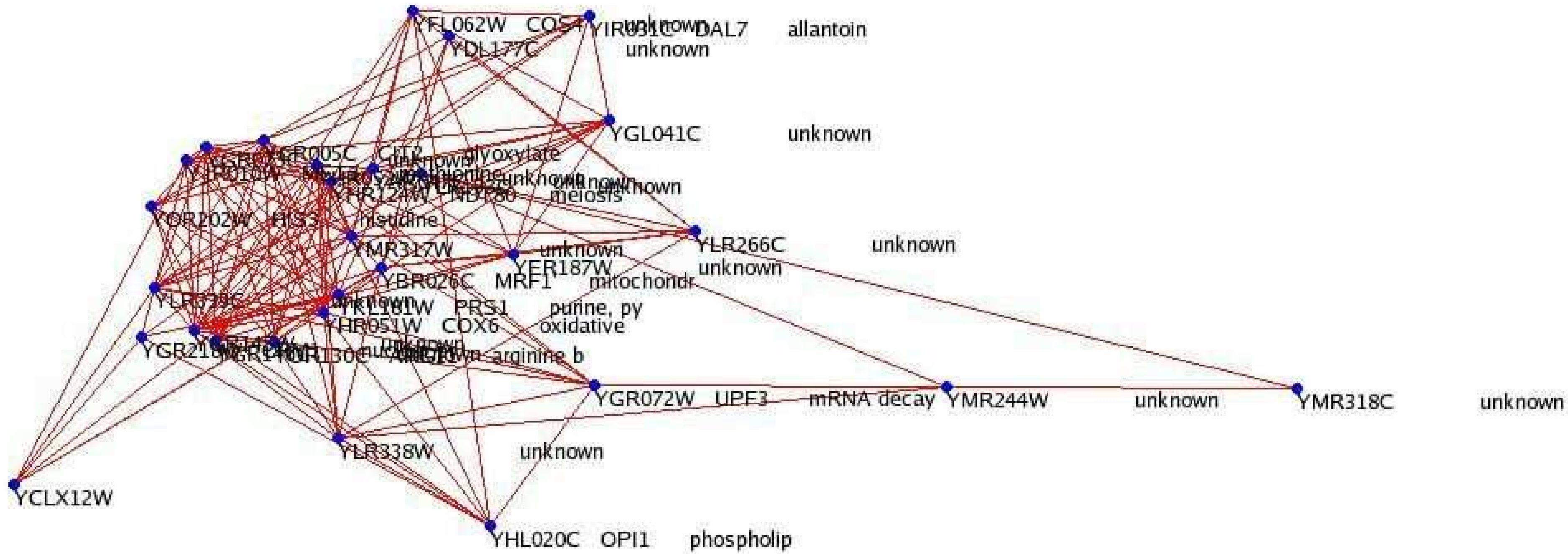
In this variation of the definition the curvature at v is computed as the *mean of the curvatures* off all the triangles with apex at v, so in a sense the curvature at each point depends on the curvatures at the points in $v_i \sim v$.

We compare the clustering performance of our (metric) curvature to that of the combinatorial curvature.

To perform clustering, one selects a curvature threshold $T_{curv} \in [0,1]*$ and selects a subgraph $H_{T_{curv}} \subseteq G$ by removing all nodes of curvature $< T_{curv}$ together with their adjacent edges.

DNA microarray data taken from
http://rana.lbl.gov/EisenData.html is made into a graph by a method of correlation based "edging". Namely, one computes the correlation between different DNA microarrays and sets an edge between them according to a (correlation) threshold. For that we used the open source Trixy (J. Rougemont and P. Hingamp).

Afterwards the obtained graph undergoes clustering according to curvature. For the metric we used gene length as vertices weights for they were shown to be relevant for the functioning of genes.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meiosis
YOR202W HIS3
histidine
YMR317W
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YLR266C
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YER187W
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mitochondr
YKL181W PRS1
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oxidative
arginine b
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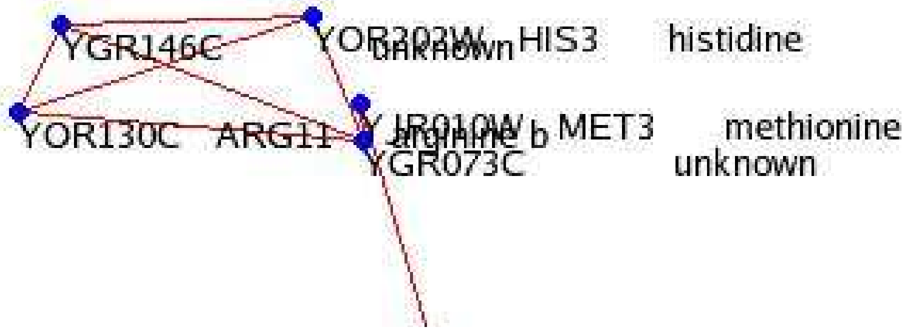
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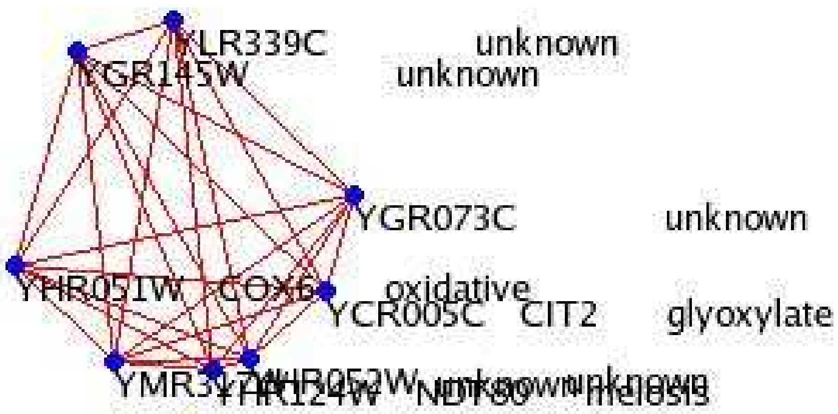
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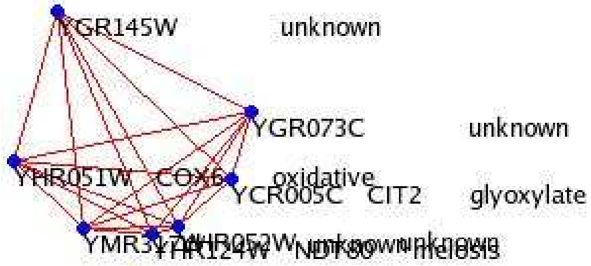
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