A $(1+\epsilon)$ -Approximation for Ultrametric Embedding in Subquadratic Time

Gabriel Bathie, Guillaume Lagarde Univ. Bordeaux, LaBRI & DI ENS PSL, France

Ultrametrics

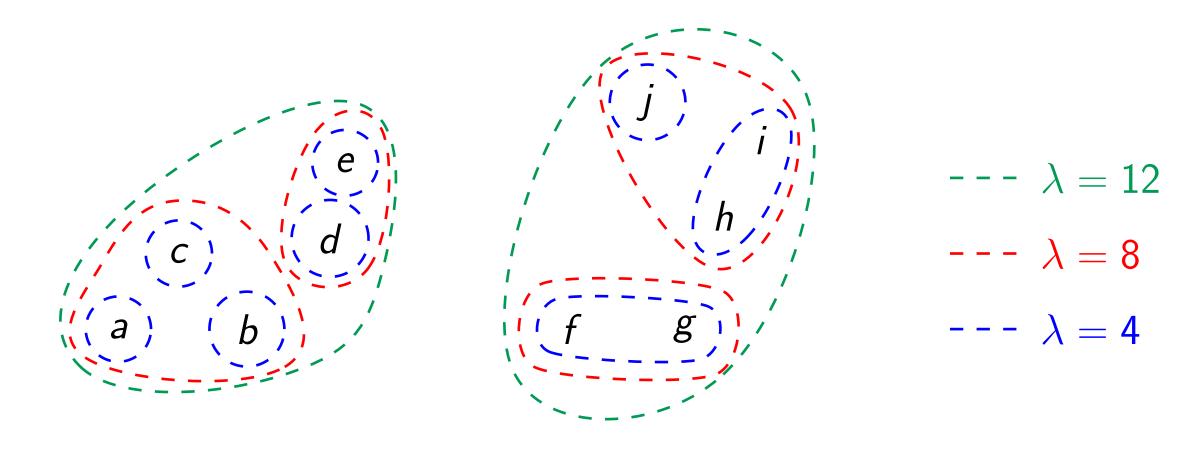
Ultrametric: *metric* + *ultrametric inequality*.

$$orall x,y,z,\Delta(x,y)\geq 0 \qquad \qquad \Delta(x,y)=0 \Longleftrightarrow x=y \ \Delta(x,y)=\Delta(y,x) \qquad \Delta(x,y)\leq \Delta(x,z)+\Delta(z,y)$$

Ultrametric: $\Delta(x, y) \leq \max(\Delta(x, z), \Delta(z, y))$

Ultrametrics and Hierarchical Clustering

Ultrametrics: Mathematical formalization of Hierarchical Clustering



Ultrametric Embedding

Goal: Given a metric space (X, d), find the ultrametric Δ that agrees the most with d.

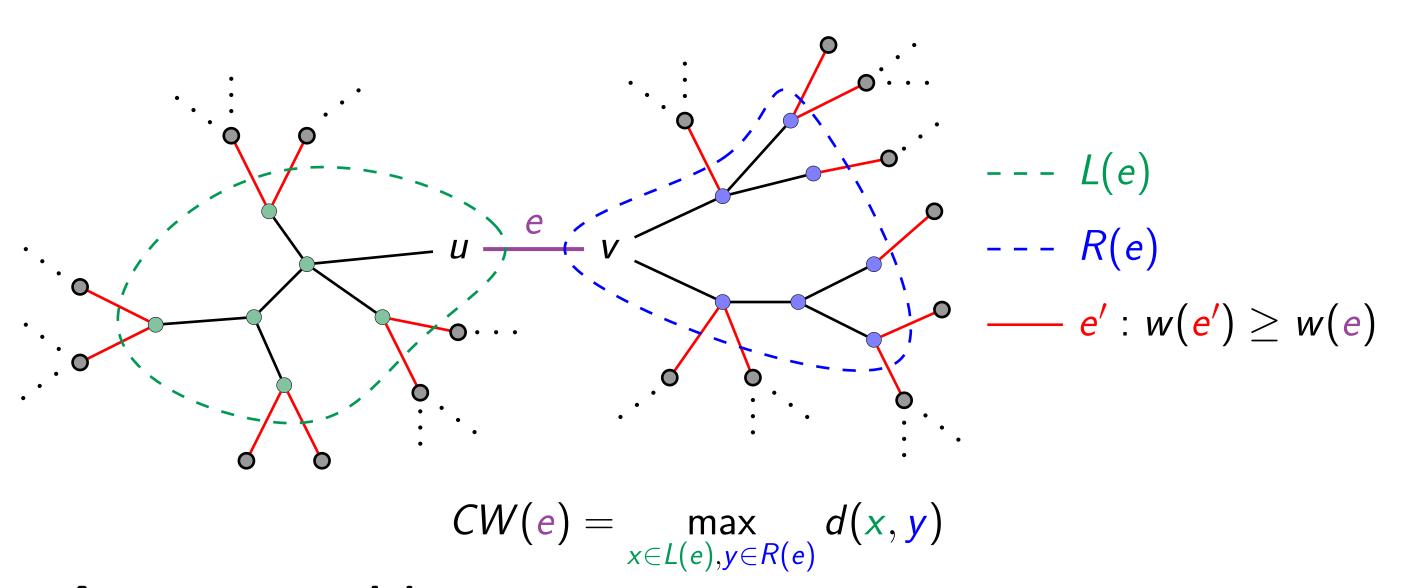
Minimize the **distortion** α :

$$\forall x, y, \Delta(x, y) \leq d(x, y) \leq \alpha \cdot \Delta(x, y).$$

Theorem: In the **Euclidean case**, for any c > 1, we can compute a c-approximation of the best ultrametric embedding in time $\mathcal{O}\left(n^{1+1/c}\right)$.

$$\forall x, y, \Delta(x, y) \leq \ell_2(x, y) \leq c \cdot \alpha \cdot \Delta(x, y).$$

Cut weights



 α -Approx. cut weights:

$$\forall e, ACW(e) \leq CW(e) \leq \alpha \cdot ACW(e)$$

Approximate Cut Weights via Approximate Farthest Neighbor

$$CW(e) = \max_{x \in L(e), y \in R(e)} d(x, y) = \max_{x \in L(e)} d(x, Farthest_{y \in R(e)}(x))$$

 $ACW(e) = \max_{x \in L(e)} d(x, ApproxFarthest_{y \in R(e)}(x))$

 \rightarrow take smallest of L(e), R(e): $\mathcal{O}(n \log n)$ queries in total.

Theorem: Dynamic data structure for α -AFN queries in time $\mathcal{O}(n^{1/\alpha^2})$. $\rightarrow \alpha$ -AFN: point $p \in S$ s.t. $d(x, p) \geq d(x, y)/\alpha$, $\forall y \in S$.

Technique:

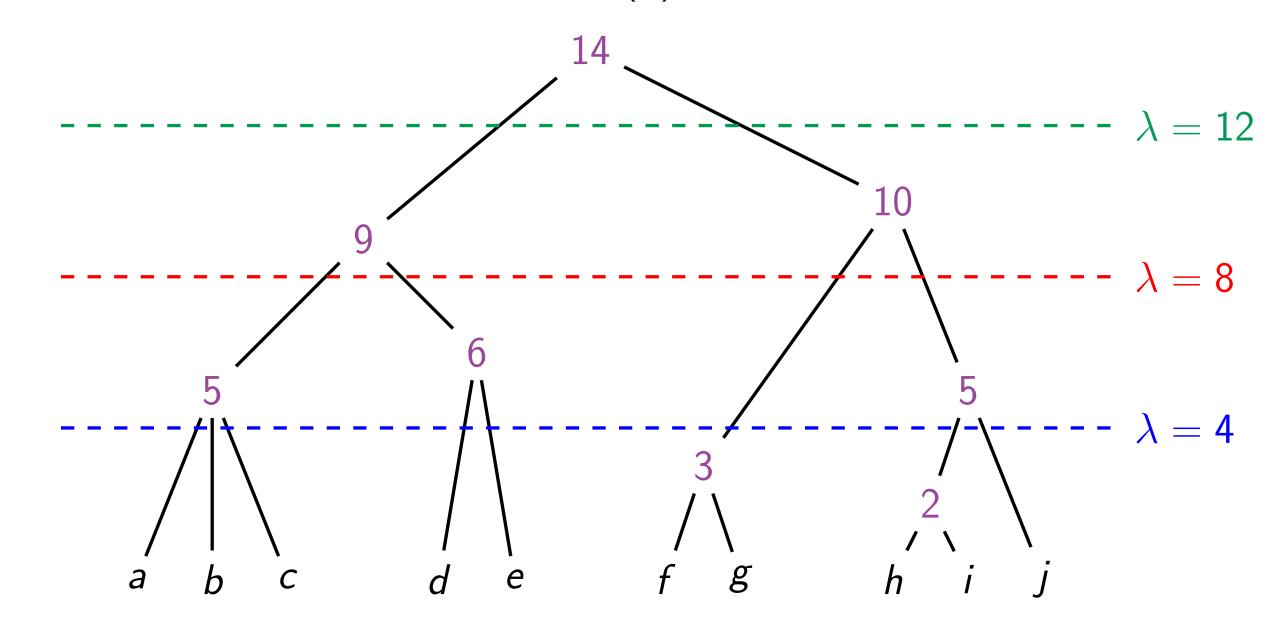
- ▶ Project all points on $\mathcal{O}(n^{1/\alpha^2})$ random lines,
- ► Keep $\mathcal{O}(n^{1/\alpha^2})$ farthest points on each line,
- ► Return farthest point among those.

Ultrametrics as Trees

 (X, Δ) is an ultrametric space $\iff \exists$ tree $T = \underbrace{N}_{\text{nodes}} \cup \underbrace{X}_{\text{leaves}}$ with weights w

s.t.
$$\forall u \in T, w(u) \leq w(parent(u))$$

 $\forall x \in X, w(x) = 0$



Mapping: $\Delta(x, y) = w(LCA(x, y))$

Algorithm for Ultrametric Embedding

 $\mathcal{O}(n^2)$ -time algorithm of Farach, Kannan and Warnow [?]:

- 1. Compute minimum spanning tree T of (X, d)
- 2. Compute the **cut weights** *CW* of *T*
- 3. Compute a cartesian tree CT of $(T, CW) \rightarrow \Delta$

Approximation algorithm:

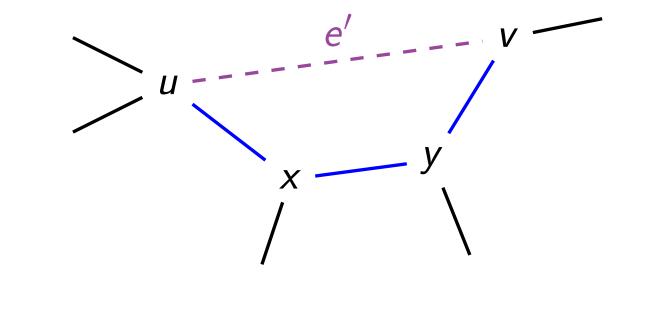
- 1. Compute a γ -Kruskal Tree T of (X, d) in $\mathcal{O}(n^{1+1/\gamma^2})$
- 2. Compute the α -approximate cut weights ACW of T in $\mathcal{O}(n^{1+1/\alpha^2})$
- 3. Compute a cartesian tree CT of $(T, ACW) \rightarrow \Delta$, $\alpha \cdot \gamma$ approx \rightarrow for $\alpha = \gamma = \sqrt{c}$, c-approx. in $\mathcal{O}(n^{1+1/c})$

γ -Kruskal Trees: Locally Approximate Minimum Spanning Trees

 $\forall e \text{ on } u\text{-}v \text{ path,}$ $MST: w(e') \geq w(e)$

 γ -KT: $w(e') \geq \frac{1}{\gamma}w(e)$

 \rightarrow Cannot take MST + long edge.



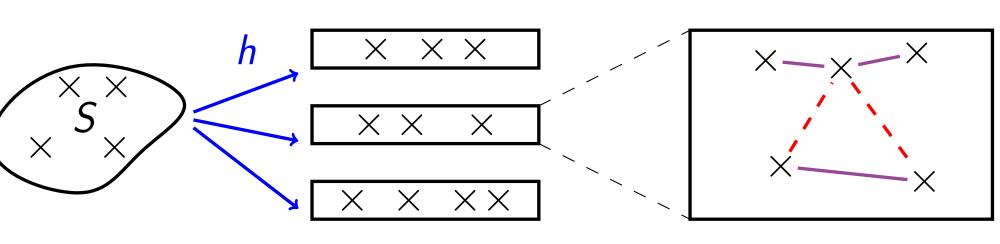
BFS over edges

 $w(e') \leq \gamma R$

γ -Kruskal Trees via Locality Sensitive Hashing

Locality Sensitive Hashing: hash function *h*

- 1. if $d(u, v) \leq R$, then h(u) = h(v) w.h.p.,
- 2. if $d(u, v) \ge \gamma R$, then $h(u) \ne h(v)$ w.h.p.,



Prop: Takes $\mathcal{O}(n^{1+1/\gamma^2})$ time.

Prop: if $w(uv) \le R$, then path with edges $w(e') \le \gamma R$ between u and v in E.

Algorithm for γ -KT:

- ightharpoonup Repeat for $R = d_{\min}, 2d_{\min}, 4d_{\min}, \dots, d_{\max}$
- \triangleright take MST of union of all E's.

References