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Asymptotic negative type properties of finite ultrametric spaces



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ABSTRACT

Negative type inequalities arise in the study of embedding properties of metric spaces, but they often reduce to intractable combinatorial problems. In this paper we study more quantitative versions of these inequalities involving the so-called p-negative type gap. In particular, we focus our attention on the class of finite ultrametric spaces which are important in areas such as phylogenetics and data mining. Let (X,d) be a given finite ultrametric space with minimum non-zero distance α . Then the p-negative type gap $\Gamma_X(p)$ of (X,d) is positive for all $p \geq 0$. In this paper we compute the value of the limit

$$\Gamma_X(\infty) := \lim_{p \to \infty} \frac{\Gamma_X(p)}{\alpha^p}.$$

It turns out that this value is positive and it may be given explicitly by an elegant combinatorial formula. This formula allows us to characterize when the ratio $\Gamma_X(p)/\alpha^p$ is a constant independent of p. The determination of $\Gamma_X(\infty)$ also leads to new, asymptotically sharp, families of enhanced p-negative type inequalities for (X,d). Indeed, suppose that $G \in (0,\Gamma_X(\infty))$. Then, for all sufficiently large p, the inequality

$$\frac{G \cdot \alpha^p}{2} \left(\sum_{k=1}^n |\zeta_k| \right)^2 + \sum_{j,i=1}^n d(z_j, z_i)^p \zeta_j \zeta_i \le 0$$

holds for each finite subset $\{z_1, \ldots, z_n\} \subseteq X$, and each scalar *n*-tuple $\zeta = (\zeta_1, \ldots, \zeta_n) \in \mathbb{R}^n$ that satisfies $\zeta_1 + \cdots + \zeta_n = 0$. Notably, these results do not extend to general finite metric spaces.

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1. Introduction and statement of results

Since the early 1990s there has been renewed interest in embedding properties of negative type metrics. One compelling reason for this is a fundamental link to the design of algorithms for cut problems [1,7,2]. The subject of this paper is the important and closely related class of *strict* negative type metrics. The first systematic treatment of strict negative type metrics appears in the elegant papers of Hjorth et al. [14,15]. Informally, a metric space is of strict negative type when all of the non-trivial negative type inequalities for the space are strict. More precisely, we have the following definition.

Definition 1.1. Let $p \geq 0$ and let (X, d) be a metric space.

(a) (X, d) is said to have *p-negative type* if and only if for each integer n > 1, each finite subset $\{z_1, \ldots, z_n\} \subseteq X$, and each scalar *n*-tuple $\boldsymbol{\zeta} = (\zeta_1, \ldots, \zeta_n) \in \mathbb{R}^n$ that satisfies $\zeta_1 + \cdots + \zeta_n = 0$, we have

$$\sum_{j,i=1}^{n} d(z_j, z_i)^p \zeta_j \zeta_i \le 0.$$
 (1.1)

(b) (X, d) is said to have *strict p-negative type* if and only if it has *p*-negative type and the inequalities (1.1) are strict except in the trivial case $\zeta = (0, \dots, 0)$.

The first hints of the negative type conditions may be traced back to an 1841 paper of Cayley [6]. Notably, a metric d on a finite set X is of 2-negative type if and only if (X, d) may be isometrically embedded into some Euclidean space. This is a well-known consequence of Theorem 1 in Schoenberg [24]. Faver et al. [13] modified Schoenberg's proof to show that a metric d on a finite set X is of strict 2-negative type if and only if (X, d) may be isometrically embedded into some Euclidean space as an affinely independent set. There is an analog of this result for infinite metric spaces that is due to Kelleher et al. [18]. Namely, a metric space of infinite cardinality ψ has strict 2-negative type if and only if it is isometric to an affinely independent subset of a real inner product space of Hamel dimension ψ .

By way of an example, given an integer n > 1, Dekster and Wilker [9] have shown that if $(X, d) = (\{x_0, x_1, \ldots, x_n\}, d)$ is an n + 1 point metric space that satisfies the inequality $1 \le d(x_j, x_i) \le v_n$ for all $j \ne i$, where

$$\upsilon_n = \begin{cases} \sqrt{1 + \frac{2n+1}{n^2 - 2}} & \text{if } n \text{ is even} \\ \sqrt{1 + \frac{2}{n-1}} & \text{if } n \text{ is odd,} \end{cases}$$

then (X,d) may be isometrically embedded into $\ell_2^{(n)}$ as an affinely independent set. Thus it follows from the result of Faver et al. [13] that such almost equilateral finite metric spaces have strict 2-negative type.

In more general settings one may simply wish to embed a finite metric space of (strict) p-negative type into a normed space such as L_1 or L_2 with minimal distortion. Being able to do so in the case p=1 has significant implications for the design of approximation algorithms. See, for instance, the papers [1, 7,2]. Lately, ultrametric spaces (or, more specifically, k-hierarchically well-separated trees) have figured prominently in work on embeddings of finite metric spaces. Interesting papers along these lines include Bartal et al. [3,4].

In this paper we examine strict p-negative type properties of finite ultrametric spaces in the limit as $p \to \infty$. Faver et al. [13] have shown that a metric space is ultrametric if and only if it has strict p-negative type for all $p \ge 0$. Doust and Weston [10] introduced a natural way to quantify the degree of strictness of the inequalities (1.1). This notion underpins the present work and may be formulated as follows.

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