

Characterization of the Distance between Subtrees of a Tree by the Associated Tight Span

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Abstract

A characterization is given to the distance between subtrees of a tree defined as the shortest path length between subtrees. This is a generalization of the four-point condition for tree metrics. For this, we use the theory of the tight span and obtain an extension of the famous result by A. Dress that a metric is a tree metric if and only if its tight span is a tree.

1 Introduction

Recently, mathematical treatments of phylogenetics have come to be increasingly important; see [2],[17]. The central problem in phylogenetics is reconstructing phylogenetic trees from given experimental data, e.g., DNA sequences. If the data is given as a distance matrix expressing dissimilarity between species, the problem is to search for a *tree metric* that “fits” the given distance matrix.

For a finite set X and a distance $d : X \times X \rightarrow \mathbf{R}$ with $d(x, x) = 0$ and $d(x, y) = d(y, x) \geq 0$ for $x, y \in X$, d is said to be a metric if it satisfies the triangle inequality, and a tree metric if there exists some weighted tree such that d can be expressed by the path metric between vertices of the tree. One of the most fundamental theorems in phylogenetics is the characterization of tree metrics.

Theorem 1.1 ([23], [18], [3], [4]). *A metric d is a tree metric if and only if it satisfies the four-point condition*

$$\forall x, y, z, w \in X, |\{x, y, z, w\}| = 4, \\ d(x, y) + d(z, w) \leq \max\{d(x, z) + d(y, w), d(x, w) + d(y, z)\}. \quad (1.1)$$

In this paper, we generalize this characterization for the distance between subtrees of a tree. We define the distance on subtrees of a tree by the shortest path length between subtrees (see Figure 1).

Our main result is as follows:

Theorem 1.2. *A distance d can be expressed as the distance between subtrees of some tree if and only if it satisfies*

$$\begin{aligned} & \forall x, y, z, w \in X, |\{x, y, z, w\}| = 4, \\ & d(x, y) + d(z, w) \leq \\ & \max \left\{ \begin{array}{l} \frac{d(x, z) + d(y, w), d(x, w) + d(y, z), d(x, y), d(z, w),}{d(x, y) + d(y, z) + d(z, x)}, \frac{d(x, y) + d(y, w) + d(w, x)}{2}, \\ \frac{d(x, z) + d(z, w) + d(w, x)}{2}, \frac{d(y, z) + d(z, w) + d(w, y)}{2} \end{array} \right\} \end{aligned} \quad (1.2)$$

If d satisfies the triangle inequality, then it can be verified that (1.2) coincides with the four-point condition (1.1) (see Remark 2.5). Hence (1.2) is a generalization of the four-point condition.

For the proof of Theorem 1.2, we use the theory of the *tight span*, which was discovered independently by J. R. Isbell [14], A. Dress [6] and M. Chrobak and L.L. Larmore [5] and developed by A. Dress and coworkers [8]. Whereas the tight span has so far been considered essentially for a metric, in this paper, we consider the tight span for a distance that may violate the triangle inequality.

This paper is organized as follows. In Section 2, we prepare definitions and notation, and present a more general version of Theorem 1.2. In Section 3, we give the proof of the theorems.

2 Definitions, Notation and Results

2.1 Distances and partial splits

Let X be a finite set. A function $d : X \times X \rightarrow \mathbf{R}$ is said to be a *distance* on X if d satisfies $d(x, x) = 0$ and $d(x, y) = d(y, x) \geq 0$ for $x, y \in X$. A distance d is said to be a *metric* if, in addition, d satisfies $d(x, y) \leq d(x, z) + d(y, z)$ for $x, y, z \in X$. For $A, B \subseteq X$ with $A \cap B = \emptyset$ and $A, B \neq \emptyset$, the unordered pair $\{A, B\}$ is called a *partial split* on X . If a partial split $\{A, B\}$ satisfies $A \cup B = X$, then $\{A, B\}$ is called a *split* on X . For a partial split $\{A, B\}$ on X , we define a *partial split distance* $\zeta_{\{A, B\}} : X \times X \rightarrow \mathbf{R}$ by

$$\zeta_{\{A, B\}}(x, y) = \begin{cases} 1 & \text{if } x \in A, y \in B \text{ or } y \in A, x \in B \\ 0 & \text{otherwise.} \end{cases} \quad (2.1)$$

Note that $\zeta_{\{A, B\}}$ is not a metric if $A \cup B \neq X$ and is a metric, called a *split metric*, if $A \cup B = X$. A pair of partial splits $\{A, B\}$ and $\{C, D\}$ on X is said to be *compatible* if it satisfies one of the following four conditions:

$$A \subseteq C \text{ and } B \supseteq D, \quad (2.2)$$

$$A \subseteq D \text{ and } B \supseteq C, \quad (2.3)$$

$$A \supseteq C \text{ and } B \subseteq D, \quad (2.4)$$

$$A \supseteq D \text{ and } B \subseteq C. \quad (2.5)$$

A collection of partial splits \mathcal{S} is said to be *compatible* if any pair of partial splits in \mathcal{S} is compatible. Note that if \mathcal{S} consists of splits, then compatibility in our sense coincides with compatibility of splits in the standard definition; see [3], [2], [17].

2.2 Graphs

For a weighted graph $G = (V, E, w)$ with a vertex set V , an edge set E , and a positive weight $w : E \rightarrow \mathbf{R}$ representing edge lengths, $D_G : V \times V \rightarrow \mathbf{R}$ denotes the path metric on G defined by the shortest length of a path. We also denote vertices of G by $V(G)$ and edges of G by $E(G)$.

2.3 Tight span of distances

Next we introduce the tight span and related concepts. For a distance $d : X \times X \rightarrow \mathbf{R}$, a polyhedron $P(X, d) \subseteq \mathbf{R}^X$ associated with d is defined as

$$P(X, d) = \{f \in \mathbf{R}^X \mid f(x) + f(y) \geq d(x, y) \ (x, y \in X)\}. \quad (2.6)$$

The tight span $T(X, d)$ is defined to be the union of bounded faces of $P(X, d)$, or equivalently,

$$T(X, d) = \{f \in \mathbf{R}^X \mid \forall x \in X, f(x) = \max_{y \in X} \{d(x, y) - f(y)\}\}. \quad (2.7)$$

The dimension of $T(X, d)$ is defined to be the maximum dimension of bounded faces of $P(X, d)$. As indicated by [6, Remark 5.4, p.370], $\dim T(X, d)$ can be characterized as follows, whether d is a metric or not.

Theorem 2.1 ([6]). *For a distance $d : X \times X \rightarrow \mathbf{R}$ and a positive integer n , the following two conditions are equivalent.*

- (a) $\dim T(X, d) \geq n$.
- (b) *There exists a $2n$ -element subset $\{x_1, x_{-1}, x_2, x_{-2}, \dots, x_n, x_{-n}\} \subseteq X$ such that*

$$\sum_{i \in I} d(x_i, x_{-i}) > \sum_{i \in I} d(x_i, x_{\sigma(i)}) \quad (2.8)$$

holds for any permutation σ of $I = \{\pm 1, \pm 2, \dots, \pm n\}$ not satisfying $\sigma(i) = -i$ for all $i \in I$.

In the appendix, we give a simple proof of Theorem 2.1 based on standard arguments in linear programming.

Let $t^d : X \rightarrow 2^{T(X, d)}$ be defined as

$$t^d(x) = T(X, d) \cap \{f \in \mathbf{R}^X \mid f(x) = 0\} \quad (x \in X), \quad (2.9)$$

which is also the union of the bounded faces of

$$\{f \in \mathbf{R}^X \mid f(y) + f(z) \geq d(y, z) \ (y, z \in X), f(x) = 0\}. \quad (2.10)$$

Then $T(X, d)$ and $t^d(x)$ are contractible since the union of the bounded faces of a polyhedron is contractible; see Lemma A.5 in Appendix. Note that contractibility of $T(X, d)$ in the case that d is a metric is shown in [6, (1.10), p.332].

We define a weighted graph $G(d)$ by the 1-skeleton of $T(X, d)$ endowed with the $\|\cdot\|_\infty$ norm of \mathbf{R}^X . For $x \in X$, let $g^d(x)$ be defined by the graph corresponding to the 1-skeleton of $t^d(x)$, which is a connected subgraph of $G(d)$.

The following shows that in the case that d is a metric, $t^d(x)$ is a single point of $T(X, d)$ that coincides with the canonical map $X \rightarrow T(X, d)$.

Lemma 2.2. *If d is a metric, then we have $t^d(x) = \{h_x\}$ for $x \in X$, where $h_x \in \mathbf{R}^X$ is defined as*

$$h_x(y) = d(x, y) \quad (y \in X). \quad (2.11)$$

Proof. Let $f \in t^d(x)$. Then we have $f(z) \geq d(x, z)$ for $z \in X$ since $f(x) = 0$. For $y \in X$, by $f \in T(X, d)$, there exists $w \in X$ such that $f(y) + f(w) = d(y, w)$. By the triangle inequality, we have $d(y, x) + d(w, x) \leq f(y) + f(w) = d(y, w) \leq d(x, y) + d(x, w)$. Hence we obtain $f(y) = d(x, y)$. \square

2.4 Results

We present a more general version of Theorem 1.2 below, which is also an extension of (a finite dimensional version of) the result of A. Dress [6] that a metric is a tree metric if and only if its tight span is a tree. In this paper, a *subtree* means a subgraph which is a tree.

Theorem 2.3. *For a distance $d : X \times X \rightarrow \mathbf{R}$, the following conditions are equivalent.*

- (a) *There exist some weighted tree T and a family of its subtrees T_x ($x \in X$) such that*

$$d(x, y) = \min\{D_T(u, v) \mid u \in V(T_x), v \in V(T_y)\} \quad (x, y \in X). \quad (2.12)$$

- (b) *There exist some compatible collection of partial splits \mathcal{S} on X and a positive weight $\alpha : \mathcal{S} \rightarrow \mathbf{R}$ such that*

$$d = \sum_{S \in \mathcal{S}} \alpha_S \zeta_S. \quad (2.13)$$

- (c) *$G(d)$ is a tree.*
 (d) *$T(X, d)$ is a tree.*
 (e) *$\dim T(X, d) \leq 1$.*
 (f) *d satisfies the condition (1.2).*

The essential part of the proof of Theorem 2.3 relies on the following, which is an extension of the fact that a finite metric space (X, d) can be isometrically embedded into $(T(X, d), \|\cdot\|_\infty)$ and realized by the 1-skeleton of $T(X, d)$ [6].

Theorem 2.4. *For a distance $d : X \times X \rightarrow \mathbf{R}$, the following holds.*

- (1) $d(x, y) = \inf\{\|f - g\|_\infty \mid f \in t^d(x), g \in t^d(y)\} \quad (x, y \in X)$.
 (2) $d(x, y) = \min\{D_{G(d)}(u, v) \mid u \in V(g^d(x)), v \in V(g^d(y))\} \quad (x, y \in X)$.

Remark 2.5. We show that the condition (1.2) reduces to the four-point condition (1.1) for a metric d . From the triangle inequality, we have

$$d(x, y) \leq \frac{1}{2}\{d(x, z) + d(z, y)\} + \frac{1}{2}\{d(x, w) + d(w, y)\}. \quad (2.14)$$

This implies that $d(x, y) \leq \max\{d(x, z) + d(y, w), d(x, w) + d(z, y)\}$. Similarly,

$$\{d(x, y) + d(y, z) + d(z, x)\}/2 \leq \{d(x, w) + d(w, y) + d(y, z) + d(z, x)\}/2 \quad (2.15)$$

implies

$$\{d(x, y) + d(y, z) + d(z, x)\}/2 \leq \max\{d(x, z) + d(y, w), d(x, w) + d(y, z)\}.$$

Remark 2.6. Every 3-point distance can be expressed as Theorem 2.3 (a). Let $d : \{1, 2, 3\} \times \{1, 2, 3\} \rightarrow \mathbf{R}$ be a distance on $\{1, 2, 3\}$. If d is a metric, then it is well known that d is a tree metric. Suppose that d does not satisfy the triangle inequality, say $d(1, 2) > d(1, 3) + d(2, 3)$. Consider a weighted tree $T = (\{i, j, k, l\}, \{ij, jk, kl\}, w)$ with edge length $w_{ij} = d(1, 3)$, $w_{jk} = d(1, 2) - d(1, 3) - d(2, 3)$ and $w_{kl} = d(2, 3)$, and a family of its subtrees $\{T_1 = (\{i\}, \emptyset), T_2 = (\{j, k\}, \{jk\}), T_3 = (\{l\}, \emptyset)\}$. Then they satisfy (2.12).

Remark 2.7. The split decomposition, due to Bandelt and Dress [1], has been extended in [12] for distances using partial split distances. A distance between subtrees of a tree, considered in this paper, is one of the examples of *totally split decomposable* distances in the sense of [12].

Remark 2.8. We give some remarks about the dual view of tight spans. Consider the point configuration $\mathcal{A}_{X,2} := \{\chi_x + \chi_y \mid x, y \in X\} \subseteq \mathbf{R}^X$; see the beginning of Section 3 for the definition of χ_x . Take the convex hull of $\{(\chi_x + \chi_y, d(x, y)) \mid x, y \in X\} \subseteq \mathcal{A}_{X,2} \times \mathbf{R}$, and project its upper faces to the convex hull of $\mathcal{A}_{X,2}$. Then we obtain a *regular subdivision* $\Delta(X, d)$ of $\mathcal{A}_{X,2}$. In fact, the tight span $T(X, d)$ is the union of dual faces of interior faces of $\Delta(X, d)$; see [12] and [20] for details. We see from this view point that $\dim T(X, d) \leq 1$ if and only if $\Delta(X, d)$ has no interior faces of codimension greater than 1. Furthermore, the condition (1.2) can be rephrased as follows:

$$\Delta(X, d) \text{ has no edge which can be represented as } [\chi_x + \chi_y, \chi_z + \chi_w] \\ \text{for some distinct } x, y, z, w \in X,$$

where $[p, q]$ denotes the closed line segment between p and q . Indeed, since the height of the upper envelope of the convex hull of $\{(\chi_x + \chi_y, d(x, y)) \mid x, y \in X\}$ at $(\chi_x + \chi_y + \chi_z + \chi_w)/2$ is given by a quarter of the optimal value of the linear program (A.7) for $Y = \{x, y, z, w\}$, we have that $[\chi_x + \chi_y, \chi_z + \chi_w]$ is an edge of $\Delta(X, d)$ if and only if the optimal value of (A.7) for $Y = \{x, y, z, w\}$ is uniquely attained by $2\chi_{\{xy, zw\}}$ if and only if $\dim T(X, d) > 1$ (see the condition (b') in Appendix). In particular, $\dim T(X, d) \leq 1$ if and only if each edge of $\Delta(X, d)$ is one of $[\chi_x + \chi_y, 2\chi_z]$, $[\chi_z + \chi_x, \chi_z + \chi_y]$, and $[2\chi_x, 2\chi_y]$. Furthermore, $[\chi_x + \chi_y, 2\chi_z]$ is an edge of $\Delta(X, d)$ if and only if $d(x, y) > d(x, z) + d(z, y)$ (consider the height of the upper envelope of the convex hull of $\{(\chi_x + \chi_y, d(x, y)) \mid x, y \in X\}$ at $(2\chi_z + \chi_x + \chi_y)/2$). Hence, d is a tree metric (d is a metric and $\dim T(X, d) \leq 1$) if and only if each edge in $\Delta(X, d)$ is parallel to $\chi_x - \chi_y$ for some $x, y \in X$. A polyhedron each of whose edges is parallel to $\chi_x - \chi_y$ is known as a *base polyhedron* or a *matroid polytope* for a $\{0, 1\}$ -polytope; see [9] and [11] for base polyhedra, and this characterization by edge vectors is due to Tomizawa [21] and Gelfand, Goresky, MacPherson, and Serganova [10]. Subdivisions consisting of base polyhedra are called *matroid subdivisions*. Hence, d is a tree metric if and only if $\Delta(X, d)$ is

a matroid subdivision. Matroid subdivisions appear in *tropical geometry* [19], *surgery on Grassmannians* [15], and *discrete convex analysis*; polyhedral convex functions whose lower faces induce a matroid subdivision are called *M-convex functions* in [16] (also see [13] for the relationship between M-convexity and tree metrics).

3 Proofs

In the following, let X be a finite set and $d : X \times X \rightarrow \mathbf{R}$ be a distance on X . For a set S , we denote by χ_S the characteristic vector of S defined as: $\chi_S(x) = 1$ if $x \in S$ and 0 otherwise. In particular we write simply χ_x instead of $\chi_{\{x\}}$ for a singleton $\{x\}$.

3.1 Preliminaries

For $f \in P(X, d)$, we define an undirected graph $K(f) = (X, E(f))$ by

$$xy \in E(f) \stackrel{\text{def}}{\iff} f(x) + f(y) = d(x, y) \quad (x, y \in X), \quad (3.1)$$

where for $x, y \in X$, xy denotes an unordered pair, which means that xy and yx are not distinguished from each other. An edge is in $K(f)$ if f is in the facet of $P(X, d)$ corresponding to that edge. Note that $E(f)$ may contain loop edges, like xx for $x \in X$. Let $F(f)$ be the face of $P(X, d)$ that contains f in its relative interior, which is also the set of solutions to the linear inequalities

$$p(x) + p(y) = d(x, y) \quad (xy \in E(f)), \quad (3.2)$$

$$p(x) + p(y) \geq d(x, y) \quad (xy \notin E(f)). \quad (3.3)$$

By the same argument in the case that d is a metric [7], it is easy to observe that

$$f \in T(X, d) \iff F(f) \text{ is bounded} \quad (3.4)$$

$$\iff K(f) \text{ does not have isolated vertices} \quad (3.5)$$

$$\iff \forall x \in X, f(x) = \max_{y \in X} \{f(y) - d(x, y)\}. \quad (3.6)$$

For the subsequent arguments, we need a characterization of the dimension of $F(f)$. Since the dimension of $F(f)$ is given by the dimension of its affine hull (3.2), $\dim F(f)$ coincides with $|X|$ minus the rank of the matrix whose column vectors are $\{\chi_x + \chi_y \mid xy \in E(f)\}$. For a connected graph (X, E) , we observe

$$\text{rank}\{\chi_x + \chi_y \mid xy \in E\} = \begin{cases} |X| - 1 & \text{if } (X, E) \text{ is bipartite,} \\ |X| & \text{if } (X, E) \text{ is nonbipartite,} \end{cases} \quad (3.7)$$

where loops are regarded as odd cycles. Therefore, if $f \in T(X, d)$, we have

$$\dim F(f) = |X| - \text{rank}\{\chi_x + \chi_y \mid xy \in E(f)\} \quad (3.8)$$

$$= \text{the number of bipartite components of } K(f). \quad (3.9)$$

In particular, we have

$$F(f) \text{ is an edge} \Leftrightarrow K(f) \text{ has only one bipartite component,} \quad (3.10)$$

$$F(f) \text{ is a vertex} \Leftrightarrow K(f) \text{ has no bipartite components.} \quad (3.11)$$

The dimension of $T(X, d)$ is given by

$$\dim T(X, d) = \max_{f \in T(X, d)} \{\text{the number of bipartite components of } K(f)\}. \quad (3.12)$$

3.2 Proof of Theorem 2.4

Theorem 2.4 says

$$d(x, y) = \inf\{\|f - g\|_\infty \mid f \in t^d(x), g \in t^d(y)\}, \quad (3.13)$$

$$= \min\{D_{G(d)}(u, v) \mid u \in V(g^d(x)), v \in V(g^d(y))\}. \quad (3.14)$$

Let D_1 and D_2 be distances on X defined by the RHS in (3.13) and (3.14), respectively. We prove $d = D_1 = D_2$.

Lemma 3.1. $d(x, y) \leq D_1(x, y) \leq D_2(x, y)$ holds for $x, y \in X$.

Proof. For any $f \in t^d(x), g \in t^d(y)$, we have

$$f(x) = 0, f(y) \geq d(x, y), g(x) \geq d(x, y), g(y) = 0. \quad (3.15)$$

Hence we have $\|f - g\|_\infty \geq d(x, y)$. We may identify the graph $G(d)$ and the 1-skeleton of $T(X, d)$. Let (f_0, f_1, \dots, f_m) be a path of $G(d)$ with $f_0 \in V(g^d(x))$ and $f_m \in V(g^d(y))$. Hence the length of the path (f_0, f_1, \dots, f_m) is $\sum_{i=0}^{m-1} \|f_i - f_{i+1}\|_\infty \geq \|f_0 - f_m\|_\infty \geq D_1(x, y)$. \square

In the following, we construct the path in $G(d)$ from $V(g^d(x))$ to $V(g^d(y))$ with its path length $d(x, y)$. This implies Theorem 2.4.

First, we take a vertex of $t^d(x)$. Let $X = \{x_1 = x, x_2 = y, x_3, \dots, x_m\}$. Then, $f \in \mathbf{R}^X$ defined by

$$\begin{aligned} f(x_1) &= 0, \\ f(x_i) &= \max(0, \max_{k=1, \dots, i-1} (d(x_i, x_k) - f(x_k))) \quad (i = 2, \dots, m) \end{aligned}$$

is a vertex of $t^d(x)$. Indeed, define $\{f^k\}_{k=1, \dots, m} \subseteq \mathbf{R}^X$ by $f^k(x_i) = f(x_i)$ for $i \leq k$ and $f^k(x_i) = +\infty$ (sufficiently large) for $i > k$. By induction on k , we see that $f^k \in P(X, d)$, $E(f^k) \subseteq E(f)$, and x_k is covered by some edge in $E(f^k)$ which is a loop ($f(x_k) = 0$), or is connected to some nonbipartite component ($f(x_k) = d(x_k, x_j) - f(x_j)$ for some $j < k$). Hence, $f = f^m$ is a vertex of $t^d(x)$ by (3.11). In particular, we have $xx, xy \in E(f)$, $f(y) = d(x, y)$, and $f(x) = 0$.

Next we try to move f toward $t^d(y)$ through edges of $T(X, d)$. If $yy \in E(f)$, then we have $f \in t^d(y)$ and $D_2(x, y) = D_1(x, y) = 0 = d(x, y)$. Hence we suppose $yy \notin E(f)$, i.e., $f(y) > 0$.

To move f in $T(X, d)$, we use stable sets of $K(f)$, where a vertex set $S \subseteq X$ is called a *stable set* of $K(f)$ if for any $x, y \in S$ we have $xy \notin E(f)$. For a subset $S \subseteq X$, we define the *neighborhood* $N(S)$ by $\{z \in X \setminus S \mid \exists w \in S, zw \in E(f)\}$. If $S \subseteq X$ is a stable set of $K(f)$, for sufficiently small $\epsilon > 0$, a vector

$f + \epsilon(\chi_{N(S)} - \chi_S)$ is also in $P(X, d)$. In particular, $\chi_{N(S)} - \chi_S$ is a feasible direction of $P(X, d)$ at f . We use this fact.

Let $S_y \subseteq X$ be a stable set of $K(f)$ constructed according to the following process, where $N(S_y \cup N(S_y))$ is the set of vertices at distance exactly 2 to S_y ,

(S0) $S_y = \{y\}$.

(S1) If there is no loopless vertex in $N(S_y \cup N(S_y))$ then output S_y and stop.

(S2) Take a loopless vertex $z \in N(S_y \cup N(S_y))$.

(S3) $S_y \leftarrow S_y \cup \{z\}$ and go to (S1).

By this construction, we see that the graph

$$G_{S_y} = (S_y \cup N(S_y), \{zw \in E(f) \mid z \in S_y, w \in N(S_y)\}) \quad (3.16)$$

is a connected bipartite subgraph of $K(f)$. For $\epsilon \geq 0$, let $f^\epsilon \in \mathbf{R}^X$ be defined as

$$f^\epsilon = f + \epsilon(\chi_{N(S_y)} - \chi_{S_y}). \quad (3.17)$$

Let $\epsilon_0 > 0$ be defined by the maximum of $\epsilon \geq 0$ such that $f^\epsilon \in P(X, d)$. Then ϵ_0 is given by

$$\min \left\{ \begin{array}{l} \min_{z, w \in S_y} (f(z) + f(w) - d(z, w))/2, \\ \min_{z \in S_y, w \notin S_y \cup N(S_y)} f(z) + f(w) - d(z, w) \end{array} \right\}. \quad (3.18)$$

Then it is seen that

- (1) $f^\epsilon \in T(X, d)$ for $0 \leq \epsilon \leq \epsilon_0$,
- (2) $K(f^\epsilon)$ has one bipartite component G_{S_y} for $0 < \epsilon < \epsilon_0$, and
- (3) $K(f^{\epsilon_0})$ has no bipartite components.

Indeed, each $z \notin S_y \cup N(S_y)$ is covered by some edge zw with $w \notin S_y \cup N(S_y)$ and each $z \in S_y \cup N(S_y)$ is covered by some edges of G_{S_y} . These edges remain in $K(f^\epsilon)$ for $0 \leq \epsilon \leq \epsilon_0$. This implies (1). For $0 < \epsilon < \epsilon_0$, any edge $zw \in E(f)$ with $z \in N(S_y), w \notin S_y$ vanishes in $(X, E(f^\epsilon))$, and each edge in G_{S_y} remains. This implies (2). In $K(f^{\epsilon_0})$, there exists some new edge $zw \in E(f^{\epsilon_0})$ such that $z, w \in S_y$ or $z \in S_y, w \notin S_y \cup N(S_y)$. In the former case, an odd cycle appears in the subgraph induced by $S_y \cup N(S_y)$. In the latter case, the bipartite component G_{S_y} is connected to some nonbipartite component. This implies (3).

By (3.10) and (3.11), the move $f \rightarrow f^{\epsilon_0}$ is on the edge of $T(X, d)$, f^{ϵ_0} is a vertex of $T(X, d)$, and we have

$$\|f^{\epsilon_0} - f\|_\infty = f^{\epsilon_0}(x) - f(x) = f(y) - f^{\epsilon_0}(y) = \epsilon_0 \quad (3.19)$$

by $y \in S_y$ and $x \in N(S_y)$. Put $f_1 = f^{\epsilon_0}$ and repeat this process for f_1 . Note that $y \in S_y$ and $x \in N(S_y)$ always hold in each step of this process. Then we have the path $(f = f_0, f_1, f_2, \dots)$ of $G(d)$. By (3.19), we have $f_0(y) > f_1(y) > \dots$. After finitely many steps, we have $f_l(y) = 0$, $f_l(x) = d(x, y)$, and $f_l \in t^d(y)$. Therefore the path length of $(f = f_0, f_1, f_2, \dots, f_l = g)$ is $\sum_{i=0}^{l-1} \|f_{i+1} - f_i\|_\infty = f(y) - g(y) = g(x) - f(x) = d(x, y)$.

3.3 Proof of Theorem 2.3

We restate six conditions of Theorem 2.3 as follows:

- (a) There exist some weighted tree T and a family of its subtrees T_x ($x \in X$) such that

$$d(x, y) = \min\{D_T(u, v) \mid u \in V(T_x), v \in V(T_y)\} \quad (x, y \in X).$$

- (b) There exist some compatible collection of partial splits \mathcal{S} on X and a positive weight $\alpha : \mathcal{S} \rightarrow \mathbf{R}$ such that

$$d = \sum_{S \in \mathcal{S}} \alpha_S \zeta_S.$$

- (c) $G(d)$ is a tree.

- (d) $T(X, d)$ is a tree.

- (e) $\dim T(X, d) \leq 1$.

- (f) d satisfies the condition (1.2).

We prove the equivalence of these conditions by showing the following:

$$\begin{array}{ccccc} (a) & \Leftarrow & (c) & \Leftarrow & (d) \\ & \Downarrow & & & \Downarrow \\ (b) & \Rightarrow & (f) & \Leftrightarrow & (e) \end{array} \quad (3.20)$$

(c) \Leftarrow (d) is obvious. (a) \Leftarrow (c) follows from Theorem 2.4. (d) \Leftrightarrow (e) follows from the contractibility of $T(X, d)$.

We show (f) \Leftrightarrow (e) from Theorem 2.1 for $n = 2$. Recall the fact that every permutation can be uniquely decomposed to disjoint cyclic permutations. For a permutation σ of a 4-point set X , $d^\sigma := \sum_{i \in X} d(i, \sigma(i))$ is given as

$$d^\sigma = \begin{cases} 0 & \text{if } \sigma = \text{identity,} \\ 2d(x, y) & \text{if } \sigma = (x \ y), \\ 2d(x, y) + 2d(z, w) & \text{if } \sigma = (x \ y)(z \ w), \\ d(x, y) + d(y, z) + d(z, x) & \text{if } \sigma = (x \ y \ z), \\ d(x, y) + d(y, z) + d(z, w) + d(w, x) & \text{if } \sigma = (x \ y \ z \ w), \end{cases} \quad (3.21)$$

where $x, y, z, w \in X$ and $\sigma = (x_0 \ x_1 \ \cdots \ x_{m-1})$ means a cyclic permutation $\sigma(x_i) = x_{i+1 \pmod m}$. Note that $d^{(x_0 \cdots x_{m-1})} = d^{(x_{m-1} \cdots x_0)}$. Hence, Theorem 2.1 for $n = 2$ says that $\dim T(X, d) \leq 1$ if and only if

$$\forall x, y, z, w \in X \text{ (all distinct)} \\ d^{(xy)(zw)} \leq \max \left\{ \begin{array}{l} d^{\text{id}}, \\ d^{(xy)}, d^{(xz)}, d^{(xw)}, d^{(yz)}, d^{(yw)}, d^{(zw)}, \\ d^{(xz)(yw)}, d^{(xw)(yz)}, \\ d^{(xyz)}, d^{(xyw)}, d^{(xzw)}, d^{(yzw)}, \\ d^{(xyzw)}, d^{(xywz)}, d^{(xzyw)} \end{array} \right\}. \quad (3.22)$$

Clearly, (1.2) implies (3.22). We show the converse. Since $d \geq 0$, $d^{(xz)(yw)} = d^{(xz)} + d^{(yw)}$ and $d^{(xw)(yz)} = d^{(xw)} + d^{(yz)}$, the terms d^{id} , $d^{(xz)}$, $d^{(yw)}$, $d^{(xw)}$ and

$d^{(yz)}$ are redundant in (3.22). Similarly, $d^{(xzyw)} = (d^{(xz)(yw)} + d^{(xw)(yz)})/2$ implies that $d^{(xzyw)}$ is also redundant. Suppose that d satisfies (3.22) and violates (1.2). Then we have $d^{(xz)(yw)} < d^{(xy)(zw)} \leq d^{(xywz)}$ or $d^{(xw)(yz)} < d^{(xy)(zw)} \leq d^{(xywz)}$. Both inequalities contradict $d^{(xywz)} = (d^{(xz)(yw)} + d^{(xy)(zw)})/2$ and $d^{(xzyw)} = (d^{(xw)(yz)} + d^{(xz)(yw)})/2$. Hence we obtain the equivalence between (1.2) and (3.22).

Next we show (a) \Rightarrow (b). Deletion of each edge e of T separates T into two trees T_e^A and T_e^B . From this, we have a disjoint pair $\{A_e, B_e\}$ defined as

$$A_e = \{x \in X \mid T_x \text{ is a subtree of } T_e^A\}, \quad (3.23)$$

$$B_e = \{x \in X \mid T_x \text{ is a subtree of } T_e^B\}. \quad (3.24)$$

For two edges $e, f \in E(T)$, we may assume that T_e^A is a subtree of T_f^A and T_f^B is a subtree of T_e^B . This implies the compatibility of $\{A_e, B_e\}$ and $\{A_f, B_f\}$. Hence we define the compatible collection of partial splits \mathcal{S} on X and its positive weight $\alpha : \mathcal{S} \rightarrow \mathbf{R}$ by

$$\mathcal{S} = \{\{A_e, B_e\} \mid e \in E(T), \{A_e, B_e\} \text{ is a partial split}\}, \quad (3.25)$$

$$\alpha_{\{A_e, B_e\}} = \text{the length of edge } e. \quad (3.26)$$

Let $d' = \sum_{S \in \mathcal{S}} \alpha_S \zeta_S$. We show $d = d'$. Let $e \in E(T)$ be an edge with $\{A_e, B_e\} \in \mathcal{S}$. For $x \in A_e$ and $y \in B_e$, any path between T_x and T_y must contain e . This implies $d \geq d'$. Next we show $d \leq d'$. For $x, y \in X$, if T_x and T_y have a common vertex, i.e., $d(x, y) = 0$, then there is no edge in T that separates T_x and T_y . Hence we have $d(x, y) = d'(x, y) = 0$. Suppose that $d > 0$. Let $e \in E(T)$ be an edge of the shortest path between T_x and T_y . Neither T_x or T_y contains the edge e . Since both T_x and T_y are trees, it must be $x \in A_e, y \in B_e$ or $y \in A_e, x \in B_e$. Hence we have $\{A_e, B_e\} \in \mathcal{S}$. This implies $d \leq d'$.

(b) \Rightarrow (f). It is sufficient to show this in the case that d is a distance on 4-point set. For this, we classify maximal compatible families of partial splits on the 4-point set $\{1, 2, 3, 4\}$. All partial splits on $\{1, 2, 3, 4\}$ are listed below, where we denote a partial split $\{\{1, 2\}, \{3\}\}$ simply by 12|3:

$$(S1): 1|234, 2|134, 3|124, 4|123,$$

$$(S2): 12|34, 13|24, 23|14,$$

$$(S3): 1|2, 1|3, 1|4, 2|3, 2|4, 3|4,$$

$$(S4): 1|23, 2|13, 3|12, 1|24, 2|14, 4|12, 1|34, 3|14, 4|13, 2|34, 3|24, 4|23.$$

The next proposition shows that maximal compatible families of partial splits on $\{1, 2, 3, 4\}$ are classified into six types. We illustrates this six types and their tree representations in Figure 2, where the line corresponding to a partial split $\{A, B\}$ separates points of A and B and meets points of $\{1, 2, 3, 4\} \setminus A \cup B$.

Two families of partial splits \mathcal{S}_1 and \mathcal{S}_2 on X are said to be *isomorphic* if there exists some bijection $\sigma : X \rightarrow X$ such that $\mathcal{S}_2 = \{\{\sigma(A), \sigma(B)\} \mid \{A, B\} \in \mathcal{S}_1\}$.

Proposition 3.2. *Any maximal compatible family of partial splits on $\{1, 2, 3, 4\}$ is isomorphic to one of the following:*

Type 1: $\{1|234, 2|134, 12|34, 3|124, 4|123\}$,

Type 2: $\{1|234, 2|134, 12|34, 12|4, 4|123\}$,

Type 3: $\{1|234, 1|34, 12|34, 12|4, 4|123\}$,

Type 4: $\{1|234, 1|34, 1|4, 13|4, 4|123\}$,

Type 5: $\{1|234, 1|34, 1|4, 12|4, 4|123\}$,

Type 6: $\{1|23, 2|13, 3|12, 1|234, 2|134, 3|124\}$.

Proof. For a family of partial splits \mathcal{S}' , the *incompatibility graph* of \mathcal{S}' is defined to be a graph whose vertex set is \mathcal{S}' and edge set is

$$\{ST \mid S \in \mathcal{S}' \text{ and } T \in \mathcal{S}' \text{ are not compatible}\}. \quad (3.27)$$

Then $\mathcal{S}'_0 \subseteq \mathcal{S}'$ is compatible if and only if \mathcal{S}'_0 is a stable set of the incompatibility graph of \mathcal{S}' .

Let \mathcal{S} be a maximal compatible family of partial splits on $\{1, 2, 3, 4\}$. Suppose that \mathcal{S} has a partial split of (S2), say $12|34$. The set of all partial splits compatible to $12|34$ is given by

$$\mathcal{S}_1 = \{12|34, 1|234, 2|134, 3|124, 4|123, 1|34, 2|14, 12|4, 12|3\}. \quad (3.28)$$

Then the incompatibility graph of \mathcal{S}_1 is (a) of Figure 3. From maximal stable sets of this graph, we see that \mathcal{S} is of Type 1, Type 2, or Type 3.

Suppose that \mathcal{S} has a partial split of (S3), say $1|2$. The set of all partial splits compatible to $1|2$ is given by

$$\mathcal{S}_2 = \{1|2, 1|234, 2|134, 1|24, 1|23, 2|34, 2|13\}. \quad (3.29)$$

Then the incompatibility graph of \mathcal{S}_2 is (b) of Figure 3. From maximal stable sets of this graph, we see that \mathcal{S} is of Type 4 or Type 5.

Suppose that \mathcal{S} has no partial splits of (S2) and (S3). If \mathcal{S} consists of partial splits of (S1), \mathcal{S} is not maximal compatible. Suppose that \mathcal{S} has a partial split of (S4), say $1|23$. The set of all partial splits of (S1) and (S4) compatible to $1|23$ is given by

$$\mathcal{S}_3 = \{1|23, 2|13, 3|12, 1|234, 2|134, 3|124, 2|14, 3|14\}. \quad (3.30)$$

Then the incompatibility graph of \mathcal{S}_3 is (c) of Figure 3. Hence all maximal stable sets of this graph are

- (1) $\{1|23, 2|13, 3|12, 1|234, 2|134, 3|124\}$,
- (2) $\{1|23, 2|14, 1|234, 2|134\}$, and
- (3) $\{1|23, 3|14, 1|234, 3|124\}$.

Neither (2) nor (3) is maximal compatible. Hence \mathcal{S} must be (1) and is of Type 6. □

Finally, we can confirm the condition (1.2) for each type in Proposition 3.2 as follows:

$$\begin{aligned} \text{(Type 1, 2, 3)} \quad & \max\{d^{(12)(34)}, d^{(13)(24)}, d^{(14)(23)}\} \text{ is attained at least twice,} \\ \text{(Type 4, 5)} \quad & \max\{d^{(12)(34)}, d^{(13)(24)}, d^{(14)(23)}\} = d^{(14)}, \\ \text{(Type 6)} \quad & \max\{d^{(12)(34)}, d^{(13)(24)}, d^{(14)(23)}\} \leq d^{(123)}, \end{aligned}$$

where we use the notation in (3.21) and the labelling corresponds to Figure 2.

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A Appendix

Proof of Theorem 2.1

Our proof is based on the fundamental duality principle in the theory of linear programming; see [22] for example for linear programming.

Lemma A.1. *Let $A = (a_1 \ a_2 \ \dots \ a_m)$ be an $n \times m$ matrix with n -dimensional column vectors $\{a_i \mid i = 1, 2, \dots, m\} \subseteq \mathbf{R}^n$. For $b \in \mathbf{R}^n$, consider the polyhedron*

$$Q = \{u \in \mathbf{R}^m \mid Au = b, u \geq 0\}. \quad (\text{A.1})$$

Then $u \in Q$ is a vertex of Q if and only if the vectors $\{a_i \mid u_i > 0\}$ are linearly independent.

Let E_X denote the set of unordered pairs defined as

$$E_X = \{xy \mid x \in X, y \in X\}. \quad (\text{A.2})$$

The following is an easy consequence of the previous lemma.

Lemma A.2. *Let $Q(X)$ be the set of nonnegative weights on E_X such that the sum of the weights around each vertex is equal to 2, i.e.,*

$$Q(X) = \{\lambda \in \mathbf{R}^{E_X} \mid \sum_{xy \in E_X} (\chi_x + \chi_y)\lambda_{xy} = 2\chi_X, \lambda_{xy} \geq 0 \ (xy \in E_X)\}. \quad (\text{A.3})$$

Then $\lambda \in Q(X)$ is a vertex of $Q(X)$ if and only if there exists some edge cover E of (X, E_X) consisting of a matching and odd cycles, pairwise vertex disjoint, such that

$$\lambda_{xy} = \begin{cases} 2 & \text{if } xy \text{ is an edge of matching of } E, \\ 1 & \text{if } xy \text{ is an edge of some odd cycle of } E, \\ 0 & \text{otherwise,} \end{cases} \quad (xy \in E_X). \quad (\text{A.4})$$

Considering the facts that a permutation of X can be decomposed as disjoint cyclic permutations, that a cyclic permutation can be regarded as a cycle of graph (X, E_X) and that an even cycle is the union two edge-disjoint matchings, the optimal value of the linear program

$$\max. \sum_{xy \in E_X} \lambda_{xy} d(x, y) \quad \text{s.t.} \quad \lambda \in Q(X) \quad (\text{A.5})$$

is given by

$$\max\left\{ \sum_{x \in X} d(x, \sigma(x)) \mid \sigma \text{ is a permutation of } X \right\}. \quad (\text{A.6})$$

Hence, the condition (b) of Theorem 2.1 can be rephrased as follows:

- (b') There exist a $2n$ -element subset $Y \subseteq X$ and a perfect matching M of (Y, E_Y) such that $2\chi_M \in \mathbf{R}^{E_Y}$ is the unique optimal solution to the linear program

$$\max. \sum_{xy \in E_Y} \lambda_{xy} d(x, y) \quad \text{s.t.} \quad \lambda \in Q(Y). \quad (\text{A.7})$$

In the following, we often use the dimension formula (3.12).

Lemma A.3. *The following holds, where $d^Y : Y \times Y \rightarrow \mathbf{R}$ denotes the restriction of d to Y .*

- (1) $\dim T(Y, d^Y) \leq \dim T(X, d)$ for $Y \subseteq X$.
- (2) If $\dim T(X, d) \geq n$, there exists $Y \subseteq X$ with $|Y| = 2n$ such that $\dim T(Y, d^Y) = n$.

Proof. For $f \in \mathbf{R}^X$ and $Y \subseteq X$, let $f^Y : Y \rightarrow \mathbf{R}$ denote the restriction of f to Y .

(1). It is sufficient to show the case $Y = X \setminus \{z\}$ for some $z \in X$. Suppose that $\dim T(Y, d^Y) = n$. Then there exists $f \in T(Y, d^Y)$ such that a graph $(Y, E(f^Y))$ has n bipartite components $(A_1 \cup B_1, E_1), \dots, (A_n \cup B_n, E_n)$ with $A_i \cap B_i = \emptyset$ and $E_i \subseteq \{xy \mid x \in A_i, y \in B_i\}$ for $i = 1, \dots, n$. We use the notation and the method in Subsection 3.2. Let $f' \in \mathbf{R}^X$ be defined as

$$f'(x) = \begin{cases} \max\{0, \max_{y \in Y} (d(z, y) - f(y))\} & \text{if } x = z, \\ f(x) & \text{otherwise.} \end{cases} \quad (\text{A.8})$$

Then some edges connecting z appear in $(X, E(f'))$ and we have $f' \in T(X, d)$. If $(X, E(f'))$ has no edges connecting $\{z\}$ and $A_1 \cup B_1 \cup \dots \cup A_n \cup B_n$, then $(X, E(f'))$ also has n bipartite components.

We suppose that there exists $y \in A_1$ with $zy \in E(f')$. Let S and S' be stable sets of $(X, E(f'))$ defined as $S = A_1 \cup A_2 \cup \dots \cup A_n$ and $S' = A_1 \cup B_2 \cup \dots \cup B_n$. Let $g \in \mathbf{R}^X$ be defined as

$$g = f' + \epsilon(\chi_{N(S)} - \chi_S) + \epsilon'(\chi_{N(S')} - \chi_{S'}) \quad (\text{A.9})$$

for sufficiently small $\epsilon, \epsilon' > 0$. Then we have $g \in T(X, d)$. Furthermore all edges in $(X, E(f'))$ connecting $\{z\}$ and $X \setminus A_1$ vanish in $(X, E(g))$. This implies that $(X, E(g))$ has n bipartite components.

(2). Since $\dim T(X, d) \geq n$, there exists $f \in T(X, d)$ such that $(X, E(f))$ has n bipartite components. Take n edges from each bipartite component, say $\{x_1 y_1, x_2 y_2, \dots, x_n y_n\}$ and put $Y = \{x_1, x_2, \dots, x_n, y_1, \dots, y_n\}$. Then it is easy to check that f^Y is in $T(Y, d^Y)$ and $(Y, E(f^Y))$ has n bipartite components. \square

Hence, it is sufficient to show the following.

Theorem A.4. *Suppose $|X| = 2n$. The following conditions are equivalent.*

- (a) $\dim T(X, d) = n$.
- (b) *There exists some perfect matching M of (X, E_X) such that $\lambda^* = 2\chi_M \in \mathbf{R}^{E_X}$ is the unique optimal solution to linear program (A.5).*

Proof. (a) \Rightarrow (b). There exists $f^* \in P(X, d)$ such that $K(f^*)$ has n bipartite components. Hence $E(f^*)$ must be a perfect matching of (X, E_X) . Consider the dual program of (A.5):

$$\min. \sum_{x \in X} f(x) \quad \text{s.t.} \quad f \in P(X, d). \quad (\text{A.10})$$

Then $\lambda^* = 2\chi_{E(f^*)}$ and f^* satisfies the (strict) complementary slackness condition

$$\lambda_{xy}^* > 0 \Leftrightarrow f^*(x) + f^*(y) = d(x, y) \quad (xy \in E_X). \quad (\text{A.11})$$

Hence λ^* and f^* are optimal solutions to (A.5) and (A.10), respectively. Conversely, any optimal solution $\tilde{\lambda}$ of (A.5) satisfies

$$\tilde{\lambda}_{xy} = 0 \quad (xy \notin E(f^*)). \quad (\text{A.12})$$

Since $\{\chi_x + \chi_y \mid xy \in E(f^*)\}$ is linearly independent, we have $\tilde{\lambda} = \lambda^*$. Hence λ^* is the unique optimal solution of linear program (A.5).

(b) \Rightarrow (a). By the strict complementary slackness theorem, there exist optimal solutions $\tilde{\lambda}$ and f^* of (A.5) and (A.10) such that

$$\tilde{\lambda}_{xy} > 0 \Leftrightarrow f^*(x) + f^*(y) = d(x, y) \quad (xy \in E_X). \quad (\text{A.13})$$

By the condition (b), we have $\tilde{\lambda} = \lambda^*$. Hence it must be that $E(f^*) = M$. This implies $\dim T(X, d) = n$. \square

Contractibility of the Union of Bounded Faces of a Polyhedron

Lemma A.5. *The union of bounded faces of a pointed polyhedron is contractible.*

Proof. Let $P \subseteq \mathbf{R}^n$ be a pointed polyhedron and B the union of bounded faces of P . We construct a continuous map (retraction) $r : P \rightarrow B$ satisfying $r(x) = x$ for $x \in B$. If such a retraction exists, r is homotopic to the identity map by a homotopy $h : P \times [0, 1] \rightarrow P$ defined as $h(x, t) = tr(x) + (1 - t)x$. Hence, B is homotopic to P which is contractible by convexity.

We may assume that P is represented as

$$P = \{x \in \mathbf{R}^n \mid \langle a_j, x \rangle \leq b_j \quad (j = 1, \dots, m)\} \quad (\text{A.14})$$

for some $\{(a_1, b_1), (a_2, b_2), \dots, (a_m, b_m)\} \subseteq \mathbf{R}^{n+1}$, where $\langle \cdot, \cdot \rangle$ denotes the standard inner product of \mathbf{R}^n . Let $\{u_1, u_2, \dots, u_k\} \subseteq \mathbf{R}^n$ be the set of extreme rays of a pointed cone $\{u \in \mathbf{R}^n \mid \langle a_j, u \rangle \leq 0 \quad (j = 1, \dots, m)\}$. Then, a face $F \subseteq P$ is bounded if and only if F does not contain each ray u_i ($i = 1, \dots, k$), where we

say " F contains a ray u_i " if it satisfies $F + tu_i \subseteq F$ for $t \geq 0$. For a ray u_i , we define a map $\phi_{u_i} : P \rightarrow P$ as

$$\begin{aligned} \phi_{u_i}(x) &:= x - u_i \sup\{t \in \mathbf{R} \mid x - tu_i \in P\} \\ &= x - u_i \sup\{t \in \mathbf{R} \mid \langle a_j, x - tu_i \rangle \leq b_j \ (j = 1, \dots, m)\} \\ &= x - u_i \inf_{j: \langle a_j, u_i \rangle < 0} \{(\langle a_j, x \rangle - b_j) / \langle a_j, u_i \rangle\} \quad (x \in P). \end{aligned} \quad (\text{A.15})$$

Since P is pointed, the infimum of (A.15) is attained. In particular, ϕ_{u_i} is continuous. Furthermore, ϕ_{u_i} is a retraction from P to the union of faces which do not contain the ray u_i . Indeed, this immediately follows from the fact that for $x \in P$, the unique minimal face F containing x does not contain the ray u_i if and only if there exists $j \in \{1, \dots, m\}$ with $\langle a_j, u_i \rangle < 0$ such that $\langle a_j, x \rangle = b_j$. Furthermore, $\phi_{u_i}(F) \subseteq F$ holds for any face F since $\langle a_j, x \rangle = b_j$ implies $\langle a_j, \phi_{u_i}(x) \rangle = b_j$. Hence, we obtain a desired retraction $r : P \rightarrow B$ defined as

$$r = \phi_{u_k} \circ \phi_{u_{k-1}} \circ \dots \circ \phi_{u_1}. \quad (\text{A.16})$$

□

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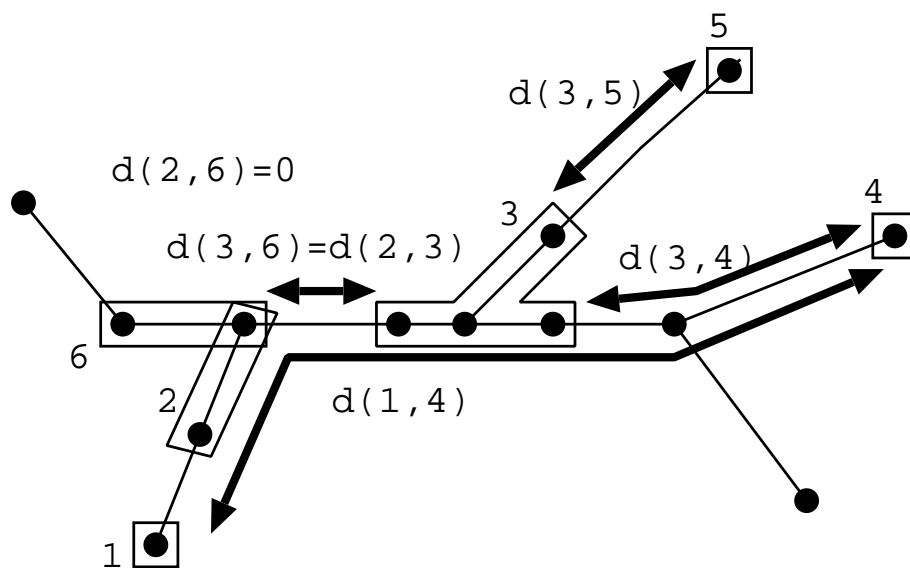


Figure 1: Shortest path lengths between six subtrees of a tree

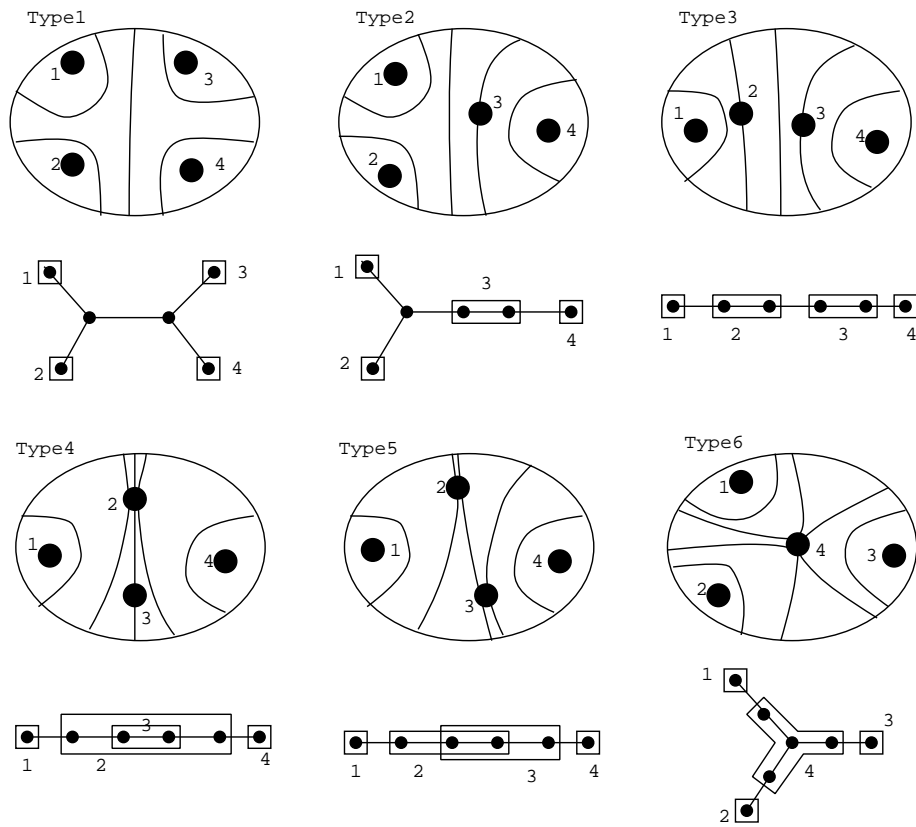


Figure 2: All types of maximal compatible families of $\{1, 2, 3, 4\}$ and their tree representations

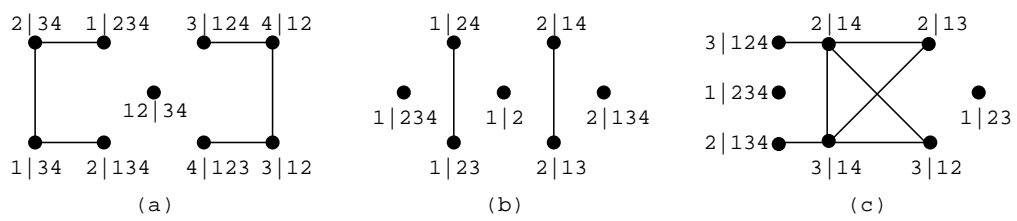


Figure 3: Incompatibility graphs