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THE COMPLEXITY OF ULTRAMETRIC PARTITIONS ON GRAPHS

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Partitioning of graphs has many practical applications namely in cluster analysis and in automated design of VLSI circuits. Using 1–1 correspondence between ultrametric partitions of a weighted complete graph $K(w)$ on a finite set X and ultrametrics on X, the computational complexity of the approximation of w by means of an ultrametric u is investigated and systematized. As a main result, a polynomial algorithm that solves the problem under some 'min–max' criterion is developed.

Keywords: Ultrametric partition, polynomial algorithm, NP-completeness

1. Introduction

Throughout this paper let $K(w)=(X, \binom{X}{2}, w)$ be a complete graph on the n-vertex set X which is edge-weighted by $w: X\times X \to R_0^+$ (positive rationals) such that $\forall x, y\in X$, $w(x, y)=w(y, x)$ and $w(x, y)=0 \Leftrightarrow x=y$. By an *ultrametric partition* π of $K(w)$ we shall understand a sequence $((P_0, l_0),\dots,(P_q, l_q))$, where

(i) $P_0,\dots, P_q$ are partitions of X, P_0 is a partition of X into singletons and $P_q=\{X\}$;
(ii) P_i is a proper refinement of P_{i+1} $(0\leqslant i\leqslant q-1)$, i.e., the partition P_{i+1} arises from P_i by joining some classes of P_i;
(iii) $0=l_0<l_1<\cdots<l_q$ are rational numbers.

Note that $q\leqslant n-1$ and $q=n-1$ exactly in the case when in (ii) the word 'some' is formally replaced by 'exactly two'.

Let π be an ultrametric partition of $K(w)$. We define the function $u_\pi: X\times X\to R_0^+$ as follows:

$$u_\pi(x, y)=\min\{l_i;\ \{x, y\} \text{ is a subset of some class in } P_i\}.$$

It is known that u_π is an ultrametric on X, i.e., u_π is a metric on X such that $\forall x, y, z\in X$, $u_\pi(x, y)\leqslant \max\{u_\pi(x, z), u_\pi(y, z)\}$ (cf. [1]). On the other hand, having an ultrametric u on X, where $R(u)=\{l_0,\dots,l_q\}$ is the range of u and $l_0<\cdots<l_q$, there is a unique ultrametric partition $\pi_u= ((P_0, l_0),\dots,(P_q, l_q))$ where each P_i is a factor set corresponding to an equivalence relation e_i on X defined as follows:

$$(x, y)\in e_i \;\Leftrightarrow\; u(x, y)\leqslant l_i, \quad i=0, 1,\dots, q.$$

Hence, there is a one-to-one correspondence between ultrametric partitions of $K(w)$ and ultrametrics on X. Therefore, the quality of an ultrametric partition π of $K(w)$ can be expressed as the approximation of a given weight function w by means of an ultrametric u on X. Since both w and u are determined by their n^2 values, they can be considered as two points in some linear space of dimension n^2. Thus, it is natural to use two objective functions σ, μ (cf. [4]):

$$\sigma(u, w)=\sum_{x<y\in X} |u(x, y)=w(x, y)|, \qquad \mu(u, w)=\max_{x, y\in X} |u(x, y)-w(x, y)|,$$

mapping the Cartesian prodı of the set of all ι ametrics $\mathscr{U}$ on X and the set of all weight functions on X into R_0^+. Note that σ, μ a in fact two extrε l cases of an 'l_p metric' ($p = 1, \infty$).

This approach will be in\ stigated in subse\ :nt sections from the point of view of computational complexity.

2. Problem formulation

In what follows we shall be interested in the ıputational complexity of six decision problems (P1), (P2), (P3), (P4), (P5), and (P6) defined as follov

INSTANCE: A graph $K(w)$, positive integer k;
QUESTION: Is there an ultrametric u on X suc ..ιι:

(P1) $u \leqslant w$ and $\mu(u, w) \leqslant k$?

(P2) $u \leqslant w$ and $\sigma(u, w) \leqslant k$?

(P3) $u \geqslant w$ and $\mu(u, w) \leqslant k$?

(P4) $u \geqslant w$ and $\sigma(u, w) \leqslant k$?

(P5) $\mu(u, w) \leqslant k$?

(P6) $\sigma(u, w) \leqslant k$ respectively, where $u \leqslant w \Leftrightarrow \forall x, y \in X, u(x, y) \leqslant w(x, y)$?

3. Solutions

Given $K(w)$, an ultrametric u on X is said to be *subdominant* (respectively *dominant*) to w if for each ultrametric u' on X the following condition is satisfied: $u \leqslant u' \leqslant w \Rightarrow u = u'$ (respectively $u \geqslant u' \geqslant w \Rightarrow u = u'$). This definition implies a straightforward lemma.

3.1. Lemma. *Let u_1, u_2, u_3, u_4 be four ultrametrics on X such that $u_1 \leqslant u_2 \leqslant w \leqslant u_3 \leqslant u_4$. Then,*

(i) $\mu(u_1, w) \geqslant \mu(u_2, w)$ *and* $\mu(u_4, w) \geqslant \mu(u_3, w)$,

(ii) $\sigma(u_1, w) \geqslant \sigma(u_2, w)$ *and* $\sigma(u_4, w) \geqslant \sigma(u_3, w)$.

By means of Lemma 3.1 we can restrict (without loss of generality) the set of all solutions of problems (P1) and (P2) (respectively (P3) and (P4)) to the set of all subdominant (respectively dominant) ultrametrics to a given weight w.

3.2. Lemma. *There exists exactly one subdominant ultrametric u_s to a given weight w while there are at most $(n-1)!$ different dominant ultrametrics to w.*

Proof. Let u_1 and u_2 be two distinct ultrametrics on X subdominant to w. Let us put

$$u_s(x, y) = \max\{u_1(x, y), u_2(x, y)\} \quad \text{for } x, y \in X.$$

Since

$$\forall x, y, z, \; u_i(x, y) \leqslant \max\{u_i(x, z), u_i(y, z)\}, \quad i = 1, 2,$$

we get

$$\begin{aligned} u_s(x, y) &\leqslant \max\{u_1(x, z), u_2(x, z), u_1(y, z), u_2(y, z)\} \\ &= \max\{\max\{u_1(x, z), u_2(x, z)\}, \max\{u_1(y, z), u_2(y, z)\}\} \\ &= \max\{u_s(x, z), u_s(y, z)\}. \end{aligned}$$

Since further $u_1 \leqslant u_s \leqslant w$ and $u_2 \leqslant u_s \leqslant w$ and moreover u_1, u_2 are subdominant ultrametrics to w, it follows that $u_1 = u_s = u_2$, a contradiction. Therefore, there is exactly one subdominant ultrametric u_s to w and

$$u_s(x, y) = \max\{u(x, y); u \in \mathscr{U} \text{ and } u \leqslant w\}, \quad x, y \in X.$$

On the other hand, let us suppose that w is an injection on $X \times X$ such that

$$w(x_i, x_j) > w(x_k, x_l) \quad \text{if } \max\{i, j\} < \max\{k, l\}.$$

Taking into account the triple x_1, x_2, x_3 there are exactly two possibilities how to construct a dominant ultrametric on this triple. Indeed, the triangle $\{x_1, x_2, x_3\}$ induced by a dominant ultrametric should have two sides equal to $w(x_1, x_2)$. This idea can easily be extended to the whole set X successively as follows: for x_j there are $j-1$ possibilities how to assign values of dominant ultrametric to edges $\{x_j, x_i\}$, $i = 1, 2, \ldots, j-1$. More precisely, let u be a dominant ultrametric to w on $\{x_1, \ldots, x_{j-1}\}$. The dominant ultrametrics u_i $(1 \leqslant i < j)$ to w on $\{x_1, \ldots, x_j\}$ are obtained by putting

$$u_i(x_j, x_i) = w(x_j, x_i) \quad \text{and} \quad u_i(x_j, x_k) = u(x_i, x_k), \qquad 1 \leqslant k \neq i < j.$$

As all these steps are mutually independent we can actually enumerate $2 \times 3 \times \cdots \times (n-1) = (n-1)!$ different ultrametrics to w on X.

This completes the proof of the lemma. □

Now, let us turn our attention to problems (P1), (P3), and (P5). First, we have the following theorem.

3.3. Theorem. *Let T be a minimum spanning tree on $K(w)$. Then it holds that*

$$\begin{aligned} \min_{u \geqslant w} \max_{x, y \in X} \{u(x, y) - w(x, y)\} &= \min_{w \geqslant u} \max_{x, y \in X} \{w(x, y) - u(x, y)\} \\ &= 2 \min_{u \in \mathscr{U}} \max_{x, y \in X} |w(x, y) - u(x, y)| = \max_{x, y \in X} \Big\{w(x, y) - \max_{e \in T(x, y)} w(e)\Big\}, \end{aligned} \tag{1}$$

where $T(x, y)$ denotes the path from x to y in T and $\mathscr{U}$ is the set of all ultrametrics on X.

Proof. Let T be a minimum spanning tree of $K(w)$. In the sequel we shall use the well-known 'bottleneck' equality [2]

$$\min_{P \in P(x, y)} \max_{e \in P} w(e) = \max_{C \in C(x, y)} \min_{e \in C} w(e) = \max_{e \in T(x, y)} w(e), \tag{2}$$

where $P(x, y)$ is the set of all paths from x to y in $K(w)$, and $C(x, y)$ is the set of all cutsets separating x and y in $K(w)$.

Note that the value $\max\{w(e); e \in T(x, y)\}$ in (2) is independent of the choice of the minimum spanning tree T of $K(w)$.

Now, let $e_1 = \{a, b\}$, $e_2 \in T(a, b)$ be two edges of $K(w)$ such that

$$w(e_1) - w(e_2) = \max_{x, y \in X} \Big\{w(x, y) - \max_{e \in T(x, y)} w(e)\Big\}. \tag{3}$$

Further, let u be an ultrame[illegible] on [illegible] vith the ordered range $l_0 < l_1 < \cdots < l_q$. We shall prove that

$$2 \max_{x,\, y \in X} | w(x,\, y \ [illegible] \ ) | \geqslant w(e_1) - w(e_2).$$

Suppose that $u(e_1) = l_i$ f[illegible]om [illegible] $= 1, 2, \ldots, q$. Let e_3 be an edge of $K(w)$ such that $w(e_3) = \min\{w(x, y);\, u(x, y) \geqslant l$ [illegible] is e[illegible] to see that there exists a cutset C_0 in $K(w)$ such that it separates a and b and $w(e_3) = \min\{$[illegible] $e \in$ [illegible]$\}$. Since

$$u(e_1) \leqslant u(e_3) \ [illegible] \ e_1) \quad w(e_3), \quad \text{and} \quad w(e_3) \leqslant \max_{C \in C(a,\, b)} \min_{e \in C} w(e) = w(e_2),$$

we have

$$\begin{aligned} \max_{x,\, y \in X} | u(x,\, y) - w(x,\, y) | &\geqslant \max\{ | u(e_1) - w(e_1) |,\, | u(e_3) - w(e_3) | \} \\ &\geqslant \tfrac{1}{2}(w(e_1) - w(e_3)) \geqslant \tfrac{1}{2}(w(e_1) - w(e_2)). \end{aligned} \tag{4}$$

In the case when we are dealing with $u \geqslant w$, this part of the proof can be done in an entirely analogous way and, moreover, the constant $\frac{1}{2}$ in (4) can be omitted. In the case when $u \leqslant w$, the situation is also simple:

$$\max_{x,\, y \in X} w(x,\, y) - u(x,\, y) \geqslant w(e_1) - u(e_1) \geqslant w(e_1) - w(e_3) \geqslant w(e_1) - w(e_2).$$

On the other hand, using equality (2) we are able to construct an ultrametric u^* on X such that

$$2 \max_{x,\, y \in X} | u^*(x,\, y) - w(x,\, y) | \leqslant w(e_1) - w(e_2). \tag{5}$$

This can be carried out by the following procedure:

***Step* 1.** Compute the minimum spanning tree T of $K(w)$.

***Step* 2.** Compute the valuation $w' : E(T) \to R_0^+$ such that

$$w'(e) = \max\{ w(x,\, y);\, w(e) = \max\{ w(f);\, f \in T(x,\, y) \} \}.$$

***Step* 3.** Compute $u^*(x,\, y) = \frac{1}{2}\max\{w(e) + w'(e);\, e \in T(x,\, y)\}$. Clearly, this procedure produces an ultrametric u^* on X. Since $w(e_2)$ is the edge value of some edge in any minimum spanning tree of $K(w)$, by virtue of (3) we get $w'(e_2) = w(e_1)$ and inequality (5) is established.

To prove the theorem it remains to examine the cases where $u^* \leqslant w$, respectively $u^* \geqslant w$. For this sake, Step 3 in the procedure outlined above is replaced by:

***Step* 3.** Compute

$$u^*(x,\, y) = \begin{cases} \max\{ w(e);\, e \in T(x,\, y) \} & \text{if } u^* \leqslant w, \\ \max\{ w'(e);\, e \in T(x,\, y) \} & \text{if } u^* \geqslant w. \end{cases}$$

Now, equality (1) is easily verified and the proof is completed. □

3.4. Corollary. *Problems* (P1), (P3), *and* (P5) *are polynomially solvable.*

Proof. Let us perform a time analysis of the procedure computing u^* as described in the proof of Theorem 3.3. Step 1 takes $O(n^2)$ time [6] and Step 3 requires $O(n^2)$ time, too. To analyze Step 2 we need the following refinement (cf. (2)):

***Step* 2.** **for each** $\{x,\, y\} \notin E(T)$ **do** $w'(x,\, y) \leftarrow \max_{e \in T(x,y)} w(e)$;
for each $e \in E(T)$ **do** $w'(e) \leftarrow \max\{ w'(f);\, f \notin E(T) \,\&\, w'(f) = w(e) \}$;

Therefore, the extension of w' on the set of edges of $K(w)$ is computable in $O(n^3)$ time. This concludes the proof. □

By virtue of Lemma 3.2 we have another corollary.

3.5. Corollary. *Problem* (P2) *is polynomially solvable.*

Proof. As in the proof of Theorem 3.3 we construct in polynomial time an ultrametric u on X such that $\forall x, y \in X$, $u^*(x, y) = \max\{w(e); e \in T(x, y)\}$. From (1) we know that $u^*(x, y)$ is determined by the minimum edge-weight in all cutsets separating x and y in $K(w)$. Hence, u^* is subdominant to w. The corollary follows via Lemmas 3.1 and 3.2. □

Finally, we shall deal with the computational complexity of problems (P4) and (P6). Recently, the NP-completeness proof for (P6) has appeared in [5]. We shall show that the same result is valid for problem (P4).

3.6. Theorem. *Problem* (P4) *is NP-complete.*

Proof. Clearly, problem (P4) is in the class NP. Now we shall exhibit a polynomial transformation from the known NP-complete problem (Δ) [3]:

(Δ) INSTANCE: A graph G, $|V(G)| = 3m$ (m is a positive integer), without subgraphs isomorphic to K_4;
QUESTION: Is there a partition $V_1, \ldots, V_m$ of $V(G)$ such that each class V_i induces a triangle in G?

Let G be an instance of (Δ). We put $X = V(G)$, $w(x, y) = 1 \Leftrightarrow \{x, y\} \in E(G)$, $w(x, y) = 0$ if $x = y$, and $w(x, y) = 2$ otherwise. Let $k = |E(G)| - |V(G)|$. Obviously, the instance of (P4) was constructed in polynomial time. Now the following equivalence is easily verified:

(P4) has "yes"-solution, i.e., $\sigma(u, w) \leqslant k$ for some u on $X \Leftrightarrow (\Delta)$ has "yes"-solution, i.e., $V(G) = V_1 \cup \cdots \cup V_m$, $V_i \cap V_j = \emptyset$ $(i \neq j)$ and each V_i induces a triangle in G.

Let (Δ) have "yes"-solution. The ultrametric u on X defined as follows:

$$u(x, x) = 0, \quad u(x, y) = 1 \quad \Leftrightarrow \quad \{x, y\} \subset V_i \text{ for some } i \quad \text{and} \quad u(x, y) = 2 \text{ otherwise},$$

yields the solution of (P4), since $\sigma(u, w) = |E(G)| - |V(G)| = k$.

Conversely, if (P4) has "yes"-solution, there are at least $|V(G)|$ pairs of $(x, y) \in X \times X$ $(x < y)$ such that $u(x, y) = 1$. Since G contains no induced subgraphs isomorphic to K_4, the classes of an equivalence relation e, $(x, y) \in e \Leftrightarrow u(x, y) = 1$, induce triangles in G. This completes the proof of the theorem. □

4. Concluding remark

In this article we have developed a new polynomial procedure of hierarchical clustering (see Theorem 3.3) which, to our knowledge, has not yet been reported in available literature. This method was successfully used in the design of multichip layouts in the Research Institute of Mathematical Machines, Prague, by the present author.

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References

[1] E. Diday, J. Lemaire, J. Pouget and F. Testu, *Elements d'Analyse des Donneés* (Dunod, Paris, 1982).

[2] J. Edmonds and D.R. Fulkerson, Bottleneck extrema, *J. Combin. Theory* **8** (1970) 299–306.

[3] M.R. Garey and D.S. Johnson, *Computers and Intractability: A Guide to the Theory of NP-Completeness* (Freeman, San Francisco, CA, 1979).

[4] N. Jardine and R. Sibson, *Mathematical Taxonomy* (Wiley, London, 1971).

[5] M. Křivánek and J. Morávek, NP-hard problems in hierarchical-tree clustering, *Acta Informatica* **23** (1986) 311–323.

[6] K. Mehlhorn, *Data Structures and Algorithms, Vol. 2* (Springer, Berlin, 1984).