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Enhanced negative type for finite metric trees

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Dedicated to Bernard Joseph Weston (and the spirit of the Eureka Stockade)
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Abstract

A finite metric tree is a finite connected graph that has no cycles, endowed with an edge weighted path metric. Finite metric trees are known to have strict 1-negative type. In this paper we introduce a new family of inequalities (1) that encode the best possible quantification of the *strictness* of the non-trivial 1-negative type inequalities for finite metric trees. These inequalities are sufficiently strong to imply that any given finite metric tree (T, d) must have strict p-negative type for all p in an open interval $(1 - \zeta, 1 + \zeta)$, where $\zeta > 0$ may be chosen so as to depend *only* upon the unordered distribution of edge weights that determine the path metric d on T. In particular, if the edges of the tree are not weighted, then it follows that ζ depends only upon the number of vertices in the tree.

We also give an example of an infinite metric tree that has strict 1-negative type but does not have p-negative type for any $p > 1$. This shows that the maximal p-negative type of a metric space can be strict.

Keywords: Finite metric trees; Strict negative type; Generalized roundness

1. Introduction and synopsis

The study of trees as mathematical objects was initiated by Cayley [6] who enumerated the isomers of the saturated hydrocarbons $C_n H_{2n+2}$. For example, an application of Cayley's formula

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shows that the number of isomers of the paraffin $C_{13}H_{28}$ is 802. More recently, mathematical studies of finite metric trees have proliferated due to myriad applications in areas as diverse as evolutionary biology and theoretical computer science. Some examples of publications which highlight this point include Weber et al. [30], Ailon and Charikar [1], Semple and Steel [29], Fakcharoenphol et al. [12], Charikar et al. [7], and Bartal [2].

Works such as those cited above illustrate two of the major themes of study pertaining to metric trees. One is to try to reconstruct metric trees from data such as DNA or protein sequences. This is the realm of so called phylogenetic tree reconstruction or (more generally) numerical taxonomy. The second major theme, driven by algorithmic considerations in computer science, is to approximate finite metrics by (small numbers of) tree metrics. The importance of finite metric trees in this context is that they are well suited to algorithms and can serve to help greatly reduce the computational hardness of certain optimization problems.

In this paper we focus on one particular aspect of the non-linear geometry of finite metric trees; namely, strict p-negative type. (See Definition 2.1.) The p-negative type inequalities arose classically in studies of isometric embeddings and remain objects of intense research scrutiny in areas ranging from functional analysis to theoretical computer science. The monographs of Wells and Williams [31], and Deza and Laurent [8], illustrate a variety of classical and contemporary applications of inequalities of p-negative type. See also the comments in Section 2 of this paper.

Hjorth et al. [14] have shown that finite metric trees have strict 1-negative type. In this paper we determine that a new and substantially stronger family of inequalities hold for finite metric trees. Namely, as we show in Theorems 4.12 and 4.16, given a finite metric tree (T,d), there is a maximal constant $\Gamma_T > 0$ so that for all natural numbers $n \geqslant 2$, all finite subsets $\{x_1, \ldots, x_n\} \subseteq T$, and all choices of real numbers $\eta_1, \ldots, \eta_n$ with $\eta_1 + \cdots + \eta_n = 0$ and $(\eta_1, \ldots, \eta_n) \neq (0, \ldots, 0)$, we have:

$$\Gamma_T + \sum_{1 \leqslant i, j \leqslant n} d(x_i, x_j)\eta_i \eta_j \leqslant 0. \tag{1}$$

We call the maximal constant Γ_T appearing in (1) the 1-negative type gap of (T,d). Theorem 4.12 includes a characterization of equality in the inequalities (1). Remark 4.17 then indicates an alternative and more direct characterization of equality in the inequalities (1). In Corollary 4.13 we compute a closed formula for the exact value of Γ_T and thereby show that it depends only upon the tree's unordered distribution of edge weights. Indeed,

$$\Gamma_T = \left\{ \sum_{(x,y) \in E(T)} d(x,y)^{-1} \right\}^{-1}$$

where the sum is taken over the set of all (unordered) edges $e = (x,y)$ in T.

The inequalities (1) are particularly strong. They imply, for example, that there is an $\zeta > 0$ so that the finite metric tree (T,d) has strict p-negative type for all $p \in (1-\zeta, 1+\zeta)$. Moreover, due to the universality of Γ_T, ζ can be chosen so that it depends only upon the tree's unordered distribution of edge weights. This is done in Theorem 5.4. So, in this context ($p = 1$), the strict negative type of finite metric trees is seen to persist on open intervals. The same cannot be said of infinite metric trees as demonstrated by the infinite necklace tree (Y,d) which is described in Example 2 and Theorem 5.7. The necklace (Y,d) has strict 1-negative type but does not have p-negative type for any $p > 1$. This example also shows that the maximal p-negative type of a metric space can be strict. It is an open question whether the maximal p-negative type of a finite metric space can be strict.

In this paper we adopt a vicarious (rather than direct) approach to p-negative type by choosing to work with the equivalent notion of generalized roundness-p. (See Definition 2.1.) We utilize this approach due to the fact that the geometric notion of generalized roundness-p seems much more well suited to the analysis of highly symmetric objects (such as metric trees) than the more analytic notion of p-negative type. The results of this paper validate this approach.

The remainder of this paper is structured as follows. Section 2 discusses all relevant background material on p-negative type and generalized roundness-p. The known equivalence of these two notions is expressed in Theorem 2.4. This equivalence constitutes the primary theoretical tool of the entire paper. Section 2 also introduces the p-negative type gap $\Gamma_{X,p}$ of a metric space (X, d). Section 3 develops some basic facts pertaining to finite metric trees (T, d) and takes some initial steps towards determining the maximal constant $\Gamma_T = \Gamma_{T,1}$ that appears in (1). Section 4 completes this process, via Lagrange's (multiplier) theorem, and this leads into the derivations of Theorems 4.12 and 4.16 (as discussed above). Section 4 also introduces the "generic algorithm" (Definition 4.4) which provides a means to characterize equality in the inequalities (1) above. Section 5 develops applications of the inequalities (1) such as Theorem 5.4 (which determines lower bounds on the p-negative type of finite metric trees) and Theorem 5.7 (which gives properties of the infinite necklace (Y, d)). Throughout this paper we use $\mathbb{N} = \{1, 2, 3, \ldots\}$ to denote the set of all natural numbers. Whenever sums are indexed over the empty set we take them to be zero by default.

2. Preliminaries on negative type and generalized roundness

The notions of negative type and generalized roundness—the formal definitions of which are given in Definition 2.1—were introduced and studied by Menger [23] and Schoenberg [27,28], and Enflo [11], respectively. In part, Schoenberg's studies were focused on determining which metric spaces can be isometrically embedded into a Hilbert space. This work was later generalized to the setting of L_p-spaces ($0 < p \leqslant 2$) by Bretagnolle et al. [5] who obtained the following celebrated characterization: a real (quasi-) normed space is linearly isometric to a subspace of some L_p-space ($0 < p \leqslant 2$) if and only if it has p-negative type. There are also results along these lines which deal with the less tractable (commutative) case $p > 2$, and with certain of the non commutative L_p-spaces. See, for example, the papers of Koldobsky and König [17], and Junge [16], respectively. General references on the interplay between p-negative type inequalities and isometric embeddings include Deza and Laurent [8], and Wells and Williams [31].

Enflo [11] was interested in a problem of Smirnov concerning uniform embeddings of metric spaces into Hilbert spaces. A uniform embedding of one metric space into another is a uniformly continuous injection whose inverse is also uniformly continuous. In other words, uniform embeddings are uniform homeomorphisms onto their range. Smirnov had asked is every separable metric space uniformly homeomorphic to a subset of a Hilbert space? In other words; is $L_2[0, 1]$ a universal uniform embedding space? Enflo answered Smirnov's question negatively by proving that universal uniform embedding spaces cannot have generalized roundness-p for any $p > 0$, and by showing that all Hilbert spaces necessarily have generalized roundness-2. In fact, it follows from Enflo's proof that the Banach space of null sequences c_0 does not embed uniformly into any Hilbert space. The ideas and constructions in Enflo [11] have proven extremely useful over time, not only within mainstream functional analysis, but also in other important areas such as coarse geometry. The recent monograph of Benyamini and Lindenstrauss [3] gives an extensive account of the non-linear classification of Banach spaces, including a chapter on uniform embeddings into Hilbert spaces.

Instigating a theory that has turned out to have a number of uncanny parallels with that of uniform embeddings, Gromov [13] introduced the notion of coarse embeddings of metric spaces. Gromov [13] asked if every separable metric space coarsely embeds into a Hilbert space? Dranishnikov et al. [9] gave a negative answer to Gromov's question by using ideas from Enflo [11]. Yu [33] showed that every discrete metric space which coarsely embeds into a Hilbert space satisfies the coarse Baum–Connes conjecture. Using the work of Dranishnikov et al. [9] as a starting point, Nowak [25] developed a number of theoretical similarities between coarse embeddings and uniform embeddings. Connections between generalized roundness, coarse embeddings and certain forms of the Baum–Connes conjecture have also been obtained by Lafont and Prassidis [18]. Given the prominence of the coarse Baum–Connes conjecture to topologists (and to mathematicians in general), and the striking result of Yu [33] (above), it is not surprising that a large number of papers have now been written on coarse embeddings. Unfortunately, many of these papers use the term "uniform embedding" when they are really referring to coarse embeddings. In addition to the source references mentioned above, the final chapters of the monograph of Roe [26] provide a good overview of recent work on asymptotic dimension and coarse embeddings into Hilbert spaces.

Definition 2.1. Let $p \geqslant 0$ and let (X, d) be a metric space. Then:

(a) (X, d) has *p-negative type* if and only if for all natural numbers $n \geqslant 2$, all finite subsets $\{x_1, \ldots, x_n\} \subseteq X$, and all choices of real numbers $\eta_1, \ldots, \eta_n$ with $\eta_1 + \cdots + \eta_n = 0$, we have

$$\sum_{1 \leqslant i,j \leqslant n} d(x_i, x_j)^p \eta_i \eta_j \leqslant 0. \tag{2}$$

(b) (X, d) has *strict p-negative type* if and only if it has p-negative type and the inequality in (a) is strict whenever the scalar n-tuple $(\eta_1, \ldots, \eta_n) \neq \vec{0}$.

(c) (X, d) has *generalized roundness-p* if and only if for all natural numbers $n \in \mathbb{N}$, and all choices of points $a_1, \ldots, a_n, b_1, \ldots, b_n \in X$, we have

$$\sum_{1 \leqslant k<l \leqslant n} \left\{ d(a_k, a_l)^p + d(b_k, b_l)^p \right\} \leqslant \sum_{1 \leqslant j,i \leqslant n} d(a_j, b_i)^p. \tag{3}$$

Remark 2.2. In making Definition 2.1(c) it is important to point out that repetitions among the a's and b's are allowed. Indeed, allowing repetitions is essential. We may, however, when making Definition 2.1(c), assume that $a_j \neq b_i$ for all i, j $(1 \leqslant i, j \leqslant n)$. This is due to an elementary cancellation of like terms phenomenon that was first observed by Andrew Tonge (unpublished).

Notice that if one restricts to $n = 2$ in Definition 2.1(c) then one gets the condition that Enflo [10] called *roundness-p*. Roundness-p can be viewed as a direct precursor to the linear Banach space notion known as Rademacher type. Since being distilled in the 1970s, the related notions of type, cotype and K-convexity have played a very prominent rôle in the development of linear Banach space theory. See, for example, the survey paper of Maurey [21]. There are also non-linear or metric notions of type and cotype due to Bourgain et al. [4], and Mendel and

Naor [22], respectively. In particular, Mendel and Naor [22] apply metric cotype to completely settle the problem of classifying when L_p embeds coarsely or uniformly into L_q. There are also connections—such as Theorem 2.3 in Lennard et al. [20]—between generalized roundness and linear cotype. A number of open problems persist in this direction.

We should point out that our Definition 2.1(c) is a cosmetic alteration of the original definition given in Enflo [11]. Enflo actually considered the supremum of all p's that satisfy Definition 2.1(c). A result of Linial and Naor, which appears in the paper of Naor and Schechtman [24], says that every metric tree has (maximal) roundness two. The results of Section 5 of this paper, which develop lower bounds on the p-negative type of finite metric trees, can be thought of as a natural extension of the work of Linial and Naor.

Papers by Lennard et al. [19] and Weston [32] have shown that Definitions 2.1(a), (c) and a third, closely related, condition are all equivalent. These equivalences are given in Theorem 2.4 (below) and, as they are quite central to the rest of this paper, we include a brief proof for easy reference. The following definition will help us to state the third condition of Theorem 2.4 succinctly and will moreover be important in its own right throughout the entire paper.

Definition 2.3. Let X be a set. Let q, t be natural numbers.

(a) A (q,t)-*simplex* in X is a $(q+t)$-vector $(a_1, \dots, a_q, b_1, \dots, b_t) \in X^{q+t}$ whose coordinates consist of $q+t$ distinct vertices $a_1, \dots, a_q, b_1, \dots, b_t \in X$. Such a simplex will be denoted $D = [a_j; b_i]_{q,t}$.
A vertex $x \in D$ is said to be of *simplex parity a* if $x = a_j$ for some j, $1 \leqslant j \leqslant q$. A vertex $y \in D$ is said to be of *simplex parity b* if $y = b_i$ for some i, $1 \leqslant i \leqslant t$. Two distinct vertices $x, y \in D$ are said to be of the *same simplex parity* if they both have simplex parity a or if they both have simplex parity b. And, *opposite simple parity* has the obvious meaning.
(b) A *load vector* for a (q,t)-simplex $D = [a_j; b_i]_{q,t}$ in X is an arbitrary vector $\vec{\omega} = (m_1, \dots, m_q, n_1, \dots, n_t) \in \mathbb{R}_+^{q+t}$ that assigns a positive weight $m_j > 0$ or $n_i > 0$ to each vertex a_j or b_i of D ($1 \leqslant j \leqslant q$, $1 \leqslant i \leqslant t$), respectively.
(c) A *loaded* (q,t)-*simplex* in X consists of a (q,t)-simplex $D = [a_j; b_i]_{q,t}$ in X together with a load vector $\vec{\omega} = (m_1, \dots, m_q, n_1, \dots, n_t)$ for D. Such a loaded simplex will be denoted $D(\vec{\omega})$ or $[a_j(m_j); b_i(n_i)]_{q,t}$ as the need arises.
(d) A *normalized* (q,t)-*simplex* in X is a loaded (q,t)-simplex $D(\vec{\omega})$ in X whose load vector $\vec{\omega} = (m_1, \dots, m_q, n_1, \dots, n_t)$ satisfies the two normalizations:

$$m_1 + \cdots + m_q = 1 = n_1 + \cdots + n_t.$$

Such a vector $\vec{\omega}$ will be called a *normalized load vector* for D.

Theorem 2.4. *(See Lennard et al. [19], Weston [32].) Let* $p \geqslant 0$. *For a metric space* (X,d)*, the following conditions are equivalent*:

(a) (X,d) *has* p*-negative type.*
(b) (X,d) *has generalized roundness-*p*.*

(c) *For all $q, t \in \mathbb{N}$ and all normalized (q,t)-simplexes $D(\vec{\omega}) = [a_j(m_j); b_i(n_i)]_{q,t}$ in X we have*:

$$\sum_{1 \leqslant j_1 < j_2 \leqslant q} m_{j_1} m_{j_2} d(a_{j_1}, a_{j_2})^p + \sum_{1 \leqslant i_1 < i_2 \leqslant t} n_{i_1} n_{i_2} d(b_{i_1}, b_{i_2})^p \leqslant \sum_{j,i=1}^{q,t} m_j n_i d(a_j, b_i)^p. \tag{4}$$

Proof. [Sketch] The equivalence of conditions (a) and (c) is an easy consequence of the following observation. Suppose $n \geqslant 2$ is a natural number. Let $\{x_1, \ldots, x_n\} \subseteq X$, and real numbers $\eta_1, \ldots, \eta_n$ (not all zero) such that $\eta_1 + \cdots + \eta_n = 0$, be given. By relabeling (if necessary) we may assume there exist $q, t \in \mathbb{N}$ such that $q + t = n$, $\eta_1, \ldots, \eta_q \geqslant 0$, and $\eta_{q+1}, \ldots, \eta_{q+t} < 0$. Clearly $\sum_{j=1}^{q} \eta_j = -\sum_{k=q+1}^{n} \eta_k$. We now make the following designations: for $1 \leqslant j \leqslant q$, set $a_j = x_j$ and $m_j = \eta_j$. Further, if $j > q$, we nominally set $m_j = 0$. For $1 \leqslant i \leqslant t$, set $b_i = x_{n-i}$ and $n_i = -\eta_{n-i}$. Further, if $i > t$, we nominally set $n_i = 0$. For all k, $1 \leqslant k \leqslant n$, we then have $\eta_k = m_k - n_k$. More importantly, for any $p \geqslant 0$, we observe that

$$\begin{aligned}
\sum_{1 \leqslant i, j \leqslant n} d(x_i, x_j)^p \eta_i \eta_j &= \sum_{1 \leqslant i, j \leqslant n} d(x_i, x_j)^p (m_i - n_i)(m_j - n_j) \\
&= \sum_{1 \leqslant j_1, j_2 \leqslant q} m_{j_1} m_{j_2} d(a_{j_i}, a_{j_2})^p + \sum_{1 \leqslant i_1, i_2 \leqslant t} n_{i_1} n_{i_2} d(b_{i_1}, b_{i_2})^p \\
&\quad - 2 \sum_{j,i=1}^{n} m_j n_i d(a_j, b_i)^p.
\end{aligned} \tag{5}$$

Clearly weights (η_k, m_j or n_i) that are equal to zero, and the vertices to which they correspond, play no rôle in the determination of (5). Moreover, we may assume that $\sum_{j=1}^{q} m_j = 1 = \sum_{i=1}^{t} n_i$ by a simple normalization. Further, the entire process is clearly symmetric. One may instead start with a normalized (q,t)-simplex and simply *reverse* all of the above designations. The equivalence of conditions (a) and (c) is now plain.

Finally, condition (c) obviously implies condition (b). The converse follows from Remark 2.2 and a simple density/continuity argument. □

Remark 2.5. One advantage of working with condition (c) in Theorem 2.4 is that it automatically excludes the trivial cases of equality that are allowed to occur in the inequalities of conditions (a) and (b). Hence Theorem 2.4(c) provides an alternate characterization of strict p-negative type when $p > 0$. Namely, a metric space (X, d) has strict p-negative type if and only if the inequality (4) is strict for each normalized (q,t)-simplex $D(\vec{\omega}) = [a_j(m_j); b_i(n_i)]_{q,t}$ in X. (This statement is a new theorem in its own right. The proof is immediate from the equality (5) derived in the proof of Theorem 2.4.) We will use this result frequently and with little further comment.

Motivated by the above inequalities (4) in the particular case $p = 1$, we now introduce two parameters $\gamma_D(\vec{\omega})$ and Γ_X that are designed to "quantify the degree of strictness" of the (strict) 1-negative type inequalities. We will see that these "gap" parameters are particularly meaningful in the context of finite metric spaces, and especially so for finite metric trees. The two relevant definitions are as follows.

Definition 2.6. Let (X, d) be a metric space. Let q, t be natural numbers. Let $D = [a_j; b_i]_{q,t}$ be a (q, t)-simplex in X. Let $N_{q,t} \subset \mathbb{R}_+^{q+t}$ denote the set of all normalized load vectors $\vec{\omega} = (m_1, \dots, m_q, n_1, \dots, n_t)$ for D. Then, the 1-*negative type simplex gap* of D is the function $\gamma_D : N_{q,t} \to \mathbb{R}$: $\vec{\omega} \mapsto \gamma_D(\vec{\omega})$, where

$$\gamma_D(\vec{\omega}) = \sum_{j,i=1}^{q,t} m_j n_i d(a_j, b_i) - \sum_{1 \leqslant j_1 < j_2 \leqslant q} m_{j_1} m_{j_2} d(a_{j_1}, a_{j_2}) - \sum_{1 \leqslant i_1 < i_2 \leqslant t} n_{i_1} n_{i_2} d(b_{i_1}, b_{i_2}),$$

for each $\vec{\omega} = (m_1, \dots, m_q, n_1, \dots, n_t) \in N_{q,t}$. If we further define the quantities

$$\mathfrak{R}_D(\vec{\omega}) = \sum_{j,i=1}^{q,t} m_j n_i d(a_j, b_i), \quad \text{and}$$

$$\mathfrak{L}_D(\vec{\omega}) = \sum_{1 \leqslant j_1 < j_2 \leqslant q} m_{j_1} m_{j_2} d(a_{j_1}, a_{j_2}) + \sum_{1 \leqslant i_1 < i_2 \leqslant t} n_{i_1} n_{i_2} d(b_{i_1}, b_{i_2}),$$

then we see that $\gamma_D(\vec{\omega}) = \mathfrak{R}_D(\vec{\omega}) - \mathfrak{L}_D(\vec{\omega})$ is the right hand side of the generalized roundness-1 inequality (4) for the normalized (q, t)-simplex $D(\vec{\omega})$ in X subtract the left-hand side of the same inequality. So, in particular, (X, d) has strict 1-negative type if and only if $\gamma_D(\vec{\omega}) > 0$ for each normalized (q, t)-simplex $D(\vec{\omega})$ in X.

Definition 2.7. Let (X, d) be a metric space with 1-negative type. We define the 1-*negative type gap* of (X, d) to be the non-negative quantity

$$\Gamma_X = \inf_{D(\vec{\omega})} \gamma_D(\vec{\omega})$$

where the infimum is taken over all normalized (q, t)-simplexes $D(\vec{\omega})$ in X.

Notice that if the 1-negative type gap $\Gamma_X > 0$, then (X, d) has strict 1-negative type. Example 2 (given in Section 5) will show that the converse is not true in general. In other words, there exist metric spaces (X, d) with strict 1-negative type and with $\Gamma_X = 0$.

Remark 2.8. More generally, and in the obvious way (again based on (4)), we can define the *p-negative type simplex gap* $\gamma_{D,p} : N_{q,t} \to \mathbb{R}$ and the resulting *p-negative type gap* $\Gamma_{X,p} = \inf \gamma_{D,p}(\vec{\omega})$ for any metric space (X, d) and any $p \geqslant 0$. (So that $\gamma_D = \gamma_{D,1}$ and $\Gamma_X = \Gamma_{X,1}$.) However, for the most part, our primary interest is the case $p = 1$.

We will see in Section 5 that if the 1-negative type gap Γ_X of a finite metric space (X, d) is positive, then there must exist a constant $\zeta > 0$ such that (X, d) has strict p-negative type for all $p \in (1 - \zeta, 1 + \zeta)$. This is done in Theorem 5.1. The proof of this theorem is independent of the following two sections and the interested reader may therefore choose to cut ahead and read it now. Moreover, Theorem 5.1, which pertains to the case $p = 1$, actually holds for any $p > 0$ provided $\Gamma_X > 0$ is replaced by $\Gamma_{X,p} > 0$, and so on. We will return to this point in Section 5.

3. Determining the simplex gap of a finite metric tree

Hjorth et al. [14] have shown that finite metric trees have strict 1-negative type. In relation to Definition 2.7 it therefore makes sense to ask if we can compute the 1-negative type gap Γ_T of an arbitrary finite metric tree (T, d)? The main purpose of these next two sections is to definitively answer this question *positively*. Our culminating result in this direction is Corollary 4.13.

Our point of entry for the above question will be to develop a key formula for the simplex gap evaluation $\gamma_D(\vec{\omega})$ of a normalized (q, t)-simplex $D(\vec{\omega})$ in a finite metric tree (T, d). This is done in Theorem 3.6 and it will eventually allow the exact computation of the 1-negative type gap $\Gamma_T = \inf \gamma_D$ of (T, d). Prior to doing this, however, it is highly germane to review some basic facts and standard notations pertaining to finite metric trees. We will also introduce some concepts and notations that are less standard.

Definition 3.1. A finite metric tree is a finite connected graph T that has no cycles, endowed with an edge weighted path metric d. Terminal vertices in T are called *leaves* or *pendants*. Given vertices $x, y \in T$, the unique shortest path from x to y is called a *geodesic* and is denoted $[x, y]$. In particular, the pair $e = (x, y)$ is an edge in T if and only if the geodesic $[x, y]$ from x to y contains no other vertices of T. If an edge e lies on a geodesic $[x, y]$, we may sometimes write $e \subseteq [x, y]$.

Notation. Given an edge $e = (x, y)$ in a finite metric tree (T, d) we will often find it convenient use the notation $|e| = d(x, y)$ to denote the metric length of the edge.

Definition 3.2. Let (T, d) be a finite metric tree.

(a) If $|e| = 1$ for all edges $e = (x, y)$ in (T, d) we will say that the path metric d is *ordinary* or *unweighted*.
(b) More generally, if $|e| \neq 1$ for at least one edge $e = (x, y)$ in (T, d), we will say that the path metric d is *edge weighted*.

Definition 3.3. Given a finite metric tree (T, d) and a set of vertices $V \subseteq T$ we can form the smallest subtree of T that contains all the vertices of V—denoted by T_V—and we can endow it with the natural restriction of the metric d. We will call (T_V, d) the *minimal subtree of* (T, d) *generated by the set of vertices* V. Clearly: if $V = \{v_1, \ldots, v_k\} \subseteq T$ then the minimal subtree T_V consists of all vertices $x \in T$ that lie on some geodesic $[v_i, v_j]$ in T. Of course, the minimal subtree (T_V, d) is a finite metric tree in its own right. Given a subset $V \subseteq T$ it is also clear that $T_V = T$ if and only if V contains all the leaves of T.

The following definition introduces a convention to "orient" the edges in any given tree. This will enable the treatment of edges as ordered pairs in a systematic and unambiguous way. Orientation will play a key rôle in determining the main results of this paper.

Definition 3.4. Let (T, d) be a finite metric tree. By way of convention, we choose and then highlight a fixed leaf $\ell \in T$. This distinguished leaf ℓ is then called the *root* of T. Once the root has been fixed we may make the following definitions.

(a) An edge $e = (x, y)$ in T is (*left/right*) *oriented* if $d(x, \ell) > d(y, \ell)$. In other words, an oriented edge in T is an ordered pair $e = (x, y)$ of adjacent vertices $x, y \in T$ where x is geodesically further from the root ℓ than y. The set of all such oriented edges e in T will be denoted $E(T)$.
(b) A vertex $v \in T$ is to the *left* of an oriented edge $e = (x, y) \in E(T)$ if $d(v, x) < d(v, y)$. If it is also the case that $v \neq x$ then we will say that v is *strictly to the left* of e. The set of all vertices $v \in T$ that are to the left of e will be denoted $L(e)$. And the set of all vertices $v \in T$ that are strictly to the left of e will be denoted $\overline{L}(e)$. Notice that we always have $x \in L(e)$ but it can happen that $\overline{L}(e) = \emptyset$. Alternately, we may think of $L(e)$ as the vertices of the subtree that is rooted at x (oriented as per T).
(c) A vertex $v \in T$ is to the *right* of an oriented edge $e = (x, y) \in E(T)$ if $d(v, y) < d(v, x)$. If it is also the case that $v \neq y$ then we will say that v is *strictly to the right of* e. The set of all vertices $v \in T$ that are to the right of e will be denoted $R(e)$. And the set of all vertices $v \in T$ that are strictly to the right of e will be denoted $\overline{R}(e)$.

Notice that each oriented edge $e \in E(T)$ partitions the vertices of T into a disjoint union $L(e) \cup R(e)$.

Henceforth, whenever we are referring to a particular finite metric tree, it will be understood that a root leaf has been chosen from the outset. So "edges" are now always ordered pairs $e = (x, y)$ with the left vertex x as the first coordinate and the right vertex y as the second coordinate. In particular, orientation affords the following compact notation.

Notation. Given an oriented edge $e = (x, y)$ in a finite metric tree (T, d) we may use its unique left vertex x to alternately denote the edge as $e(x)$. Note that, under this scheme, $e(\ell)$ is not defined because the root leaf ℓ is not the left vertex of any oriented edge. All other vertices in T appear (uniquely) as the left vertex of some oriented edge.

Definition 3.5. Let $D = [a_j; b_i]_{q,t}$ be a fixed (q, t)-simplex in a finite metric tree (T, d). Let T_D be the minimal subtree of T generated by the vertices a_j, b_i of D. Orient the edges of T_D by fixing a root leaf $\ell \in T_D$. For each oriented edge $e \in E(T_D)$ and each load vector $\vec{\omega} = (m_1, \ldots, m_q, n_1, \ldots, n_t) \in \mathbb{R}_+^{q+t}$ for D, we define the following *partition sums of* $\vec{\omega}$:

(a) $\alpha_L(\vec{\omega}, e) = \sum_{j \in A_L(e)} m_j$ where $A_L(e) = \{j \in [q]\colon a_j \in L(e)\}$.
(b) $\alpha_R(\vec{\omega}, e) = \sum_{j \in A_R(e)} m_j$ where $A_R(e) = \{j \in [q]\colon a_j \in R(e)\}$.
(c) $\beta_L(\vec{\omega}, e) = \sum_{i \in B_L(e)} n_i$ where $B_L(e) = \{i \in [t]\colon b_i \in L(e)\}$.
(d) $\beta_R(\vec{\omega}, e) = \sum_{i \in B_R(e)} n_i$ where $B_R(e) = \{i \in [t]\colon b_i \in R(e)\}$.

If, in the above definitions, we replace $L(e)$ and $R(e)$ with $\overline{L}(e)$ and $\overline{R}(e)$ (respectively), then we obtain the *strict partition sums of* $\vec{\omega}$: $\bar{\alpha}_L(\vec{\omega}, e)$, $\bar{\alpha}_R(\vec{\omega}, e)$, $\bar{\beta}_L(\vec{\omega}, e)$ and $\bar{\beta}_R(\vec{\omega}, e)$. For example:

(e) $\bar{\alpha}_L(\vec{\omega}, e) = \sum\{m_j\colon a_j \in \overline{L}(e)\}$.
(f) $\bar{\beta}_L(\vec{\omega}, e) = \sum\{n_i\colon b_i \in \overline{L}(e)\}$.

Notice that if the load vector $\vec{\omega}$ is normalized, then we obtain the innocuous looking (but important) identities $\alpha_L(\vec{\omega}, e) + \alpha_R(\vec{\omega}, e) = 1 = \beta_L(\vec{\omega}, e) + \beta_R(\vec{\omega}, e)$.

Notation. In relation to Definition 3.5, if we want to emphasize the (fixed) underlying (q,t)-simplex D, we may sometimes write $\alpha_L(D,\vec{\omega},e)$ in place of $\alpha_L(\vec{\omega},e)$, and so on. (See, for example, Lemma 4.11.)

Theorem 3.6. *Let $D=[a_j;b_i]_{q,t}$ be a given (q,t)-simplex in a finite metric tree (T,d). Let T_D denote the minimal subtree of T generated by the vertices of D. Let $N_{q,t}\subset\mathbb{R}_+^{q+t}$ denote the set of all normalized load vectors for D. Then, for each such normalized load vector $\vec{\omega}=(m_1,\ldots,m_q,n_1,\ldots,n_t)\in N_{q,t}$, the simplex gap evaluation $\gamma_D(\vec{\omega})$ is given by the following formulas*:

$$\gamma_D(\vec{\omega})=\sum_{e\in E(T_D)}\big(\alpha_L(\vec{\omega},e)-\beta_L(\vec{\omega},e)\big)^2\cdot|e|$$
$$=\sum_{e\in E(T_D)}\big(\alpha_R(\vec{\omega},e)-\beta_R(\vec{\omega},e)\big)^2\cdot|e|.$$

In particular it follows that the simplex gap functions $\gamma_D:N_{q,t}\to\mathbb{R}$ are positive valued for all possible (q,t)-simplexes $D\subseteq T$.

Proof. Fix a normalized load vector $\vec{\omega}=(m_1,\ldots,m_q,n_1,\ldots,n_t)$ for the given (q,t)-simplex $D=[a_j;b_i]_{q,t}$. The idea of the proof is to calculate the contribution of each oriented edge $e\in E(T_D)$ to the simplex gap evaluation $\gamma_D(\vec{\omega})$, and then to sum over all such oriented edges.

As per Definition 2.6, $\gamma_D(\vec{\omega})=\mathfrak{R}_D(\vec{\omega})-\mathfrak{L}_D(\vec{\omega})$, where

$$\mathfrak{L}_D(\vec{\omega})=\sum_{1\leqslant j_1<j_2\leqslant q}m_{j_1}m_{j_2}d(a_{j_1},a_{j_2})+\sum_{1\leqslant i_1<i_2\leqslant t}n_{i_1}n_{i_2}d(b_{i_1},b_{i_2}),\quad\text{and}$$
$$\mathfrak{R}_D(\vec{\omega})=\sum_{j,i=1}^{q,t}m_jn_id(a_j,b_i).$$

Notice that if $[x,y]$ is a geodesic in the minimal subtree T_D, then

$$d(x,y)=\sum\big\{|f|:\ f\in E(T_D)\text{ and }f\subseteq[x,y]\big\}.\tag{6}$$

This is because (T_D,d) is a metric tree. Due to the geodesic decompositions (6) we may therefore rewrite the sums $\mathfrak{L}_D(\vec{\omega})$ and $\mathfrak{R}_D(\vec{\omega})$ as

$$\mathfrak{L}_D(\vec{\omega})=\sum_{e\in E(T_D)}\mathfrak{L}_D^{(e)}(\vec{\omega})\cdot|e|,\quad\text{and}\quad\mathfrak{R}_D(\vec{\omega})=\sum_{e\in E(T_D)}\mathfrak{R}_D^{(e)}(\vec{\omega})\cdot|e|,$$

where the coefficients $\mathfrak{L}_D^{(e)}(\vec{\omega})$ and $\mathfrak{R}_D^{(e)}(\vec{\omega})$ are yet to be determined.

Now consider a fixed oriented edge $e\in E(T_D)$. Notice that if the edge e lies on the geodesic $[a_{j_1},a_{j_2}]$ then the term $m_{j_1}m_{j_2}\cdot|e|$ appears in the sum $\mathfrak{L}_D(\vec{\omega})$ (and so on). For this to happen, a_{j_1} must be to the left of e (that is, $j_1\in A_L(e)$) and a_{j_2} must be to the right of e (that is, $j_2\in A_R(e)$) or, vice versa. This and similar such comments, together with the definitions of $\mathfrak{L}_D(\vec{\omega})$ and $\mathfrak{R}_D(\omega)$, imply:

$$\begin{aligned}\mathfrak{L}_D^{(e)}(\vec{\omega}) &= \Bigl(\sum_{j_1 \in A_L(e)} m_{j_1}\Bigr)\Bigl(\sum_{j_2 \in A_R(e)} m_{j_2}\Bigr) + \Bigl(\sum_{i_1 \in B_L(e)} n_{i_1}\Bigr)\Bigl(\sum_{i_2 \in B_R(e)} n_{i_2}\Bigr)\\ &= \alpha_L(\vec{\omega}, e) \cdot \alpha_R(\vec{\omega}, e) + \beta_L(\vec{\omega}, e) \cdot \beta_R(\vec{\omega}, e)\\ &= \alpha_L(\vec{\omega}, e) \cdot \bigl(1 - \alpha_L(\vec{\omega}, e)\bigr) + \beta_L(\vec{\omega}, e) \cdot \bigl(1 - \beta_L(\vec{\omega}, e)\bigr), \quad \text{and}\\ \mathfrak{R}_D^{(e)}(\omega) &= \Bigl(\sum_{j \in A_L(e)} m_j\Bigr)\Bigl(\sum_{i \in B_R(e)} n_i\Bigr) + \Bigl(\sum_{j \in A_R(e)} m_j\Bigr)\Bigl(\sum_{i \in B_L(e)} n_i\Bigr)\\ &= \alpha_L(\vec{\omega}, e) \cdot \beta_R(\vec{\omega}, e) + \alpha_R(\vec{\omega}, e) \cdot \beta_L(\vec{\omega}, e)\\ &= \alpha_L(\vec{\omega}, e) \cdot \bigl(1 - \beta_L(\vec{\omega}, e)\bigr) + \bigl(1 - \alpha_L(\vec{\omega}, e)\bigr) \cdot \beta_L(\vec{\omega}, e).\end{aligned}$$

We can now define $\gamma_D^{(e)}(\vec{\omega})$, the contribution of the oriented edge $e \in E(T_D)$ to the simplex gap evaluation $\gamma_D(\vec{\omega})$, in a natural and obvious way:

$$\gamma_D^{(e)}(\vec{\omega}) = \bigl(\mathfrak{R}_D^{(e)}(\vec{\omega}) - \mathfrak{L}_D^{(e)}(\vec{\omega})\bigr) \cdot |e|.$$

As a result we get the following simplex gap decomposition automatically:

$$\gamma_D(\vec{\omega}) = \mathfrak{R}_D(\vec{\omega}) - \mathfrak{L}_D(\vec{\omega}) = \sum_{e \in E(T_D)} \gamma_D^{(e)}(\vec{\omega}).$$

Setting $\alpha = \alpha_L(\vec{\omega}, e)$ and $\beta = \beta_L(\vec{\omega}, e)$ we see, from the preceding computations, that:

$$\begin{aligned}\gamma_D^{(e)}(\vec{\omega}) &= \bigl(\mathfrak{R}_D^{(e)}(\vec{\omega}) - \mathfrak{L}_D^{(e)}(\vec{\omega})\bigr) \cdot |e|\\ &= \bigl(\alpha \cdot (1 - \beta) + (1 - \alpha) \cdot \beta - \alpha \cdot (1 - \alpha) - \beta \cdot (1 - \beta)\bigr) \cdot |e|\\ &= \bigl(\alpha^2 - 2\alpha\beta + \beta^2\bigr) \cdot |e|\\ &= (\alpha - \beta)^2 \cdot |e|\\ &= \bigl(\alpha_L(\vec{\omega}, e) - \beta_L(\vec{\omega}, e)\bigr)^2 \cdot |e|\\ &= \bigl(\alpha_R(\vec{\omega}, e) - \beta_R(\vec{\omega}, e)\bigr)^2 \cdot |e|.\end{aligned}$$

Now sum $\gamma_D^{(e)}(\vec{\omega})$ over all $e \in E(T_D)$ to get the stated formulas for $\gamma_D(\vec{\omega})$.

If either vertex of an oriented edge e is a leaf in the minimal subtree T_D, then clearly $\gamma_D^{(e)}(\vec{\omega}) > 0$ and hence the simplex gap $\gamma_D(\vec{\omega}) > 0$, establishing the final statement of the theorem. □

Notation. As introduced in the proof of Theorem 3.6, given a normalized (q, t)-simplex $D(\vec{\omega})$ in a finite metric tree (T, d), we will continue to use the notation $\gamma_D^{(e)}(\vec{\omega})$ to denote the contribution of an oriented edge $e \in E(T_D)$ to the simplex gap evaluation $\gamma_D(\vec{\omega})$. So, according to Theorem 3.6, we have the following formulas:

(a) $\gamma_D^{(e)}(\vec{\omega}) = (\alpha_L(\vec{\omega}, e) - \beta_L(\vec{\omega}, e))^2 \cdot |e| = (\alpha_R(\vec{\omega}, e) - \beta_R(\vec{\omega}, e))^2 \cdot |e|$ for each oriented edge $e \in E(T_D)$, and
(b) $\gamma_D(\vec{\omega}) = \sum_{e \in E(T_D)} \gamma_D^{(e)}(\vec{\omega})$.

Remark 2.5, Definition 2.6 and Theorem 3.6 automatically furnish a new and elementary proof of the following result of Hjorth et al. [14].

Corollary 3.7. *Every finite metric tree has strict* 1*-negative type.*

In addition to finite metric trees, Hjorth et al. [15] and Hjorth et al. [14] have elaborated and studied several other classes of finite metric spaces which have strict 1-negative type. These include—under appropriate restrictions—finite metric spaces whose elements have been chosen from a Riemannian manifold (and endowed with the natural inherited distances).

4. Determining the negative type gap of a finite metric tree

In this section we compute the exact value of the 1-negative type gap Γ_T (see Definition 2.7) of a finite metric tree (T, d), and then explore some consequences of this computation. We begin with an upper bound

$$\left\{ \sum_{e \in E(T)} |e|^{-1} \right\}^{-1}$$

for Γ_T that is determined via an algorithm, and then proceed to show that this upper bound is also a lower bound for Γ_T. Isolating the value of Γ_T leads to an entirely new class of inequalities for finite metric trees which may be termed *inequalities of enhanced* 1*-negative type*. These inequalities are developed in Theorems 4.12 and 4.16. Not surprisingly, we need to introduce some more definitions and concepts before computing Γ_T. These are as follows.

Definition 4.1. Let T be a finite tree. Let $\ell \in T$ be the designated root leaf for T. Let d denote the ordinary path metric on T and set

$$k_0 = \max_{x \in T} d(x, \ell).$$

Let k be any integer such that $0 \leqslant k \leqslant k_0$. Then we say that a vertex $v \in T$ is a *level k vertex of T* if $d(v, \ell) = k_0 - k$.

The introduction of levels has the effect of partitioning T into k_0 disjoint sets of vertices.

We will now focus on a particular subclass of normalized (q, t)-simplexes $D(\vec{\omega})$ that turn out to be pivotal in the determination of the 1-negative type gap Γ_T of a finite metric tree (T, d). The condition we introduce depends only upon the underlying tree T and the vertices of D. The path metric d on T and the normalized load vectors $\vec{\omega}$ for D play no (immediate) rôle. The relevant definition is as follows.

Definition 4.2. Let T be a finite tree. Let D be a (q, t)-simplex in T. Let T_D be the minimal subtree of T generated by the vertices of D. We say that D is *generically labeled* if:

(a) $D = T_D$ as sets (in other words, every vertex of T_D belongs to D), and
(b) for all edges $e = (x, y) \in E(T_D)$, x and y have opposite simplex parity.

Notice that we can restate condition (b) in terms of levels:

(c) For all vertices $x, y \in T_D$, if x is in an even level of T_D and if y is in an odd level of T_D, then x and y have opposite simplex parity.

Remark 4.3. Let T be a finite tree. Suppose T has been oriented via the designation of a root leaf $\ell \in T$. We can always generically label the vertices of T. The easiest way to describe this process is to use levels. Simply assign parity a to all vertices of T that lie in even numbered levels, and parity b to all vertices of T that lie in odd numbered levels. This realizes the whole tree T as a generically labeled (q,t)-simplex with:

(a) $q = |\{x \in T\colon\ x \text{ is in an even numbered level of } T\}|$, and
(b) $t = |\{y \in T\colon\ y \text{ is in an odd numbered level of } T\}|$.

Clearly there is (essentially) only one way to generically label the vertices of T. The only other possible labeling of the vertices of T that is generic is the trivial one whereby we switch all of the parity assignments given above: $a_j \leftrightarrow b_i$. We may therefore refer to *the* generic labeling of the vertices of T.

In short, generic labeling a finite tree T amounts to little more than a 2-coloring of the vertices of T.

Definition 4.4. Let T be a finite tree. Let $\ell \in T$ be the designated root leaf of T. Partition the vertices of T into $k_0 + 1$ levels as per Definition 4.1. Let $D = [a_j; b_i]_{q,t}$ denote the (essentially) unique (q,t)-simplex in T that generically labels the vertices of T as per Remark 4.3. We may assume that the level 0 vertices in T have parity a in the simplex D.

Let k_1 be an arbitrary odd natural number such that $k_1 \leqslant k_0$, and let k_2 be an arbitrary even natural number such that $k_2 \leqslant k_0$. We may denote the level k_1 vertices of T as $b_i^{(k_1)}$ where i ranges over a suitable segment of the natural numbers, and we may denote the level k_2 vertices of T as $a_j^{(k_2)}$ where j ranges over a suitable segment of the natural numbers. This notation allows us to "rewrite" the generically labeled simplex $D = T$ in the form $D = [a_j^{(k_2)}; b_i^{(k_1)}]_{q,t}$.

Now, given $\delta > 0$, we define the following *generic algorithm* that assigns a unique vector $\vec{\omega}_\delta = (m_j^{(k_2)}, n_i^{(k_1)}) \in \mathbb{R}^{q+t}$ to the generically labeled simplex $D = T$.

(a) Set each level 0 weight to be

$$m_j^{(0)} = \frac{\delta}{|e(a_j^{(0)})|}.$$

(b) If $k_1 < k_0$ is odd and if weights have been assigned by the algorithm to all level k vertices of T for all $k < k_1$, then set

$$n_i^{(k_1)} = \alpha_L\big(e\big(b_i^{(k_1)}\big)\big) - \overline{\beta}_L\big(e\big(b_i^{(k_1)}\big)\big) + \frac{\delta}{|e(b_i^{(k_1)})|}$$

for each value of the subscript i.

(c) If $k_2 < k_0$ is even and if weights have been assigned by the algorithm to all level k vertices of T for all $k < k_2$, then set

$$m_j^{(k_2)} = \beta_L\big(e\big(a_j^{(k_2)}\big)\big) - \bar{\alpha}_L\big(e\big(a_j^{(k_2)}\big)\big) + \frac{\delta}{|e(a_j^{(k_2)})|}$$

for each value of the subscript j.

(d) If k_0 is odd, then set

$$n_1^{(k_0)} = 1 - \sum_{\substack{i,k \\ k<k_0}} n_i^{(k)}.$$

(e) If k_0 is even, then set

$$m_1^{(k_0)} = 1 - \sum_{\substack{j,k \\ k<k_0}} m_j^{(k)}.$$

Lemma 4.5. *Let T be a finite tree. Let $\ell \in T$ be the designated root leaf of T. Let $e_\ell = (z, \ell)$ denote the unique oriented edge in $E(T)$ whose right vertex is ℓ. Let $D = [a_j^{(k_2)}; b_i^{(k_1)}]_{q,t}$ denote the* (*essentially*) *unique (q,t)-simplex in T that generically labels the vertices of T.* (*Here, as in Definition* 4.4*, superscripts are being used to denote the level of each vertex in the (q,t)-simplex $D = T$.*) *For each $\delta > 0$, let $\vec{\omega}_\delta = (m_j^{(k_2)}, n_i^{(k_1)}) \in \mathbb{R}^{q+t}$ be the vector assigned to the (q,t)-simplex D by the generic algorithm. Then*:

(a) *$\vec{\omega}_\delta$ is a load vector for the (q,t)-simplex D if and only if*

$$\delta < \Bigg\{ \sum_{e \in E(T) \setminus \{e_\ell\}} |e|^{-1} \Bigg\}^{-1}.$$

(b) *$\vec{\omega}_\delta$ is a normalized load vector for the (q,t)-simplex D if and only if*

$$\delta = \Bigg\{ \sum_{e \in E(T)} |e|^{-1} \Bigg\}^{-1}.$$

Proof. Let $\delta > 0$ be given. For simplicity, and using the notations of Definitions 4.1 and 4.4, we will assume that k_0 is even. (The case where k_0 is odd is entirely similar and is omitted.)

According to the definition of the generic algorithm, only

$$m_1^{(k_0)} = 1 - \sum_{\substack{j,k \\ k<k_0}} m_j^{(k)}$$

is possibly non positive. So $\vec{\omega}_\delta$ is a load vector for D if and only if $m_1^{(k_0)} > 0$. With this in mind, we shall address both parts of the lemma simultaneously. Applying the definition of the generic algorithm repeatedly leads to the following observations.

If we sum $m_j^{(0)}$ for all level zero vertices in T we obtain

$$\sum_j m_j^{(0)} = \delta \cdot \sum_j \bigl|e\bigl(a_j^{(0)}\bigr)\bigr|^{-1}.$$

If we sum $n_i^{(1)}$ for all level one vertices in T we obtain

$$\begin{aligned}\sum_i n_i^{(1)} &= \sum_j m_j^{(0)} + \delta \cdot \sum_i \bigl|e\bigl(b_i^{(1)}\bigr)\bigr|^{-1} \\ &= \delta \cdot \sum_i \bigl|e\bigl(b_i^{(1)}\bigr)\bigr|^{-1} + \delta \cdot \sum_j \bigl|e\bigl(a_j^{(0)}\bigr)\bigr|^{-1},\end{aligned}$$

where the last line follows by the previous computation.

If we sum $m_j^{(2)}$ for all level two vertices we obtain

$$\begin{aligned}\sum_j m_j^{(2)} &= \Bigl\{\sum_i n_i^{(1)} - \sum_j m_j^{(0)}\Bigr\} + \delta \cdot \sum_j \bigl|e\bigl(a_j^{(2)}\bigr)\bigr|^{-1} \\ &= \delta \cdot \sum_i \bigl|e\bigl(b_i^{(1)}\bigr)\bigr|^{-1} + \delta \cdot \sum_j \bigl|e\bigl(a_j^{(2)}\bigr)\bigr|^{-1},\end{aligned}$$

where the last line follows by the previous computation.

We therefore obtain the following recursive formulas by induction:

$$\sum_i n_i^{(k_1)} = \delta \cdot \sum_i \bigl|e\bigl(b_i^{(k_1)}\bigr)\bigr|^{-1} + \delta \cdot \sum_j \bigl|e\bigl(a_j^{(k_1-1)}\bigr)\bigr|^{-1}$$

for all odd natural numbers k_1 such that $k_1 < k_0$, and

$$\sum_j m_j^{(k_2)} = \delta \cdot \sum_j \bigl|e\bigl(a_j^{(k_2)}\bigr)\bigr|^{-1} + \delta \cdot \sum_i \bigl|e\bigl(b_i^{(k_2-1)}\bigr)\bigr|^{-1}$$

for all even natural numbers k_2 such that $0 < k_2 < k_0$. Hence

$$x = \sum_{\substack{j,k \\ k<k_0}} m_j^{(k)} = \delta \cdot \Bigl\{\sum_{e \in E(T)\setminus\{e_\ell\}} |e|^{-1}\Bigr\}.$$

And so

$$1 - x > 0 \quad \text{if and only if} \quad \delta < \Bigl\{\sum_{e \in E(T)\setminus\{e_\ell\}} |e|^{-1}\Bigr\}^{-1},$$

establishing part (a).

Moreover, our recursive formulas show that

$$\sum_{i,k} n_i^{(k)} = \delta \cdot \left\{ \sum_{e \in E(T)} |e|^{-1} \right\}.$$

Therefore $\vec{\omega}_\delta$ is normalized if and only if $\delta = \{\sum_{e \in E(T)} |e|^{-1}\}^{-1}$. □

Theorem 4.6. *Let (T, d) be a finite metric tree. Let Γ_T denote the 1-negative type gap of (T, d). Then*

$$\Gamma_T \leqslant \left\{ \sum_{e \in E(T)} |e|^{-1} \right\}^{-1}.$$

Proof. For any given normalized (q, t)-simplex $D(\vec{\omega})$ in T, the simplex gap evaluation $\gamma_D(\vec{\omega})$ provides an upper bound for Γ_T (by definition).

Let D denote the (essentially) unique (q, t)-simplex in T that generically labels the vertices of T. Let $\vec{\omega}_G$ denote the unique normalized load vector for D that is generated by the generic algorithm. By Lemma 4.5, $\vec{\omega}_G = \vec{\omega}_\delta$ where

$$\delta = \left\{ \sum_{e \in E(T)} |e|^{-1} \right\}^{-1}.$$

Consider the resulting normalized (q, t)-simplex $D(\vec{\omega}_G)$ in T. The generic algorithm is structured so that

$$\left| \alpha_L(\vec{\omega}_G, e) - \beta_L(\vec{\omega}_G, e) \right| = \frac{\delta}{|e|}$$

for all oriented edges $e \in E(T)$.

Hence by Theorem 3.6,

$$\gamma_D(\vec{\omega}_G) = \sum_{e \in E(T)} \frac{\delta^2}{|e|^2} \cdot |e| = \delta^2 \cdot \sum_{e \in E(T)} |e|^{-1} = \delta^2 \cdot \delta^{-1} = \left\{ \sum_{e \in E(T)} |e|^{-1} \right\}^{-1}. \qquad \square$$

Theorem 4.6 already gives an indication that the generic algorithm is going to be very important in the context of this paper. We therefore isolate the following natural definition.

Definition 4.7. To say that a finite metric tree (T, d) is *generically labeled and generically weighted* means we are considering the (essentially) unique normalized (q, t)-simplex $D(\vec{\omega}_G)$ in T with the following properties:

(a) $q + t = |T|$,
(b) D is generically labeled, and
(c) $\vec{\omega}_G$ is the unique normalized load vector for D that is generated by the generic algorithm.

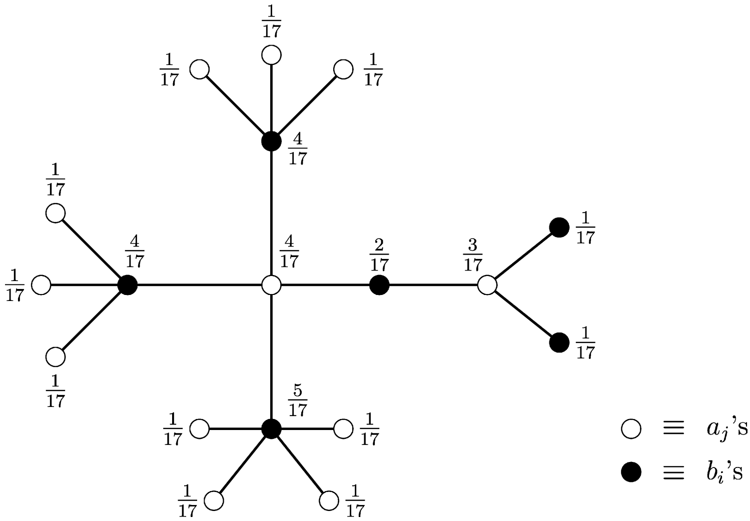

Fig. 1. A generically labeled and generically weighted finite metric tree (endowed with the ordinary path metric).

Fig. 1 gives an example of a generically labeled and generically weighted metric tree.

Suppose $D = [a_j; b_i]_{q,t}$ is a (q,t)-simplex in a finite metric tree (T,d). Currently, the domain of the simplex gap function γ_D is restricted to the surface of normalized load vectors $N_{q,t} \subset \mathbb{R}_+^{q+t}$. We would like to extend the domain of definition of γ_D to all of the open set $\mathbb{R}_+^{q+t}$ in such a way that the extended simplex gap function (which we will denote $\gamma_D^{\times}$) retains an accessible encoding of the geometry of the underlying tree T. We do this by "formally" adapting the formulas of Theorem 3.6.

Definition 4.8. Let (T,d) be a finite metric tree. Let $D = [a_j; b_i]_{q,t}$ be a (q,t)-simplex in T. The *extended simplex gap function* $\gamma_D^{\times} : \mathbb{R}_+^{q+t} \to \mathbb{R}$ is defined as follows:

$$\gamma_D^{\times}(\vec{\omega}) = \sum_{e \in E(T_D)} \left\{ \left(\alpha_L(\vec{\omega}, e) - \beta_L(\vec{\omega}, e)\right)^2 + \left(\alpha_R(\vec{\omega}, e) - \beta_R(\vec{\omega}, e)\right)^2 \right\} \cdot \frac{|e|}{2}$$

for all $\vec{\omega} = (m_1, \ldots, m_q, n_1, \ldots, n_t) \in \mathbb{R}_+^{q+t}$. Notice that we have $\gamma_D^{\times}(\vec{\omega}) = \gamma_D(\vec{\omega})$ for all of the normalized load vectors $\vec{\omega} \in N_{q,t}$ on account of Theorem 3.6.

Notation. In relation to Definition 4.8, given an oriented edge $e \in E(T_D)$, we will denote the "e-term" of the extended gap $\gamma_D^{\times}(\vec{\omega})$ by $\gamma_{D,e}^{\times}(\vec{\omega})$. That is,

$$\gamma_{D,e}^{\times}(\vec{\omega}) = \frac{((\alpha_L(\vec{\omega}, e) - \beta_L(\vec{\omega}, e))^2 + (\alpha_R(\vec{\omega}, e) - \beta_R(\vec{\omega}, e))^2) \cdot |e|}{2}.$$

According to this notation,

$$\gamma_D^{\times}(\vec{\omega}) = \sum_{e \in E(T_D)} \gamma_{D,e}^{\times}(\vec{\omega}) \quad \text{for each } \vec{\omega} \in \mathbb{R}_+^{q+t}.$$

This notation is used in the proof of the next lemma. This lemma points out that provided the (q,t)-simplex D is generically labeled, the partial derivatives of the extended gap function $\gamma_D^\times$ pack together like Russian dolls when constrained to $N_{q,t}$, the surface of normalized load vectors for D. The lemma will help us compute $\min_{\vec{\omega}\in N_{q,t}} \gamma_D^\times(\vec{\omega})$ in this (generically labeled) setting.

Lemma 4.9. *Let (T,d) be a finite metric tree. Let $D=[a_j;b_i]_{q,t}$ be a generically labeled (q,t)-simplex in T. Let $\gamma_D^\times$ denote the extended gap function associated with the (q,t)-simplex D. Then, for all oriented edges $e\in E(T_D)$ and all normalized load vectors $\vec{\omega}\in N_{q,t}$, we have the following relationships*:

(a) *If $e=(a_j,b_i)$, then*

$$\frac{\partial\gamma_D^\times}{\partial m_j}(\vec{\omega}) = 2\big(\alpha_L(\vec{\omega},e)-\beta_L(\vec{\omega},e)\big)\cdot|e| - \frac{\partial\gamma_D^\times}{\partial n_i}(\vec{\omega}).$$

(b) *If $e=(b_i,a_j)$, then*

$$\frac{\partial\gamma_D^\times}{\partial n_i}(\vec{\omega}) = 2\big(\beta_L(\vec{\omega},e)-\alpha_L(\vec{\omega},e)\big)\cdot|e| - \frac{\partial\gamma_D^\times}{\partial m_j}(\vec{\omega}).$$

Proof. The proofs of parts (a) and (b) are very similar, so we will just concentrate on part (a). This requires us to consider a fixed oriented edge $e\in E(T_D)$ of the form $e=(a_j,b_i)$.

Suppose $f\neq e$ is some other oriented edge in the minimal subtree T_D. Then f is either to the left of a_j or to the right of b_i. Let us assume, for arguments sake, that f is to the left of a_j. (The other case is entirely similar.) In this context we have both a_j and b_i on the right of f. That is, $j\in A_R(f)$ and $i\in B_R(f)$. (See Definition 3.5.) Consequently,

$$\frac{\partial\gamma_{D,f}^\times}{\partial m_j}(\vec{\omega}) = \big(\alpha_R(\vec{\omega},f)-\beta_R(\vec{\omega},f)\big)\cdot|f|, \quad \text{and}$$
$$\frac{\partial\gamma_{D,f}^\times}{\partial n_i}(\vec{\omega}) = \big(\beta_R(\vec{\omega},f)-\alpha_R(\vec{\omega},f)\big)\cdot|f|,$$

for all $\vec{\omega}\in\mathbb{R}_+^{q+t}$. By adding these two formulas we see that

$$\left(\frac{\partial}{\partial m_j}+\frac{\partial}{\partial n_i}\right)\gamma_{D,f}^\times(\vec{\omega}) = 0 \tag{7}$$

for all oriented edges $f\neq e$ and all $\vec{\omega}\in\mathbb{R}_+^{q+t}$.

On the other hand, because a_j and b_i are on opposite sides of e, we see that

$$\frac{\partial\gamma_{D,e}^\times}{\partial m_j}(\vec{\omega}) = \big(\alpha_L(\vec{\omega},e)-\beta_L(\vec{\omega},e)\big)\cdot|e|, \quad \text{and}$$
$$\frac{\partial\gamma_{D,e}^\times}{\partial n_i}(\vec{\omega}) = \big(\beta_R(\vec{\omega},e)-\alpha_R(\vec{\omega},e)\big)\cdot|e|,$$

for any $\vec{\omega} \in \mathbb{R}_+^{q+t}$. Therefore

$$\left(\frac{\partial}{\partial m_j} + \frac{\partial}{\partial n_i}\right)\gamma_{D,e}^{\times}(\vec{\omega}) = \big(\big(\alpha_L(\vec{\omega}, e) - \alpha_R(\vec{\omega}, e)\big) + \big(\beta_R(\vec{\omega}, e) - \beta_L(\vec{\omega}, e)\big)\big) \cdot |e|$$

for all $\vec{\omega} \in \mathbb{R}_+^{q+t}$. If, in particular, we evaluate this last formula for a normalized load vector $\vec{\omega} \in N_{q,t}$, then we get the following simplifications:

$$\begin{aligned}\left(\frac{\partial}{\partial m_j} + \frac{\partial}{\partial n_i}\right)\gamma_{D,e}^{\times}(\vec{\omega}) &= \big(\alpha_L(\vec{\omega}, e) - \big(1 - \alpha_L(\vec{\omega}, e)\big)\big) \cdot |e| + \big(\big(1 - \beta_L(\vec{\omega}, e)\big) - \beta_L(\vec{\omega}, e)\big) \cdot |e| \\ &= 2\big(\alpha_L(\vec{\omega}, e) - \beta_L(\vec{\omega}, e)\big) \cdot |e|. \end{aligned} \tag{8}$$

The lemma now follows from Eq. (8), which holds for the oriented edge e on $N_{q,t}$, and equations (7), which hold on $\mathbb{R}_+^{q+t}$ for all oriented edges $f \neq e$, by summing these equations over all such edges. □

Given a generically labeled (q, t)-simplex D in a finite metric tree (T, d) we now show how to minimize the simplex gap $\gamma_D = \gamma_D(\vec{\omega})$ as a function of the normalized load vectors $\vec{\omega} \in N_{q,t}$.

Theorem 4.10. *Let (T, d) be a finite metric tree. Let $D = [a_j; b_i]_{q,t}$ be a generically labeled (q, t)-simplex in T. Let $\gamma_D^{\times}$ denoted the extended gap function associated with the simplex D. Let $N_{q,t} \subset \mathbb{R}_+^{q+t}$ denoted the set of all normalized load vectors for D. Then*

$$\min_{\vec{\omega} \in N_{q,t}} \gamma_D^{\times}(\vec{\omega}) = \left\{\sum_{e \in E(T_D)} |e|^{-1}\right\}^{-1}.$$

In particular, if d is just the ordinary path metric on T (so that $|e| = 1$ for all $e \in E(T_D)$), then we get

$$\min_{\vec{\omega} \in N_{q,t}} \gamma_D^{\times}(\vec{\omega}) = \frac{1}{q + t - 1}.$$

Moreover, in general and in particular, the above minimums are attained if and only if $\vec{\omega} \in N_{q,t}$ is the generic load vector $\vec{\omega}_G$ for D which is assigned by the generic algorithm.

Proof. The idea of the proof is to use Lagrange's (multiplier) theorem on a large scale. In relation to using this theorem, note that the extended gap function $\gamma_D^{\times}$ is defined on an open set (namely, $\mathbb{R}_+^{q+t}$) that contains the constraint surface $N_{q,t}$, which consists of all normalized load vectors for D. We may assume (although it is not strictly necessary) that the level zero vertices of the minimal subtree T_D ($= D$, as sets) all have parity a.

Accordingly, we introduce two Lagrange multipliers λ_1, λ_2 and proceed to solve the system

$$\begin{cases} \dfrac{\partial}{\partial m_j}\left(\gamma_D^{\times}(\vec{\omega}) - \lambda_1 \cdot \displaystyle\sum_{j_1=1}^{q} m_{j_1} - \lambda_2 \cdot \displaystyle\sum_{i_1=1}^{t} n_{i_1}\right) = 0, & 1 \leqslant j \leqslant q, \\ \dfrac{\partial}{\partial n_i}\left(\gamma_D^{\times}(\vec{\omega}) - \lambda_1 \cdot \displaystyle\sum_{j_1=1}^{q} m_{j_1} - \lambda_2 \cdot \displaystyle\sum_{i_1=1}^{t} n_{i_1}\right) = 0, & 1 \leqslant i \leqslant t, \end{cases} \tag{9}$$

subject to the two constraints imposed by the condition $\vec{\omega} \in N_{q,t}$.

Obviously we may rewrite the system of equations (9) as follows:

$$\begin{cases} \dfrac{\partial \gamma_D^{\times}}{\partial m_j}(\vec{\omega}) = \lambda_1, & 1 \leqslant j \leqslant q, \\ \dfrac{\partial \gamma_D^{\times}}{\partial n_i}(\vec{\omega}) = \lambda_2, & 1 \leqslant i \leqslant t, \\ \vec{\omega} \in N_{q,t}. \end{cases} \tag{10}$$

Now consider an arbitrary oriented edge $e \in E(T_D)$. If $e = (a_j, b_i)$ then system (10) in tandem with Lemma 4.9 gives

$$\big(\alpha_L(\vec{\omega}, e) - \beta_L(\vec{\omega}, e)\big) \cdot |e| = \frac{\lambda_1 + \lambda_2}{2}.$$

Recalling that $\alpha_L(\vec{\omega}, e) = \bar{\alpha}_L(\vec{\omega}, e) + m_j$ then gives

$$m_j = \beta_L(\vec{\omega}, e) - \bar{\alpha}_L(\vec{\omega}, e) + \frac{\lambda_1 + \lambda_2}{2|e|}.$$

On the other hand, if $e = (b_i, a_j)$, we (similarly) get

$$n_i = \alpha_L(\vec{\omega}, e) - \bar{\beta}_L(\vec{\omega}, e) + \frac{\lambda_1 + \lambda_2}{2|e|}.$$

Hence the solution vector $\vec{\omega} = (m_1, \ldots, m_q, n_1, \ldots, n_t) \in N_{q,t}$ to system (10) satisfies the generic algorithm of Definition 4.4 with $\delta = (\lambda_1 + \lambda_2)/2$. In particular, by applying Lemma 4.5(b), we conclude that the solution vector $\vec{\omega} \in N_{q,t}$ is uniquely determined and must be the generic load vector $\vec{\omega}_G$ assigned to the (q, t)-simplex D by the generic algorithm. Moreover, by Lemma 4.5(b) and Theorem 3.6, in conjunction with the computation in the latter part of the proof of Theorem 4.6 (with T replaced by T_D in the obvious way), we conclude:

$$\frac{\lambda_1 + \lambda_2}{2} = \delta = \left\{\sum_{e \in E(T_D)} |e|^{-1}\right\}^{-1} = \gamma_D(\vec{\omega}_G).$$

Appealing to Lagrange's (multiplier) theorem completes the proof. □

Let $D(\vec{\omega})$ be a normalized (q, t)-simplex in a finite metric tree and let $T_D \subseteq T$ be the minimal subtree generated by the vertices of D. If D is not generically labeled there are two ways we can prune the minimal subtree T_D that lead (after a finite number of steps) to a generically labeled normalized (q', t')-simplex $D_*(\vec{\omega}_*)$ in a modified finite metric tree (T_*, d) with a smaller simplex gap: $\gamma_D(\vec{\omega}) > \gamma_{D_*}(\vec{\omega}_*)$. These pruning operations are described in Lemma 4.11 and illustrated in Fig. 2.

Lemma 4.11. *Let (T, d) be a finite metric tree. Let $D(\vec{\omega}) = [a_j(m_j); b_i(n_i)]_{q,t}$ be a normalized (q, t)-simplex in T. Let T_D denoted the minimal subtree of T generated by the vertices of D. Suppose $e_* = (x, y)$ is an oriented edge in T_D with one of the following two properties*:

(a) *$x, y \in D$ and x, y have the same simplex parity, or*
(b) *$x \notin D$ or $y \notin D$.*

Form a new normalized (q', t')-simplex $D_*(\vec{\omega}_*)$ and corresponding minimal subtree T_{D_*}—within a modified tree (T_*, d)—by identifying vertex x with vertex y and by adding the simplex weights associated with x and y, if any. (*In other words, to form T_*, delete the oriented edge e_* from T and paste. And so on.*) *Then, recalling the more precise notation introduced after Definition* 3.5, *we have*:

$$\begin{aligned}\gamma_{D_*}(\vec{\omega}_*) &= \gamma_D(\vec{\omega}) - \big(\alpha_L(D, \vec{\omega}, e_*) - \beta_L(D, \vec{\omega}, e_*)\big)^2 \cdot |e_*| \\ &= \sum_{e \in E(T_D)\setminus\{e_*\}} \big(\alpha_L(D, \vec{\omega}, e) - \beta_L(D, \vec{\omega}, e)\big)^2 \cdot |e|.\end{aligned}$$

In particular, we see that $\gamma_D(\vec{\omega}) > \gamma_{D_*}(\vec{\omega}_*)$.

Proof. Assume condition (a) or (b) holds. Let e be an oriented edge in T_D such that $e \neq e_*$. Obviously e is an edge in T_{D_*} too. Moreover, all edges in T_{D_*} arise this way. Checking four simple cases shows that the left (and right) partition sums for e are invariant under the identification $x \equiv y$. That is to say, $\alpha_L(D, \vec{\omega}, e) = \alpha_L(D_*, \vec{\omega}_*, e)$ and $\beta_L(D, \vec{\omega}, e) = \beta_L(D_*, \vec{\omega}_*, e)$. [There are four cases because (a) or (b) might hold and because e is either to the left of x or to the right of y. Whatever the case, when we delete the oriented edge e_*, no simplex weight shifts from the left to the right of e, or vice versa.] So $\gamma_D^{(e)}(\vec{\omega}) = \gamma_{D_*}^{(e)}(\vec{\omega}_*)$. Now apply Theorem 3.6 to get the formulas in the statement of the lemma. □

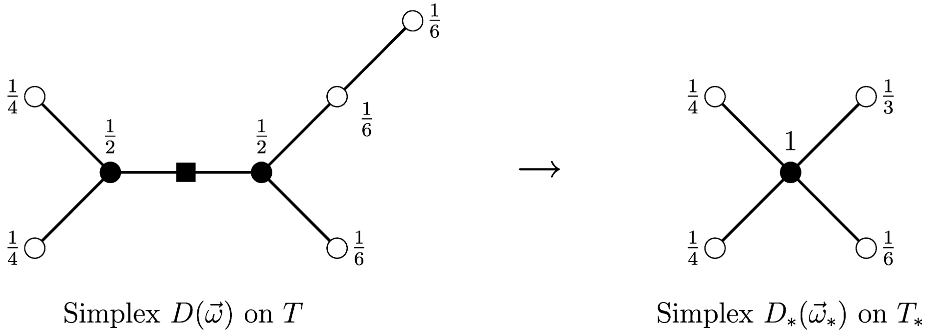

Fig. 2. A three-step reduction to a generically labeled simplex: $\gamma_D > \gamma_{D_*}$.

Theorem 4.12. *Let* (T, d) *be a finite metric tree. For all normalized* (q, t)*-simplexes* $D(\vec{\omega}) = [a_j(m_j); b_i(n_i)]_{q,t}$ *in* T *we have*:

$$\sum_{j_1<j_2} m_{j_1} m_{j_2} d(a_{j_1}, a_{j_2}) + \sum_{i_1<i_2} n_{i_1} n_{i_2} d(b_{i_1}, b_{i_2}) + \left\{ \sum_{e\in E(T)} |e|^{-1} \right\}^{-1} \leqslant \sum_{i,j} m_j n_i d(a_j, b_i). \quad (11)$$

Moreover, we have equality in (11) *if and only if* $D = T$ (*as sets*) *and* D *is both generically labeled and generically weighted.*

Proof. If $D(\vec{\omega})$ is generically labeled, then (11) holds by Theorem 4.10 because

$$\left\{ \sum_{e\in E(T)} |e|^{-1} \right\}^{-1} \leqslant \left\{ \sum_{e\in E(T_D)} |e|^{-1} \right\}^{-1} = \inf_{N_{q,t}} \gamma_D \leqslant \gamma_D(\vec{\omega}).$$

If $D(\vec{\omega})$ is not generically labeled, we may apply Lemma 4.11 a finite number of times to produce a possibly smaller normalized (q', t')-simplex $D_*(\vec{\omega}_*)$ in a modified tree (T_*, d) that is generically labeled and which satisfies (by Lemma 4.11 in the first instance and Theorem 4.10 in the second instance):

$$\gamma_D(\vec{\omega}) > \gamma_{D_*}(\vec{\omega}_*) \geqslant \left\{ \sum_{e\in E(T_{D_*})} |e|^{-1} \right\}^{-1} \geqslant \left\{ \sum_{e\in E(T_D)} |e|^{-1} \right\}^{-1} \geqslant \left\{ \sum_{e\in E(T)} |e|^{-1} \right\}^{-1}.$$

From these two cases—generically labeled, or not—we conclude that (11) holds in general. Moreover, the characterization of equality in (11) is clear from the statement and proof of Theorem 4.10, together with the observation that the minimum

$$\min_{E\subseteq E(T)} \left\{ \sum_{e\in E} |e|^{-1} \right\}^{-1}$$

is uniquely attained when $E = E(T)$. □

As an automatic corollary to Theorem 4.12 we can compute the 1-negative type gap of any finite metric tree *exactly*.

Corollary 4.13. *Let* (T, d) *be a finite metric tree. Let* $\Gamma_T = \inf_{D(\vec{\omega})} \gamma_D(\vec{\omega})$ *denote the* 1*-negative type gap of* (T, d)*. Then*

$$\Gamma_T = \left\{ \sum_{e\in E(T)} |e|^{-1} \right\}^{-1}.$$

Notice that the constant Γ_T in Corollary 4.13 is independent of the internal geometry of the tree T and depends only upon the unordered distribution of the tree's edge weights. By way of analogy, the situation we are encountering in Corollary 4.13 is to be compared to having a box of matches of unequal lengths. No matter how we construct a metric tree T by using all of the matches in the box, we invariably get the same value for the 1-negative type gap Γ_T. The same phenomenon applies to the inequalities (11) of Theorem 4.12: they are independent of the particular finite metric tree's internal geometry. This seems remarkable.

It is also the case that the above formula for Γ_T holds for any countable metric tree (T, d). Simply note that since trees are connected (by definition), the minimal subtree generated by any finite subset of a countable tree T must be finite. This then allows one to invoke Corollary 4.13 and make a simple limiting argument. No proof is therefore necessary for the following corollary.

Corollary 4.14. *Let (T, d) be a countable metric tree. Then the* 1*-negative type gap Γ_T of (T, d) is given by the formula*

$$\Gamma_T = \left\{ \sum_{e \in E(T)} |e|^{-1} \right\}^{-1}$$

where it is understood that Γ_T is taken to be zero if the series in the parentheses diverges.

Corollary 4.14 makes it clear that, given any $\Gamma \geqslant 0$, we can construct a countable metric tree (T, d) whose 1-negative type gap $\Gamma_T = \Gamma$. The simplest way to do this is to consider an internal node, denoted 0, surrounded by countably many leaves, denoted n where $n \in \mathbb{N}$. Using Corollary 4.14 we can then drive the 1-negative type gap of this star with $\aleph_0$ leaves by varying the edge weights $d(0, n)$, $n \in \mathbb{N}$, accordingly. In summary, we have the following.

Corollary 4.15. *For each non-negative real number $\Gamma \geqslant 0$ there exists a countable metric tree (T, d) such that the* 1*-negative type gap Γ_T of (T, d) equals Γ.*

We now return to the context of finite metric trees as they are the primary objects of interest in this paper. In particular, Theorem 4.12 and Corollary 4.13 are seen to be key results of this paper. The inequalities (11) of Theorem 4.12 can be rephrased using Theorem 2.4 as follows.

Theorem 4.16. *Let (T, d) be a finite metric tree. Then for all natural numbers $n \geqslant 2$, all finite subsets $\{x_1, \ldots, x_n\} \subseteq T$, and all choices of real numbers $\eta_1, \ldots, \eta_n$ with $\eta_1 + \cdots + \eta_n = 0$ and $(\eta_1, \ldots, \eta_n) \neq \vec{0}$, we have*

$$\Gamma_T + \sum_{1 \leqslant i, j \leqslant n} d(x_i, x_j)\eta_i \eta_j \leqslant 0 \tag{12}$$

where

$$\Gamma_T = \left\{ \sum_{e \in E(T)} |e|^{-1} \right\}^{-1}.$$

Remark 4.17. Because the constant Γ_T appearing on the left-hand side of (12) is maximal we see that Theorem 4.16 (alternately, Theorem 4.12) provides the *optimal enhancement* of the 1-negative type inequalities for finite metric trees. Moreover, it is clear from the proof of Theorem 2.4 (and, particularly, the equality (5) given in that proof) that one may characterize the case of equality in (12) *directly* in terms of $\{x_1, \ldots, x_n\}$ and $(\eta_1, \ldots, \eta_n)$. Although this characterization is visibly apparent, we leave the precise formulation to the interested reader.

5. Applications of the negative type gap

In this section we determine some applications of the negative type gap of a finite metric space (X, d). The main point is that if $|X| < \infty$ and if the p-negative type gap $\Gamma_{X,p}$ of (X, d) is positive, then (X, d) must have strict s-negative type for some $s > p$. In such a way, the negative type gap provides a new technique for obtaining lower bounds on the maximal p-negative of certain finite metric spaces. We will illustrate this technique in the case of finite metric trees, and then complete this section by constructing some basic examples to make a few final technical points.

This is perhaps a good time to recall that p-negative type holds on closed intervals of the form $[0, \wp]$. Specifically, if (X, d) is a metric space (finite or otherwise), then (X, d) has p-negative type for all p such that $0 \leqslant p \leqslant \wp$, where $\wp = \max\{p_*\colon (X, d) \text{ has } p_*\text{-negative type}\}$. See, for example, Wells and Williams [31].

We mentioned the following theorem at the end of Section 2. The estimate (17) derived in the proof of this theorem is of independent interest and we will refer back to it later in this section.

Theorem 5.1. *Let (X, d) be a finite metric space with $|X| \geqslant 3$. Assume (X, d) has a positive 1-negative type gap $\Gamma_X = \Gamma_{X,1} > 0$. Then there exists an $\zeta > 0$ such that (X, d) has strict p-negative type for all $p \in (1 - \zeta, 1 + \zeta)$. Moreover, ζ may be chosen so that it depends only upon Γ_X and the set of non-zero distances in (X, d).*

Proof. We may assume that the metric d is not a positive multiple of the discrete metric on X. (Otherwise, (X, d) has strict p-negative type for all $p > 0$.) And we will let n denote $|X|$, the cardinality of X (which is assumed to be at least three). Our focus will be on determining the interval $[1, 1 + \zeta)$. (Arguing the interval $(1 - \zeta, 1]$ is entirely similar.)

It is helpful to begin with a simple estimate which will be used later in the proof. Namely, if $b > 1$, $k \in \mathbb{N}$ and $\varepsilon > 0$, then

$$b^{1+\varepsilon} - b < \frac{\Gamma_X}{2k} \quad \text{if and only if} \quad \varepsilon < \frac{\ln(1 + \frac{\Gamma_X}{2kb})}{\ln b}. \tag{13}$$

Let

$$\mathfrak{s} = \min_{x \neq y} d(x, y) \quad \text{and} \quad \mathfrak{w} = \max_{x \neq y} d(x, y)$$

denote the shortest and longest non-zero distances in (X, d). Our opening assumption on d in this proof is that $\mathfrak{s} < \mathfrak{w}$. By scaling (if necessary) we may further assume that $\mathfrak{s} \geqslant 1$.

Consider an arbitrary normalized (q, t)-simplex $D(\vec{\omega}) = [a_j(m_j); b_i(n_i)]_{q,t}$ in X. Note that both $q, t \leqslant n - 1$ because $q + t \leqslant n$. Given $p \geqslant 0$, we will use the following abbreviated notation throughout the remainder of this proof:

$$\mathfrak{L}(p) = \sum_{j_1 < j_2} m_{j_1} m_{j_2} d(a_{j_i}, a_{j_2})^p + \sum_{i_1 < i_2} n_{i_1} n_{i_2} d(b_{i_1}, b_{i_2})^p, \quad \text{and}$$

$$\mathfrak{R}(p) = \sum_{j,i} m_j n_i d(a_j, b_i)^p.$$

Our 1-negative type gap hypothesis on (X, d), applied to the simplex $D(\vec{\omega})$, is therefore:

$$\mathfrak{L}(1) + \Gamma_X \leqslant \mathfrak{R}(1). \tag{14}$$

The overall idea of the proof is to exploit the 1-negative type gap $\Gamma_X > 0$ to show

$$\mathfrak{L}(1+\varepsilon) < \mathfrak{L}(1) + \frac{\Gamma_X}{2} \quad \text{and} \quad \mathfrak{R}(1) - \frac{\Gamma_X}{2} < \mathfrak{R}(1+\varepsilon)$$

provided $\varepsilon > 0$ is sufficiently small. If so, we then have $\mathfrak{L}(1+\varepsilon) < \mathfrak{R}(1+\varepsilon)$ by (14), provided $\varepsilon > 0$ is sufficiently small, and (hence) the theorem follows.

In the current context we have $\mathfrak{R}(1) < \mathfrak{R}(1+\varepsilon) < \mathfrak{R}(1+\varepsilon) + \frac{\Gamma_X}{2}$ for all $\varepsilon > 0$ because all of the non-zero distances in (X, d) are at least one. Moreover, for all $\ell = d(x, y) \neq 0$ and all $\varepsilon > 0$, we have $\ell^{1+\varepsilon} - \ell \leqslant \mathfrak{w}^{1+\varepsilon} - \mathfrak{w}$. This is because (for any fixed $\varepsilon > 0$) the function $f(x) = x^{1+\varepsilon} - x$ increases as x ($\geqslant 1$) increases.

Now, recalling that we need to show that $\mathfrak{L}(1+\varepsilon) < \mathfrak{L}(1) + \frac{\Gamma_X}{2}$ for all sufficiently small $\varepsilon > 0$, observe that we have

$$\begin{aligned}
\mathfrak{L}(1+\varepsilon) - \mathfrak{L}(1) &= \sum_{j_1 < j_2} m_{j_1} m_{j_2} \bigl(d(a_{j_1}, a_{j_2})^{1+\varepsilon} - d(a_{j_1}, a_{j_2})\bigr) \\
&\quad + \sum_{i_1 < i_2} n_{i_1} n_{i_2} \bigl(d(b_{i_1}, b_{i_2})^{1+\varepsilon} - d(b_{i_1}, b_{i_2})\bigr) \\
&\leqslant (n-1)(n-2)\bigl(\mathfrak{w}^{1+\varepsilon} - \mathfrak{w}\bigr)
\end{aligned} \tag{15}$$

on the basis of the preceding comments. And, according to (13), we have:

$$\mathfrak{w}^{1+\varepsilon} - \mathfrak{w} < \frac{\Gamma_X}{2(n-1)(n-2)} \quad \text{iff} \quad \varepsilon < \frac{\ln(1 + \{\frac{\Gamma_X}{2\mathfrak{w}(n-1)(n-2)}\})}{\ln \mathfrak{w}}. \tag{16}$$

If we now set

$$\zeta = \frac{\ln(1 + \{\frac{\Gamma_X}{2\mathfrak{w}(n-1)(n-2)}\})}{\ln \mathfrak{w}}, \tag{17}$$

then it is clear that (15) and (16) establish the theorem. □

Looking at the statement and proof of Theorem 5.1 it is clear that a more general theorem can be formulated. This more general theorem, which we will now state, follows from simple modifications and adaptations of the proof of Theorem 5.1.

Theorem 5.2. *Let (X, d) be a finite metric space with $|X| \geqslant 3$. Let $p_1 \geqslant 0$. If the p_1-negative type gap $\Gamma_{X,p_1} > 0$, then there exists an $\zeta > 0$ such that (X, d) has strict p-negative type for all $p \in (p_1 - \zeta, p_1 + \zeta)$. Moreover, ζ may be chosen so that it depends only upon Γ_{X,p_1} and the set of non zero distances in (X, d). Note, however, that in the case $p_1 = 0$ one must naturally work with the interval $p \in (0, \zeta)$.*

We mentioned in Section 1 that it is not known if the maximal p-negative type of a finite metric space (X, d) can be strict. The following automatic corollary of Theorem 5.2 provides some information on this open question.

Corollary 5.3. *Let (X, d) be a finite metric space with $|X| \geqslant 3$. Let $\wp$ denote the maximal p-negative type of (X, d). If (X, d) has strict $\wp$-negative type, then the $\wp$-negative type gap $\Gamma_{X,\wp}$ of (X, d) must equal to zero.*

Theorem 5.1 and Corollary 4.13 automatically imply the following generalization of Corollary 3.7. Recall that Corollary 3.7 is due to Hjorth et al. [14].

Theorem 5.4. *Let (T, d) be a finite metric tree with $n = |T| \geqslant 3$. Then there exists an $\zeta > 0$ such that (T, d) has strict p-negative type for all $p \in (1 - \zeta, 1 + \zeta)$. Moreover, ζ may be chosen so that it depends only upon the unordered distribution of the tree's edge weights.*

Looking at Theorem 5.4 and referring back to the estimate (17) in the proof of Theorem 5.1, we can extract the following interesting corollary. This corollary gives a lower bound on the maximal p-negative type of any finite tree T endowed with the ordinary path metric. Importantly, these lower bounds depend only on $|T|$.

Corollary 5.5. *Let T be a finite tree with $|T| = n \geqslant 3$. Let $\wp_T$ denote the maximal p-negative type of (T, d). Then*

$$\wp_T \geqslant 1 + \frac{\ln(1 + \frac{1}{(n-1)^3(n-2)})}{\ln(n-1)}.$$

Proof. Simply observe that, in the notation of the proof of Theorem 5.1, we have $\mathfrak{s} = 1$, $\mathfrak{w} \leqslant n - 1$, and that $\Gamma_X = \Gamma_T = 1/(n - 1)$ by Corollary 4.13, so we may apply (17) to obtain the stated lower bound on $\wp_T$. We should point out that in applying (17) in this context we have removed a factor of 2 from the expression for ζ. It is clear that this can always be done in the proof of Theorem 5.1. $\square$

For certain classes of finite metric trees (T, d), such as "stars," it is possible to compute the maximum of all p such that (T, d) has p-negative type. Such examples may then be strung together to form further interesting metric trees (with sometimes pathological properties) such as the "infinite necklace" which is described in Example 2.

Example 1 *(A star with n leaves).* Let $n \geqslant 2$ be a natural number. Let Y_n denote the unique tree with $n + 1$ vertices and n leaves. In other words, Y_n consists of an internal node, which we will denote r_n, surrounded by n leaves. We endow Y_n with the ordinary path metric d. Consequently, there are only two non-zero distances in this tree; 1 & 2. The following theorem computes the maximal p-negative type of Y_n.

Theorem 5.6. *For all natural numbers $n \geqslant 2$, the maximal p-negative type $\wp_n$ of the metric tree (Y_n, d) is given by*

$$\wp_n = 1 + \frac{\ln(1 + \frac{1}{n-1})}{\ln 2}.$$

Proof. Consider a normalized (q,t)-simplex $D = D(\vec{\omega}) = [a_j(m_j); b_i(n_i)]_{q,t}$ in Y_n.

If the internal node $r_n \neq a_j, b_i$ for all j and i then the generalized roundness inequalities (4) become:

$$\sum_{j_1<j_2} m_{j_1}m_{j_2}\cdot 2^p + \sum_{i_1<i_2} n_{i_1}n_{i_2}\cdot 2^p \leqslant \sum_{j,i} m_j n_i \cdot 2^p,$$

and these obviously hold for any $p \geqslant 0$. So we may assume that the internal node r_n of Y_n is represented in the normalized simplex D without any loss of generality. Say, $r_n = b_1$.

Now suppose that $t \geqslant 2$. Form a modified normalized $(q, t-1)$-simplex $D_* = D_*(\vec{\omega}_*)$ in Y_n by replacing the pair $b_1(n_1), b_2(n_2)$ in D with $b_1(n_1+n_2)$. In other words, remove the vertex b_2 from D and add its simplex weight n_2 to that of b_1. Consider an arbitrary $p \geqslant 0$. Let $\Delta_{\mathfrak{L}}$ and $\Delta_{\mathfrak{R}}$ denote the net change in the left-hand and the right-hand sides of the generalized roundness-p inequality (4) when we pass from the modified normalized simplex D_* to the original normalized simplex D. It is not hard to see that

$$\Delta_{\mathfrak{L}} = n_1n_2 + \sum_{2<i\leqslant t} n_2n_i\cdot\big(2^p-1\big) \leqslant n_2(1-n_2)\cdot\big(2^p-1\big), \quad \text{and}$$

$$\Delta_{\mathfrak{R}} = \sum_{j=1}^{q} m_j n_2\cdot\big(2^p-1\big) = n_2\cdot\big(2^p-1\big).$$

Because $\Delta_{\mathfrak{L}} < \Delta_{\mathfrak{R}}$ it follows that if $p \geqslant 0$ satisfies the generalized roundness-p inequality (4) for the modified normalized simplex D_*, then p must also satisfy the generalized roundness-p inequality (4) for the original normalized simplex D. Hence, by applying this rationale a finite number of times (as necessary), we may assume that the normalized simplex D is generically labeled. That is, $t = 1$ and $b_1 = r_n$.

Now consider an arbitrary p for which (Y_n, d) has p-negative type. Referring to our now generically labeled normalized simplex D we see that p must satisfy

$$\sum_{1\leqslant j_1<j_2\leqslant q} m_{j_1}m_{j_2}\cdot 2^p \leqslant \sum_{j=1}^{q} m_j\cdot 1^p = 1.$$

That is,

$$\left(1-\sum_{j=1}^{q} m_j^2\right)\cdot 2^p \leqslant 2.$$

But $\max(1-\sum_{j=1}^{q} m_j^2) = 1-\frac{1}{q}$, which is realized when each weight $m_j = \frac{1}{q}$ (in which case D is also generically weighted), and so p must satisfy $(1-\frac{1}{q})\cdot 2^{p-1} \leqslant 1$. In other words:

$$p \leqslant 1 + \frac{\ln(1+\frac{1}{q-1})}{\ln 2}.$$

The right-hand side of this last expression minimizes when $q = n$ and this implies

$$\wp_n = 1 + \frac{\ln(1 + \frac{1}{n-1})}{\ln 2}. \qquad \square$$

Using Example 1 and Theorem 5.6 we can construct an infinite metric tree that has strict 1-negative type but does not have p-negative for any $p > 1$.

Example 2. We can form an infinite tree Y as follows: for each natural number $n \geqslant 2$ connect Y_n to Y_{n+1} by introducing a new edge which connects the internal node r_n of Y_n to the internal node r_{n+1} of Y_{n+1}. Endow Y with the ordinary path metric d.

Theorem 5.7. *The infinite metric tree (Y, d) described in Example 2 has strict 1-negative type but does not have p-negative type for any $p > 1$. Moreover, the 1-negative type gap $\Gamma_Y = 0$.*

Proof. Each normalized (q, t)-simplex D in (Y, d) spans a minimal subtree T_D of Y which is finite. By Corollary 3.7, (T_D, d) has strict 1-negative type. Therefore (Y, d) has strict 1-negative type.

For all n, (Y_n, d) is a subtree of (Y, d) and by Theorem 5.6 it has maximal p-negative type $\wp_n = 1 + \frac{\ln(1+\frac{1}{n-1})}{\ln 2}$. As $n \to \infty$ we see that $\wp_n \to 1^+$. Hence (Y, d) does not have p-negative type for any $p > 1$. Moreover, $\Gamma_Y = 0$ by Corollary 4.14. $\square$

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