Ultrametrization and its applications in GH geometry

Lecture 2 of the minicourse "Gromov–Hausdorff distance: applications and lower bounds"

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Lecture outline

1. Ultrametric spaces and their properties.
2. Ultrametrization $\mathcal{U}(X)$ of a metric space.
3. Main theorem: $d_{GH}(X,Y) \geq d_{GH}\big(\mathcal{U}(X),\mathcal{U}(Y)\big)$.
4. Applications: distances $d_{GH}(P_n, S^1)$ and $d_{GH}(P_m, P_n)$.
5. Ultrametrization and metric trees.
6. Ultrametrization, Jung's constant and MST-spectrum.

Ultrametrics: definition and properties

Definition

A metric space (X, d) is called *ultrametric* if its distance function satisfies the *strong triangle inequality*:

$$d(x, z) \le \max\{d(x, y),\ d(y, z)\} \qquad \forall x, y, z \in X.$$

Properties

1. *Polygon inequality*: $d(x_0, x_n) \le \max_{1 \le i \le n} d(x_{i-1}, x_i)$.
2. *Isosceles*: among $d(x, y)$, $d(y, z)$, $d(z, x)$ two are equal, and the third does not exceed them.
3. *Property of balls*: every ball of non-zero radius is open and closed; if two balls intersect, one is contained in the other.
4. *Diameter of component*: if $d(x, y) = \operatorname{diam} X$, then for any z either $d(x, z) = \operatorname{diam} X$ or $d(y, z) = \operatorname{diam} X$.
5. *Center of the ball*: every point on the ball is its center.

Examples of ultrametric spaces

1. *Discrete metric*: $d(x,y) = 1$ for $x \neq y$.
2. *Trees with maximum edge metric*: for a tree T with weights $\omega(e) > 0$ we set

$$d(v,w) = \max\{\omega(e) : \ e \text{ lies on the path from } v \text{ to } w\}.$$

   This is an ultrametric, and vice versa: any finite ultrametric space can be represented in this way.
3. *p-adic numbers*: for $x = p^k \frac{m}{n} \in \mathbb{Q}$ with p not dividing mn, put $|x|_p = p^{-k}$, $|0|_p = 0$; the metric $|x-y|_p$ on $\mathbb{Q}_p$ is ultrametric.
4. *Function spaces*: for $f\colon X \to (0,\infty)$ the function $d(x,y) = \max\{f(x), f(y)\}$, $x \neq y$, is an ultrametric.

Definition (ultrametrization: step 1)

A polyline in the metric space (X, d) is a finite sequence of points $x_0, x_1, \ldots, x_n \in X$. Its *ultra-length* is

$$|L|_u := \max_{1 \le i \le n} d(x_{i-1}, x_i).$$

The *ultradistance* between $x, y \in X$ is defined by

$$d_u(x, y) := \inf\big\{|L|_u : \ L \text{ is a polyline in } X, \text{ connecting } x \text{ and } y\big\}.$$

Unlike regular length, ultra-length is not additive: it is equal to the maximum link, so small links "do not accumulate".

Ultra-distance: pseudometric

Proposition

The function d_u is a pseudometric on X and satisfies the strong triangle inequality:

$$d_u(x,z) \le \max\bigl\{d_u(x,y),\ d_u(y,z)\bigr\}.$$

Proof. The symmetry is obvious. The triangle inequality follows from the concatenation of polylines: if L_{xy} connects x to y, and L_{yz} connects y to z, then

$$|L_{xy} + L_{yz}|_u = \max\bigl\{|L_{xy}|_u,\ |L_{yz}|_u\bigr\},$$

whence

$$d_u(x,z) \le \inf_{L_{xy},L_{yz}} \max\bigl\{|L_{xy}|_u,\ |L_{yz}|_u\bigr\} = \max\bigl\{d_u(x,y),\ d_u(y,z)\bigr\}.$$

Positive definiteness may be violated: $d_u(x,y) = 0$ is possible for $x \ne y$ (for example, for a connected space).

Ultrametrization $\mathcal{U}(X)$

Definition

An *Ultrametrization* of a metric space X is a quotient space

$$\mathcal{U}(X) := X/\sim, \qquad x \sim y \iff d_u(x,y) = 0,$$

with the metric induced by d_u.

Note

The space $\mathcal{U}(X)$ is ultrametric. If X is already ultrametric, then $\mathcal{U}(X) = X$ (up to isometry), since $d_u = d$.

Examples of ultrametrization

Examples

- If X is connected and any two points are connected by a curve of finite length, then $\mathcal{U}(X) = \Delta_1$: for any x, y and any $\varepsilon > 0$ there is a polyline of ultralength $< \varepsilon$.
- For circle S^1: $\mathcal{U}(S^1) = \Delta_1$.
- For the set P_n of vertices of a regular n-gon inscribed in a unit circle (the metric is induced from the intrinsic metric of the circle): $\mathcal{U}(P_n) = (2\pi/n)\Delta_n$.

Correspondences (recall)

Definition

A *correspondence* between X and Y is a set $R \subset X \times Y$ whose projections onto X and onto Y are surjective. Its *distortion* is

$$\operatorname{dis} R = \sup\bigl\{\,|\,|xx'|_X - |yy'|_Y\,|\,:\ (x,y),(x',y') \in R\bigr\},$$

and the Gromov–Hausdorff distance is expressed as

$$d_{GH}(X,Y) = \frac{1}{2} \inf_{R \in \mathcal{R}(X,Y)} \operatorname{dis} R.$$

This is the characteristic we shall use: it allows us to "transfer" a correspondence from $X \times Y$ to $\mathcal{U}(X) \times \mathcal{U}(Y)$.

The main theorem about ultrametrization

Theorem

For any non-empty metric spaces X and Y,

$$d_{GH}(X,Y) \geq d_{GH}\big(\mathcal{U}(X),\mathcal{U}(Y)\big).$$

- Ultrametrization does not increase the GH-distance: the operation $\mathcal{U}$ is a 1-Lipschitz (more precisely, non-stretching) mapping $\mathcal{GH} \to \mathcal{GH}$.
- This provides a way to obtain *lower* estimates: we calculate the distance between (simpler) ultrametrizations.

Proof: correspondence construction

If $d_{GH}(X,Y)=\infty$, the inequality is trivial. Let $d:=d_{GH}(X,Y)<\infty$ and $\varepsilon>0$. According to the characteristic through correspondences, there is $R\in\mathcal{R}(X,Y)$ with $\operatorname{dis} R<2d+\varepsilon$.

We denote by $[x]$ the class of the point x in $\mathcal{U}(X)$ and by $[y]$ the class of the point y in $\mathcal{U}(Y)$, and set

$$R_u:=\big\{\big([x],[y]\big):\ (x,y)\in R\big\}\subset\mathcal{U}(X)\times\mathcal{U}(Y).$$

The projections of R onto X and onto Y are surjective, which means that both projections R_u are also surjective, that is, R_u is a correspondence between $\mathcal{U}(X)$ and $\mathcal{U}(Y)$.

Proof: distortion estimate

It is enough to check that for any $(x, y), (x', y') \in R$

$$d_u(y, y') \le d_u(x, x') + \operatorname{dis} R.$$

(The second symmetric inequality is obtained by applying the same reasoning to R^{-1}.)

1. Let us take $\delta > 0$ and the polyline $L = (x_0 = x, x_1, \dots, x_n = x')$ in X with $|L|_u < d_u(x, x') + \delta$.
2. For each $i = 1, \dots, n-1$ we choose y_i with $(x_i, y_i) \in R$; let us put $y_0 := y$, $y_n := y'$. We get the polyline $L' = (y_0, \dots, y_n)$ in Y.
3. From the distortion: $|y_i y_{i+1}|_Y \le |x_i x_{i+1}|_X + \operatorname{dis} R$ for all i, therefore

$$d_u(y, y') \le |L'|_u = \max_i |y_i y_{i+1}|_Y \le \max_i |x_i x_{i+1}|_X + \operatorname{dis} R$$
$$= |L|_u + \operatorname{dis} R < d_u(x, x') + \delta + \operatorname{dis} R.$$

4. Due to the arbitrariness of $\delta > 0$, we have $d_u(y, y') \le d_u(x, x') + \operatorname{dis} R$, that is, $\operatorname{dis} R_u \le \operatorname{dis} R < 2d + \varepsilon$. Passing to the infimum and to the limit at $\varepsilon \to 0$, we obtain $d_{GH}\big(\mathcal{U}(X), \mathcal{U}(Y)\big) \le d$.

Corollaries of the main theorem

Corollary 1

If $d_{GH}(X,Y)=0$, then $d_{GH}\big(\mathcal{U}(X),\mathcal{U}(Y)\big)=0$.

Corollary 2

For any metric space X

$$\operatorname{diam}\mathcal{U}(X)\leq\operatorname{diam}X.$$

If X is connected and any two of its points are connected by a curve of finite length, then $\operatorname{diam}\mathcal{U}(X)=0$.

The second corollary shows that ultrametrization cannot increase the diameter, but it contracts connected spaces with finite path lengths to a point.

Corollary: lower bound for the GH-distance

Corollary 3

If in a metric space X any two points are connected by a curve of finite length, then for any metric space Y

$$d_{GH}(X,Y) \geq \frac{1}{2}\operatorname{diam}\mathcal{U}(Y).$$

In particular, this is true for any normed space X and any subset $Y \subseteq X$.

Proof. By Corollary 2 we have $\mathcal{U}(X) = \Delta_1$, and $d_{GH}(\Delta_1, Y) = \frac{1}{2}\operatorname{diam} Y$; hence by the main theorem $d_{GH}(X,Y) \geq d_{GH}\big(\mathcal{U}(X),\mathcal{U}(Y)\big) = \frac{1}{2}\operatorname{diam}\mathcal{U}(Y)$.

Note

Such a lower bound cannot be derived from the Hausdorff estimate: if $Y \subseteq X$, then $d_{GH}(X,Y) \leq d_H(X,Y)$, so d_H gives an estimate *from above*.

Circle and regular polygon

Theorem

Let S^1 be a standard circle with intrinsic metric, and $P_n \subset S^1$ be the set of vertices of a regular n-gon. Then

$$d_{GH}(P_n, S^1) = \frac{\pi}{n}.$$

Proof.

- *Upper bound*: The Hausdorff distance between P_n and S^1 is π/n, so $d_{GH}(P_n, S^1) \leq \pi/n$.
- *Lower bound*: S^1 is connected, which means $\mathcal{U}(S^1) = \Delta_1$; for the space P_n, we get $\mathcal{U}(P_n) = (2\pi/n)\Delta_n$. According to the main theorem

$$d_{GH}(P_n, S^1) \geq d_{GH}\Big(\frac{2\pi}{n}\Delta_n, \Delta_1\Big) = \frac{1}{2} \cdot \frac{2\pi}{n} = \frac{\pi}{n}.$$

Combining the estimates, we obtain equality.

Regular polygons: lower bound

Theorem

Let P_m and P_n be the sets of vertices of regular m- and n-gons inscribed in the same circle, $m \le n$. Then

$$d_{GH}(P_m, P_n) \ge \frac{\pi}{m} - \frac{\pi}{n}.$$

If n is divisible by m, then the inequality becomes an equality.

Lower bound. Both ultrametrizations are simplices: $\mathcal{U}(P_m) = (2\pi/m)\Delta_m$ and $\mathcal{U}(P_n) = (2\pi/n)\Delta_n$, therefore, by the main theorem

$$d_{GH}(P_m, P_n) \ge d_{GH}\Big(\frac{2\pi}{m}\Delta_m, \frac{2\pi}{n}\Delta_n\Big).$$

For $\lambda = 2\pi/m$ and $\mu = 2\pi/n$ (so $\mu < \lambda$) the formula for the distance between simplexes gives $2d_{GH}(\lambda\Delta_m, \mu\Delta_n) = \max\{\mu, \lambda - \mu\} \ge \lambda - \mu$, that is $d_{GH}(P_m, P_n) \ge \pi/m - \pi/n$.

Regular polygons: upper bound

Upper estimate for $n = pm$. Let us construct the correspondence $R \in \mathcal{R}(P_m, P_n)$:

$$R = \bigcup_{i=0}^{m-1} \big\{(u_i, v_{pi+k}) : \ k = 0, \dots, p-1\big\},$$

where u_i are the vertices of the m-gon, v_j are the vertices of the n-gon. Direct check gives

$$\operatorname{dis} R = \frac{2\pi}{m} - \frac{2\pi}{n}, \qquad \text{whence} \qquad d_{GH}(P_m, P_n) \le \frac{\pi}{m} - \frac{\pi}{n}.$$

Together with the lower estimate, this gives the equality $d_{GH}(P_m, P_n) = \pi/m - \pi/n$ with $m \mid n$.

Metric trees

Definition

Metric tree is a connected graph without cycles, each edge of which is a segment of a given length, and the distance between points is equal to the length of the only path connecting them.

Proposition

If T is a metric tree, then $\mathcal{U}(T) = \Delta_1$ (one-point space).

Rationale: the tree is linearly connected, and the lengths of all paths are finite, so any two points are connected by a polyline of arbitrarily small ultralength.

Lower estimate of the GH distance from the tree

Corollary

For any metric tree T and any metric space X

$$d_{GH}(T, X) \geq \frac{1}{2} \operatorname{diam} \mathcal{U}(X).$$

This is a special case of Corollary 3: a metric tree is linearly connected, and all paths in it have finite length. The resulting lower bound for the distance from a tree to an arbitrary space is sharp; the following example shows this.

Example: tripod and its ends

Let T be the union of three unit segments $[o,a]$, $[o,b]$, $[o,c]$ emanating from one point o (tripod), with the intrinsic metric; $X=\{a,b,c\}$ the set of ends, with the metric induced from T. Then

$$d_X(a,b)=d_X(b,c)=d_X(c,a)=2,$$

since the path from a to b goes through o. Let us calculate $d_{GH}(T,X)$.

Lower bound. Any polyline in X connecting two distinct points consists of links of length 0 or 2, so its ultralength is 2; this means $d_u(x,y)=d_X(x,y)$ and $\mathcal{U}(X)=X$. In particular, $\operatorname{diam}\mathcal{U}(X)=2$, and the corollary gives

$$d_{GH}(T,X)\geq\frac{1}{2}\operatorname{diam}\mathcal{U}(X)=1.$$

Example: tripod (end)

Upper bound. Since $X \subset T$, let us estimate the Hausdorff distance, considering both sets to be subsets of T. Each point $t \in T$ lies on one of the segments $[o, x]$, so $d_T(t, x) \leq 1$; in this case $d_T(o, X) = 1$, which means $d_H(T, X) = 1$ and

$$d_{GH}(T, X) \leq d_H(T, X) = 1.$$

Conclusion. $d_{GH}(T, X) = 1$: the estimate of the corollary $d_{GH}(T, X) \geq \frac{1}{2} \operatorname{diam} \mathcal{U}(X)$ is achieved here.

Circumsphere radius and Jung's constant

Definition

For a non-empty bounded $A \subset Z$ *radius of a circumscribed ball* is

$$R_Z(A) := \inf_{z \in Z} \sup_{a \in A} |za|_Z.$$

Jung constant of the space Z is

$$J(Z) := \sup_{\substack{A \subseteq Z \\ \operatorname{diam} A > 0}} \frac{R_Z(A)}{\operatorname{diam} A}.$$

Jung's constant: basic properties

Note

If Z contains at least two points, then $\frac{1}{2} \leq J(Z) \leq 1$: the lower bound is the triangle inequality, the upper bound is the ball of radius $\operatorname{diam} A$ with center at any point $a \in A$ contains A. In particular, $J(Z) > 0$ always.

For $X \subset Z$ the value $d_H(X, Z) = \sup_{z \in Z} |zX|$ is the smallest radius at which $Z \subseteq U_r(X)$; the condition $d_H(X, Z) < \infty$ means that X is a net in Z. If $d_H(X, Z) = \infty$, the estimates from below are trivial, so the main interest is in the case $d_H(X, Z) < \infty$. Our task is to obtain a lower estimate for $d_H(X, Z)$: to this end we relate the Hausdorff distance to the ultrametrization diameter $\operatorname{diam} \mathcal{U}(X)$, which in concrete examples is computed directly.

Lemma: ultrametrization diameter in terms of d_H and J

Lemma

Let Z be a metric space, $X \subseteq Z$ and $d_H(X, Z) < \infty$. Then:

1. if $J(Z) < 1$, then
$$\operatorname{diam} \mathcal{U}(X) \leq \frac{d_H(X, Z)}{1 - J(Z)};$$
2. if any two points $a, b \in Z$ have a midpoint at Z (an $m \in Z$ such that $|am|_Z = |mb|_Z = \frac{1}{2}|ab|_Z$) — for example, it is true for a normed space, a metric tree or a sphere with an intrinsic metric, then
$$\operatorname{diam} \mathcal{U}(X) \leq 2\, d_H(X, Z).$$

Idea of the proof of the lemma

Set $r := d_H(X,Z)$; then for any $\delta > 0$ and any $z \in Z$ there is $x \in X$ with $|zx|_Z < r + \delta$.

Item 1. First we show that for any different $a, b \in X$ there is $x \in X$ with

$$\max\bigl\{|ax|_Z,\ |xb|_Z\bigr\} \le J(Z)|ab|_Z + r + \delta.$$

We take a point $z \in Z$ that almost realizes the circumscribed radius $R_Z(\{a,b\}) \le J(Z)|ab|_Z$, i.e. such that $\max\{|az|_Z, |zb|_Z\} < J(Z)|ab|_Z + \delta/2$, and then a point $x \in X$ with $|zx|_Z < r + \delta/2$; by the triangle inequality this gives the required estimate. Now let $a, b \in X$ be arbitrary; we construct by induction a sequence of polylines L_k connecting a and b with ultralength $\le D_k$, where

$$D_0 = |ab|_Z, \qquad D_{k+1} = JD_k + r + \delta :$$

each link L_k is replaced by a pair of links through "almost the middle" in X. Since $J < 1$, we have $D_k \to \frac{r+\delta}{1-J}$ and

$$d_u(x,y) \le \frac{r+\delta}{1-J}, \qquad \text{that is} \qquad \operatorname{diam}\mathcal{U}(X) \le \frac{d_H(X,Z)}{1-J(Z)}.$$

Item 2 is obtained by the same iteration, but with midpoints in Z (without the factor J).

Example: uniform net in a segment

Let $Z = [0,1]$ and $X = \left\{\frac{k}{n} : \ k = 0, \dots, n\right\} \subset Z$. For any $A \subset Z$ we have $R_Z(A) = \frac{1}{2}\operatorname{diam} A$, therefore $J(Z) = \frac{1}{2}$; in addition, $d_H(X, Z) = \frac{1}{2n}$. According to the first item of the lemma

$$\operatorname{diam} \mathcal{U}(X) \le \frac{d_H(X,Z)}{1 - J(Z)} = \frac{1}{n}.$$

The estimate is exact. Neighboring points of X are separated by $\frac{1}{n}$, and any two distinct points of it are separated by at least $\frac{1}{n}$. Therefore, in any polyline connecting different $x, y \in X$, there is a link of length $\ge \frac{1}{n}$, while the polyline through all intermediate nodes consists of links of length exactly $\frac{1}{n}$. This means $d_u(x, y) = \frac{1}{n}$ and

$$\operatorname{diam} \mathcal{U}(X) = \frac{1}{n} = 2\, d_H(X, Z).$$

Example: net in a segment (end)

The segment is connected, therefore $\mathcal{U}(Z) = \Delta_1$, and by the main theorem

$$d_{GH}(Z, X) \geq d_{GH}\big(\Delta_1, \mathcal{U}(X)\big) = \frac{1}{2} \operatorname{diam} \mathcal{U}(X) = \frac{1}{2n}.$$

Since, in addition, $d_{GH}(Z, X) \leq d_H(Z, X) = \frac{1}{2n}$, we obtain the equality $d_{GH}(Z, X) = \frac{1}{2n}$.

For $J(Z) > \frac{1}{2}$, the factor $\frac{1}{1-J(Z)}$ is greater than 2: for example, $J(\mathbb{R}^2) = \frac{1}{\sqrt{3}}$ (Jung's theorem), and the first estimate of the lemma gives $\operatorname{diam} \mathcal{U}(X) \leq \frac{3+\sqrt{3}}{2} d_H(X, \mathbb{R}^2) \approx 2.37\, d_H(X, \mathbb{R}^2)$.

Ultrametrization and MST-spectrum

Theorem

Let X be a finite metric space and $\sigma(X) = (\sigma_1, \ldots, \sigma_{n-1})$ be its MST-spectrum. Then $\mathcal{U}(X)$ is an ultrametric space in which all non-zero distances belong to the set $\{\sigma_1, \ldots, \sigma_{n-1}\}$.

More precisely, let T be the minimum spanning tree on X. Then for any σ_k from the MST-spectrum, the partition of X into classes with respect to the relation $d_u(x, y) < \sigma_k$ coincides with the partition into sets of vertices of the components obtained from T by removing all edges of length $\geq \sigma_k$; in this case, the smallest distance in $\mathcal{U}(X)$ between points from different components is equal to σ_k.

The theorem is based on a classical fact of cluster analysis: the ultrametric of a single linkage, coinciding with d_u, for a finite metric space is calculated from MST of the complete graph as the maximum length of edges on the path between points.

Ultrametrization diameter and σ_1

Corollary

For a finite metric space X

$$\operatorname{diam} \mathcal{U}(X) = \sigma_1 \leq \operatorname{diam} X,$$

where σ_1 is the largest number of the MST-spectrum. Moreover, $\sigma_1 = \operatorname{diam} X$ if and only if the diameter X is reached on the edge of some minimum spanning tree.

An example when the inequality is strict. Let $X = \{0, 1, 2\}$ be the vertices of the path 0—1—2 with the usual distance on the line. Then $\operatorname{diam} X = 2$, and the minimum spanning tree consists of edges $\{0, 1\}$ and $\{1, 2\}$ of length 1, so $\sigma_1 = 1 < 2 = \operatorname{diam} X$.

Lecture summary

1. Definition of ultrametric space and its basic properties (polygon inequality, isosceles, properties of spheres).
2. Ultrametrization $\mathcal{U}(X) = X/\sim$, where $x \sim y \iff d_u(x,y) = 0$, and its connection with the usual metric.
3. Main theorem: $d_{GH}(X,Y) \geq d_{GH}\big(\mathcal{U}(X),\mathcal{U}(Y)\big)$.
4. Applications: $d_{GH}(P_n, S^1) = \pi/n$ and $d_{GH}(P_m, P_n) \geq \pi/m - \pi/n$ (equality for $m \mid n$).
5. Metric trees: $\mathcal{U}(T) = \Delta_1$, whence $d_{GH}(T,X) \geq \frac{1}{2}\operatorname{diam}\mathcal{U}(X)$; The tripod example shows the sharpness.
6. Radius of the circumscribed ball, Jung's constant and estimates $\operatorname{diam}\mathcal{U}(X) \leq \frac{d_H(X,Z)}{1-J(Z)}$, $\operatorname{diam}\mathcal{U}(X) \leq 2d_H(X,Z)$.
7. Corollary for a normed V: $d_{GH}(V,X) \geq \frac{1}{2}\operatorname{diam}\mathcal{U}(X)$.
8. The ultrametrization of a finite X is described by its MST-spectrum: $\operatorname{diam}\mathcal{U}(X) = \sigma_1$.

Open questions

1. *Sharpness of the estimate* $d_{GH}(X,Y) \geq d_{GH}\big(\mathcal{U}(X),\mathcal{U}(Y)\big)$. In what cases is it sharp? It is known that for $X = P_n$, $Y = S^1$ the estimate is exact; are there other such classes of spaces?
2. *Ultrametrization and the Gromov–Wasserstein distance.* How is ultrametrization related to the Gromov–Wasserstein distance?
3. *Continuity of ultrametrization.* Is the mapping $\mathcal{U}\colon \mathcal{GH} \to \mathcal{GH}$ continuous? The main theorem only implies 1-Lipschitz property.
4. *Infinite spaces.* Is it possible to extend the theory to non-compact spaces?
5. *Characterization of images.* Which ultrametric spaces are ultrametrizations of some metric spaces?