Topological k-Metrics

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Abstract

Metric spaces (X, d) are ubiquitous objects in mathematics and computer science that allow for capturing pairwise distance relationships $d(x, y)$ between points $x, y \in X$. Because of this, it is natural to ask what useful generalizations there are of metric spaces for capturing "k-wise distance relationships" $d(x_1, \ldots, x_k)$ among points $x_1, \ldots, x_k \in X$ for $k > 2$. To that end, Gähler (Math. Nachr., 1963) (and perhaps others even earlier) defined *k-metric spaces*, which generalize metric spaces, and most notably generalize the triangle inequality $d(x_1, x_2) \leq d(x_1, y) + d(y, x_2)$ to the "simplex inequality" $d(x_1, \ldots, x_k) \leq \sum_{i=1}^{k} d(x_1, \ldots, x_{i-1}, y, x_{i+1}, \ldots, x_k)$. (The definition holds for any fixed $k \geq 2$, and a 2-metric space is just a (standard) metric space.)

In this work, we introduce *strong k-metric spaces*, k-metric spaces that satisfy a topological condition stronger than the simplex inequality, which makes them "behave nicely." We also introduce *coboundary k-metrics*, which generalize ℓ_p metrics (and in fact all finite metric spaces induced by norms) and *minimum bounding chain k-metrics*, which generalize shortest path metrics (and capture all strong k-metrics). Using these definitions, we prove analogs of a number of fundamental results about embedding finite metric spaces including Fréchet embedding (isometric embedding into ℓ_∞) and isometric embedding of all tree metrics into ℓ_1. We also study relationships between families of (strong) k-metrics, and show that natural quantities, like simplex volume, are strong k-metrics.

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1 Introduction

Metric spaces (X, d) consist of a set of points X and a metric function d that specifies pairwise distances between elements in X. Metric spaces capture and abstract most familiar notions of distance, such as the ℓ_p distance between pairs of points in $\mathbb{R}^m$ and the length of the shortest path between pairs of vertices in a weighted graph. A major line of research has studied *metric embeddings*, which work to relate different families of metrics and classify them according to their "richness." Formally, it seeks to construct isometric or low-distortion embeddings between different families of metric spaces. Well-known examples of such results are Fréchet embedding into ℓ_∞ [13], Bourgain's theorem for embedding into ℓ_1 [5], the Johnson-Lindenstrauss lemma for dimension reduction in ℓ_2 [20], the embeddability of tree metrics into ℓ_1 [24], and Bartal's theorem for embedding into a distribution of tree metrics [3]. See Matoušek [25] for a survey. Besides being inherently mathematically interesting, these results have many applications in computer science, including most notably in the design of approximation algorithms for problems involving flows and cuts, as well as for problems in network design. See, e.g., [2, 22, 3, 21, 1].

Generalizing to larger k. Although metrics capture pairwise distance relationships between points, they do not (directly) capture relationships among more points. Moreover, notions of "distance" that capture such relationships among $k > 2$ points have been studied less extensively, and much less is known about their structural properties and possible applications. In fact, it is not even a priori clear what the right way to generalize metric spaces to $k > 2$ points is. Potentially the most notable and natural generalization of metric spaces is *k-metric spaces*, which were apparently introduced by [17]. [1] (In fact, the definition of k-metrics may have been introduced even earlier, e.g., by Menger [26].) The theory of k-metric spaces is rich (although somewhat disjointed). Indeed, Deza and Rosenberg [8] in their work on the subject state that Gähler created an (apparently unpublished) bibliography of hundreds of works that discuss k-metrics. See also [9]. These k-metric spaces are defined analogously to normal metric spaces, as the following definition makes precise.

Let $k \geq 2$ be an integer, let X be a finite set, and let $d : X^k \to \mathbb{R}$. We call (X, d) a ***k-metric space***, and d a ***k-metric function*** if for any $x_1, \ldots, x_k \in X$:

(1) $d(x_1, \ldots, x_k) \geq 0$.
(2) $d(x_1, \ldots, x_k) = 0$ if and only if the values $x_1, \ldots, x_k$ are not all distinct.
(3) $d(x_1, \ldots, x_k) = d(x_{\pi(1)}, \ldots, x_{\pi(k)})$ for any permutation $\pi : [k] \to [k]$.
(4) $d(x_1, \ldots, x_k) \leq \sum_{i=1}^{k} d(x_1, \ldots, x_{i-1}, y, x_{i+1}, \ldots, x_k)$ for any $y \in X$.

It is straightforward to check that plugging $k = 2$ into the above definition yields the definition of a "standard" metric space, and so k-metrics do in fact capture and generalize metric spaces. Perhaps the most interesting aspect of this definition is its generalization of the triangle inequality $d(x_1, x_2) \leq d(x_1, y) + d(y, x_2)$ to the ***simplex inequality*** $d(x_1, \ldots, x_k) \leq \sum_{i=1}^{k} d(x_1, \ldots, x_{i-1}, y, x_{i+1}, \ldots, x_k)$ in Item 4. However, the condition in the simplex inequality is not the only natural generalization of the triangle inequality, and is not obviously strong enough to prove good analogs of many of the core embedding results for finite metric spaces mentioned above.

Strong k-metric spaces. In this work, we introduce *strong k-metrics*, which replace the simplex inequality (Item 4) in the definition of k-metric spaces with a stronger, topological condition. Furthermore, we introduce strong k-metric analogs of norm metrics (that is, metrics in which $d(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|$ for some norm $\|\cdot\|$) called *coboundary k-metrics*, and of graph shortest path metrics called *minimum bounding chain k-metrics*. We show that these strong k-metric spaces "behave nicely," and have many properties of regular metric spaces, which allows us to prove analogs of a number of well-known embedding results for metric spaces, including Fréchet embedding and isometric embedding of tree metrics into ℓ_1. See Table 2 for a summary and Section 1.1 for a more detailed discussion of these results.

[1] We note that some other work on k-metrics – including [8] and [9], which calls them *m-hemi-metrics* – defines them in an off-by-one way from this work. In this work, the k in k-metric refers to the arity of the function d, whereas in some other works it refers to the dimension k of the simplex spanned by $k + 1$ affinely independent points. I.e., a k-metric space in this work is a $(k - 1)$-metric space in [8, 9], and in particular a (standard) metric space is a 2-metric space in this work but a 1-metric in theirs.

Table 1 Five families of (pseudo) k-metric spaces together with the corresponding family of metric space (i.e., 2-metric space) that they generalize. The family of minimum bounding chain k-metrics is equivalent to the family of strong k-metrics $\mathcal{S}_k$ (analogously to how the family of shortest path metric spaces is equivalent to the family of finite metric spaces).

Symbol	k-metric space	Corresponding (2-)metric space
$\mathcal{W}_k$	Weak k-metrics	Finite metric spaces
$\mathcal{S}_k$	Strong k-metrics	Finite metric spaces
	Minimum bounding chain k-metrics	Shortest path metrics on graphs
$\mathcal{T}_k$	Hypertree k-metrics	Shortest path metrics on trees
$\mathcal{C}_{k,\|\cdot\|}$	Coboundary k-metrics	Norm metric spaces (with $d(\boldsymbol{x},\boldsymbol{y}) = \|\boldsymbol{x}-\boldsymbol{y}\|$)
$\mathcal{V}_k$	$(k-1)$-dimensional volume	Euclidean distance

Table 2 A list of our strong k-metric embedding results and the corresponding results for (standard) metrics that they generalize. The last result concerns embedding ℓ_2 (respectively, $\mathcal{C}_{k,2}$) into ℓ_p (respectively, $\mathcal{C}_{k,p}$) for $p \in [1,\infty)$ with $(1+\varepsilon)$ distortion.

The k-metric generalization	The (2-)metric embedding result
$\mathcal{C}_{k,\infty} = \mathcal{S}_k$	ℓ_∞ metrics contain all finite metrics
$\mathcal{C}_{k,p\neq\infty} \subsetneq \mathcal{S}_k$	$\ell_{p\neq\infty}$ metrics do not contain all finite metrics
$\mathcal{T}_k \subseteq \mathcal{C}_{k,1}$	Any tree metric is an ℓ_1 metric
Dimension reduction in $\mathcal{C}_{k,2}$	Johnson-Lindenstrauss lemma
$\mathcal{C}_{k,2}$ $(1+\varepsilon)$-embeds into $\mathcal{C}_{k,p}$	ℓ_2 $(1+\varepsilon)$-embeds into ℓ_p

Future work and applications. We view this paper as initial work on strong k-metrics, coboundary k-metrics, and minimum bounding chain k-metrics. We hope that this work and further work in the area will result in valuable tools for solving problems in computational topology. For example, our hope is that a strong k-metric analog of Bourgain's theorem [5] would result in a good approximation algorithm for the topological sparsest cut problem [28, 29]. [2] Moreover, a variant of the Bartal tree theorem [3] could be used to solve problems about chains, such as the minimum bounding chain problem [4], via embedding into topological hypertrees.

1.1 Summary of Results and Techniques

In this section, we give a summary of our results and the techniques we use to show them. We refer the interested reader to the full version of this paper cited on the first page. Table 1 and Table 2 give summaries of the notation that we use as well as some of the results in the paper. In this summary, we use standard terminology from algebraic topology and metric geometry. We quickly review some of this terminology, but refer the reader to the full version of this paper for detailed definitions.

1.1.1 Strong k-metrics

Item 4 in the definition of k-metrics is called the ***(weak) simplex inequality***. As motivation for the definition of strong k-metrics, we start by noting that the triangle inequality in "standard" metric spaces actually enforces a stronger structural property than the weak

[2] There is also a more combinatorial generalization of the sparsest cut problem, for which we refer the reader to [14, 15, 16].

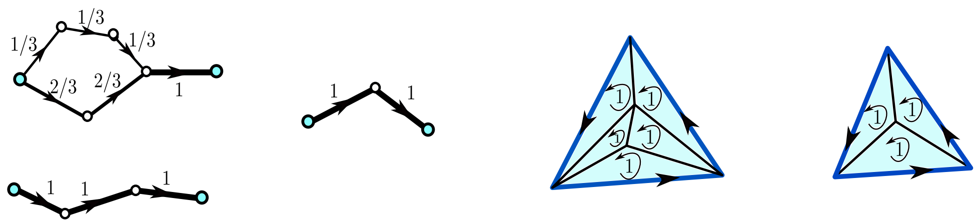

Figure 1 Left: two s, t-flows, the top one splits the unit flow between two paths, the bottom one is just a path. Both are checked by the strong triangle inequality but not the weak one. Middle-left: an s, t-flow that happens to be a path of length two, checked by the strong and weak triangle inequality. Middle-right: a 2-chain whose boundary is the blue triangle, checked by the strong simplex inequality but not the weak one. Right: a simpler 2-chain whose boundary is a the blue triangle, checked by the strong and weak simplex inequality.

simplex inequality does when $k > 2$ in a precise sense. Let (X, d) be a finite (2-)metric space, and let $G = (X, E, d)$ be the complete graph whose edges are weighted according to d (i.e., with edge weights $d(u, v)$ for $(u, v) \in E$). Specifically, we note that for any $s, t \in X$, $d(s, t)$ is at most the cost of any unit (s, t)-flow.

A ***unit*** (s,t)***-flow*** $f : E \to \mathbb{R}$ is a function on (directed) edges of G where (1) the total flow out of the source s is 1, (2) the total flow into the sink t is 1, and (3) flow is conserved at all vertices $v \in V \setminus \{s, t\}$. The ***cost*** of a (unit) (s, t)-flow f is $\sum_{(u,v)\in E} |f(u, v)| \cdot d(u, v)$. An (s, t)-path is captured by the special case of a unit flow where the flow values are binary, i.e., where $f(u, v) \in \{0, 1\}$ for all $u, v \in V$. Thus, $d(s, t)$ being at most the cost of any unit (s, t)-*flow* is a (not necessarily strictly) stronger condition than $d(s, t)$ being at most the length of any (s, t)-*path* in G, which in turn is a (not necessarily strictly) stronger condition than the triangle inequality (which considers paths of length 2). We call the first of these conditions – that $d(s, t)$ is at most the cost of any unit (s, t)-flow – the *strong* triangle inequality. Yet, for (standard) metrics one can show that these three conditions – the strong triangle inequality, that $d(s, t)$ is at most the length of any (s, t)-path, and the (standard) triangle inequality – are all equivalent. Moreover, many metric embedding results crucially rely on this equivalence. However, unfortunately, the analogous equivalence does not hold for k-metrics with $k > 2$.

The strong simplex inequality. We next define a notion of k-metrics that *does* enforce the higher-dimensional analog of the strong triangle inequality, which we call the *strong simplex inequality*. To give this definition, we first need to define the higher-dimensional analog of flows. To do this, we use the language of algebraic topology.

A ***simplicial complex*** K of a point set X is a set of downward-closed subsets of X (i.e., if $Y \in K$ and $Y' \subseteq Y$ then $Y' \in K$). Subsets of X of cardinality i are called $(i-1)$***-simplices*** of K (e.g., vertices are 0-simplices and edges are 1-simplices). We denote the set of all i-simplices of K by K_i. An i***-chain*** α is a real-valued function on the (oriented) i-simplices of K (e.g., flows are 1-chains). Equivalently, one can view i-chains as vectors $\boldsymbol{\alpha} \in \mathbb{R}^{K_i}$, i.e., as real-valued vectors indexed by the $|K_i|$ elements of K_i. [3] [4] We denote the space of all

[3] i-chains are defined on oriented i-simplices t of K, i.e., on i-simplices whose vertices are ordered. However, the value of an i-chain on one orientation of a simplex induces values of the chain on all other orientations of the simplex, and so it suffices to specify the value of an i-chain on an arbitrary orientation of each i-simplex. Because of this, we identify i-chains with $|K_i|$-dimensional vectors and not $(i! \cdot |K_i|)$-dimensional vectors. See the full version for more details.

[4] We will use boldface symbols like $\boldsymbol{\alpha}$ to emphasize that a variable, such as a chain, is a vector.

i-chains in K by $C_i(K)$. We will use $\boldsymbol{e}_t$ for i-simplices $t \subseteq K$ to denote the i-chain that has value 1 on t and value 0 on all other i-simplices (i.e., $\boldsymbol{e}_t \in C_i(K)$ with $\boldsymbol{e}_t[t] = 1$ and $\boldsymbol{e}_t[t'] = 0$ on non-equivalent simplices t').

The ***boundary*** of an i-simplex t is an $(i-1)$-chain that is ± 1 (according to the orientation of t) on all $(i-1)$-faces of t (all subsets of t with cardinality i) and 0 everywhere else. We also extend the definition of boundary from individual simplices to chains by defining the boundary of an i-chain α to be the weighted sum of the boundaries of its simplices. We denote the boundary of $\boldsymbol{\alpha}$ by $\partial_{k-1} \cdot \boldsymbol{\alpha}$, and remark that ∂_{k-1} is a linear operator.

With each k-metric (X, d), we associate a ***complete*** $(k-1)$***-simplicial complex*** K, i.e., the set of all subsets of X with cardinality at most k. We define the *cost* of an $(k-1)$-chain $\boldsymbol{\alpha}$ to be the dot product $|\boldsymbol{\alpha}| \cdot \boldsymbol{d} = \sum_{\tau \in K_i} |\alpha[\tau]| \cdot d(\tau)$, where $|\boldsymbol{\alpha}| := (|\alpha[\tau]|)_{\tau \in K_{k-1}}$ and $\boldsymbol{d} := (d(\tau))_{\tau \in K_{k-1}}$.

See also Figure 1 for examples of unit (s,t)-flows (which are 1-chains) and of 2-chains whose boundaries are three-edge-cycles (i.e., cycles of length three). These help illustrate (chains quantified by) the strong simplex inequality when k is 2 and 3. We now formally present the definition of the *strong simplex inequality* and *strong k-metric spaces*.

Let X be a finite set, and let $d : X^k \to \mathbb{R}$. We call (X, d) a ***strong k-metric space***, and d a ***strong k-metric function*** if any elements $x_1, \ldots, x_k \in X$ satisfy Items 1–3 in the definition of a k-metric space, and the following ***strong simplex inequality***.

4′. Let K be the complete $(k-1)$-dimensional simplicial complex on the vertex set X. Let t be the $(k-1)$-simplex in K with vertices $x_1, \ldots, x_k$, and let $\boldsymbol{\alpha} \in C_{k-1}(K)$ be such that $\partial_{k-1} \cdot \boldsymbol{\alpha} = \partial_{k-1} \cdot \boldsymbol{e}_t$ (i.e., the boundary of the $(k-1)$-chain $\boldsymbol{\alpha}$ is the same as the boundary of $\boldsymbol{e}_t$). Then

$$d(x_1, \ldots, x_k) = d(t) \leq |\boldsymbol{\alpha}| \cdot \boldsymbol{d} = \sum_{\tau \in K_{k-1}} |\boldsymbol{\alpha}[\tau]| \cdot d(\tau) \ ,$$

where $|\boldsymbol{\alpha}| := (|\alpha[\tau]|)_{\tau \in K_{k-1}}$ and $\boldsymbol{d} := (d(\tau))_{\tau \in K_{k-1}}$.

Following standard terminology for metrics, we say that (X, d) is a (strong) ***pseudo*** k-metric if Item 2 is replaced with the weaker property $d(x_1, \ldots, x_k) = 0$ *if* $x_i = x_j$ for any $i \neq j$, and that it is a ***meta*** (strong) k-metric if Item 2 is replaced with the weaker property $d(x_1, \ldots, x_k) = 0$ *only if* $x_i = x_j$ for some $i \neq j$. Following standard practice, we sometimes drop the word "pseudo" and do not differentiate between pseudo and non-pseudo k-metric spaces in what follows.

We use $\mathcal{S}_k$ to denote the family of all strong pseudo k-metric spaces. We use $\mathcal{W}_k$ to denote the family of all pseudo k-metric spaces, which we sometimes call ***weak pseudo k-metric spaces*** for contrast with strong pseudo k-metric spaces. We show that, as the names suggest, the strong simplex inequality is in fact stronger than (at least as tight as) the (weak) simplex inequality and therefore that $\mathcal{S}_k \subseteq \mathcal{W}_k$. We additionally show that $\mathcal{S}_2 = \mathcal{W}_2$ coincides with the family of all finite pseudo metric spaces and therefore strong k-metric spaces generalize (standard) metrics spaces. On the other hand, we show that $\mathcal{S}_k \subsetneq \mathcal{W}_k$ for $k \geq 3$. We also show that it can be verified whether a k-metric space is a strong k-metric space in polynomial time, via solving multiple linear programs.

Similar to graph shortest paths metrics, we can define ***minimum bounding chain k-metrics*** for a given $(k-1)$-simplicial complex with positive weights on its $(k-1)$-simplices, with complete $(k-2)$-skeleton, in which every $(k-2)$-cycle is a boundary cycle. Let K be such a complex with vertex set X. The minimum bounding chain k-metric d, assigns to a simplex $t = (x_1, \ldots, x_k)$ the minimum cost of any $(k-1)$-chain with boundary ∂t. A minimum bounding chain satisfies the strong simplex inequality by its definition, as well as other properties of a strong k-metric. If we allow (non-negatively) weighted $(k-1)$-simplices, then the minimum bounding chain k-metrics can express all (finite) strong k-metrics.

Examples of strong k-metrics. We next give several simple examples of strong (potentially pseudo or meta) k-metrics. An important and intuitive example of a pseudo k-metric space (x, d) is what we call a *volume k-metric* $\mathcal{V}_k$. Specifically, for a finite subset X of m-dimensional Euclidean space ($X \subset \mathbb{R}^m$ for some m), we define $d(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k)$ to be the $(k-1)$-dimensional volume of the convex hull of $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k \in X$, which is a k-simplex. In the special case where $k = 3$, $d(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$ is the area of the triangle spanned by points $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in X$, and we call (X, d) an *area metric.* We focus on studying volume k-metrics (i.e., $\mathcal{V}_k$ metrics) in this paper, where in particular we show that volume k-metrics are strong (pseudo) k-metrics.

The following theorem describes a few other natural examples that satisfy the strong simplex inequality, and some that are strong *meta* k-metrics. See the full version for its proof.

▶ **Theorem 1.** *For any $k \geq 2$, the following four (X, d) pairs satisfy the strong simplex inequality:*

(1) *$X \subset \mathbb{R}^m$, and $d(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k)$ is the maximum length of an edge in the simplex spanned by $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k \in X$.*

(2) *$X \subset \mathbb{R}^m$, and $d(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k)$ is the minimum diameter of a Euclidean ball containing $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k \in X$.*

(3) *$X \subset \mathbb{R}^m$, and $d(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k)$ is the surface area of the simplex spanned by $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k \in X$.* [5]

(4) *$G = (X, E)$ is a graph with positive edge weights, and $d(x_1, \ldots, x_k)$ is the weight of the minimum Steiner tree of $x_1, \ldots, x_k \in X$.*

Moreover, Item 1, Item 2 and Item 4 are meta k-metrics, and Item 3 is a meta 3-metric when $k = 3$.

We note that the $(k-1)$-simplices in the Vietoris–Rips and Čech complexes of X are exactly the k-tuples of distinct points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k \in X$ such that $d(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k) \leq c$ for some constant $c > 0$ with respect to the k-metric functions d defined in Items 1 and 2, respectively. These two simplicial complexes are extensively studied in topological data analysis.

1.1.2 Norms and Coboundary k-metrics

We next introduce *coboundary k-metric spaces*, a family of strong k-metric spaces that generalize (finite) metric spaces induced by norms. (We show that coboundary k-metrics as defined are strong (pseudo) k-metrics in the full version of the paper.) That is, coboundary k-metrics generalize metric spaces (X, d) satisfying $X \subseteq \mathbb{R}^m$ and $d(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|$ for all $\boldsymbol{x}, \boldsymbol{y} \in X$ and some norm $\|\cdot\|$. In particular, coboundary k-metric spaces generalize (finite) ℓ_p spaces. We then discuss how coboundary k-metrics relate to other k-metrics (including other coboundary k-metrics). In particular, we show generalizations of some key embedding results for ℓ_p spaces to coboundary k-metrics.

A ***coboundary k-metric*** (X, d) of dimension m with respect to a given vector norm $\|\cdot\|$ is defined roughly as follows. (See Figure 2 for examples of 2- and 3-coboundary metrics of dimension $m = 2$ with respect to the ℓ_2 norm, and see the full version of the paper for a formal definition.) Let K be the complete $(k-1)$-simplicial complex on vertex set X (i.e., K contains all simplices corresponding to sets of k or fewer points in X), and assign fixed orientations to the $(k-2)$-simplicies in K. Additionally, assign vectors in $\mathbb{R}^m$ to the $(k-2)$-simplices of K. These vectors can be arranged as the rows of a matrix F; in particular, the rows of F are indexed by the $(k-2)$-simplices of K. We also note that the columns

[5] The surface area of the $(k-1)$-simplex K spanned by $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k$ is equal to $\sum_{i=1}^{k} \mathrm{vol}_{k-2}(K \setminus \{\boldsymbol{x}_i\})$, i.e., the sum of the $(k-2)$-dimensional volumes of the faces of K.

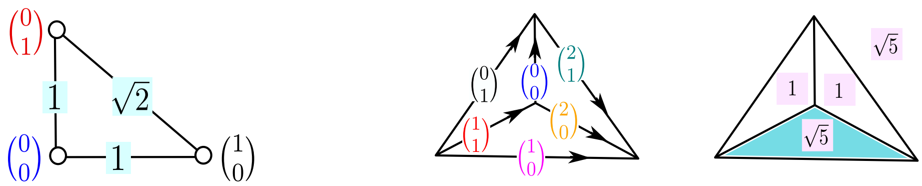

Figure 2 Left: The labeling corresponds to a pair of 0-chains and its implied 2-coboundary metric with the ℓ_2 norm; $F = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}^T$, Right: The labeling corresponds to a pair of 1-chains and its implied 3-metric with ℓ_2 norm, for example, the norm of the shaded triangle is $\left\| \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 2 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right\|_2 = \sqrt{5}$; $F = \begin{pmatrix} 0 & 1 & 0 & 1 & 2 & 2 \\ 1 & 1 & 0 & 0 & 1 & 0 \end{pmatrix}^T$.

of F are $(k-2)$-chains of K. Then, apply the coboundary operator δ_{k-2} (column-wise) to F to obtain $F' := \delta_{k-2}F$, where the rows of F' are indexed by the $(k-1)$-simplices of K. The row of F' indexed by a $(k-1)$-simplex s is a (± 1)-linear combinations of the vectors assigned to the $(k-2)$-faces of s. (The columns of F' are $(k-1)$-chains of K.) Finally, to obtain our metric value on a $(k-1)$-simplex t, we compute the norm of the row of F' that corresponds to t, i.e., set $d(t) = \|\boldsymbol{e}_t^T \cdot F'\| = \|\boldsymbol{e}_t^T \cdot \delta_{k-2} \cdot F\|$ (multiplying by $\boldsymbol{e}_t^T$ is to select the row that corresponds to t).

We remark that coboundary 2-metrics with respect to $\|\cdot\|$ are equivalent to (standard) metrics induced by $\|\cdot\|$. Indeed, as shown in Figure 2, if one labels the vertices $\boldsymbol{v}$ of a complete graph with vectors $\boldsymbol{x}_v \in \mathbb{R}^m$, then the induced coboundary metric d satisfies $d(u,v) = \|\boldsymbol{x}_u - \boldsymbol{x}_v\|$.

We denote the space of all coboundary k-metrics in m dimensions with respect to norm $\|\cdot\|$ by $\mathcal{C}^m_{k,\|\cdot\|}$. We slightly simplify notation for ℓ_p norms and write $\mathcal{C}^m_{k,p}$ for $\mathcal{C}^m_{k,\|\cdot\|_p}$. Furthermore, we define $\mathcal{C}_{k,\|\cdot\|} = \bigcup_{m \in \mathbb{Z}^+} \mathcal{C}^m_{k,\|\cdot\|}$ and $\mathcal{C}_{k,p} = \bigcup_{m \in \mathbb{Z}^+} \mathcal{C}^m_{k,p}$. As noted above, it is straightforward to show that $\mathcal{C}^m_{2,p}$ is the family of (finite) ℓ_p^m metrics in the usual sense, and that, analogously, $\mathcal{C}_{2,p}$ is the family of ℓ_p metrics. So, coboundary k-metrics generalize (standard) metrics induced by norms. There is a wealth of results regarding embeddings from and to different ℓ_p metrics [25]. We attempt to generalize some of these results to our coboundary metrics.

1.1.3 The Power of ℓ_∞

It is well-known that any (finite) metric space is isometrically embedabble into ℓ_∞, via a map that is usually known as the Fréchet embedding. We next describe a generalization of this result that we show for coboundary metrics. Specifically, we show that any strong pseudo k-metric belongs to $\mathcal{C}_{k,\infty}$, and therefore $\mathcal{C}_{k,\infty} = \mathcal{S}_k$).

Fréchet's isometric embedding of finite metric spaces into ℓ_∞ is simple and elegant. We sketch the idea here. Let (X,d) be a finite metric space, and fix $x, x' \in X$. The main idea is that there is an embedding of X into the line ($\mathbb{R}^1$) that (1) does not expand any distance and (2) exactly preserves the distance from x to x'. For example, the embedding that maps each $y \in X$ to $d(x,y)$ has this property. To obtain an isometric embedding of (X,d) with $n := |X|$ into ℓ_∞, one can concatenate the $\binom{n}{2}$ line embeddings corresponding to distinct pairs of elements $x, x' \in X$. [6] Note that each distance is never expanded and is preserved at least once, and so this does in fact give an isometric embedding into ℓ_∞.

[6] In fact, it suffices to use n line embeddings in the Frćhet embedding as each line embedding preserve all distances to a single point. But, we find this embedding (which uses $\binom{n}{2}$ line embeddings) more conducive to generalization to k-metrics.

We follow the outline of the proof above to show that any strong k-metric (X, d) is in $\mathcal{C}^m_{k,\infty}$, where $m = \binom{n}{k}$. First, we construct analogs of the line embeddings used above. Namely, for each k-tuple $t = (x_1, \dots, x_k) \in X^k$ we construct a k-metric ϕ_t in $\mathcal{C}^1_{k,\infty}$ that preserves the value of $d(t)$ and does not increase the value of $d(t')$ for any other such k-tuple t'. Then, we concatenate the $m = \binom{n}{k}$ functions ϕ_t to obtain a k-metric ϕ in $\mathcal{C}^m_{k,\infty}$ that preserves all d values.

While the latter step is straightforward and similar to the case of standard metrics, the former presents a greater challenge as explicit constructions, like the mapping $y \mapsto d(x, y)$ used for standard metrics, are not readily available.

Instead, we show how to obtain such a coboundary k-metric as the solution of a certain (feasible) linear program. To that end, let $t = (x_1, \dots, x_k)$. We will attempt to find a k-metric in $\mathcal{C}^1_{k,\infty} = \mathcal{C}^1_{k,|\cdot|}$ that preserves the value of $d(t)$ and does not expand the d value on other simplices. [7] Equivalently, we look for a $(k-2)$-chain $\boldsymbol{f}$ such that $|\delta_{k-2} \cdot \boldsymbol{f}| \leq \boldsymbol{d}$, i.e., such that $|\delta_{k-2} \cdot \boldsymbol{f}|$ assigns one non-negative value to each $(k-1)$-simplex s that is not larger than $d(s)$, hence not expanding. (Here $|\cdot|$ and $\leq$ are treated element-wise.) On the other hand, we want $\delta_{k-2} \cdot \boldsymbol{f}$ at t to be as large as possible and ideally equal to $d(t)$. So, we try to maximize $\boldsymbol{e}_t^T \cdot \delta_{k-2} \cdot \boldsymbol{f}$ by solving the following linear program with variables $\boldsymbol{f}$ corresponding to the $\binom{n}{k-1}$ many $(k-2)$-simplices.

$$
\begin{aligned}
\max \quad & \boldsymbol{e}_t^T \cdot \delta_{k-2} \cdot \boldsymbol{f} \\
\text{s.t.} \quad & -\boldsymbol{d} \leq \delta_{k-2} \cdot \boldsymbol{f} \leq \boldsymbol{d} \\
& \partial_{k-2} \cdot \boldsymbol{f} = 0 \ .
\end{aligned}
$$

The equality is added for technical reasons. Namely, it ensures that the feasible region of the linear program is bounded while maintaining the same optimal value. We refer the reader to the full version of this paper for details. Because its feasible region is a (bounded) polytope, this linear program has an optimal solution that is a vertex of this polytope. We show that this optimal solution corresponds to a "non-expanding" d, in which $d(t)$ is preserved.

Using the fact that $\delta_{k-2} = \partial_{k-1}^T$, we rewrite the objective function of the linear program as $(\partial_{k-1} \cdot \boldsymbol{e}_t)^T \cdot \boldsymbol{f}$, and the first set of constraints as $-d(\tau) \leq (\partial_\tau \cdot \boldsymbol{e}_\tau)^T \cdot \boldsymbol{f} \leq d(\tau)$ for all $(k-1)$-simplices τ. We let $\{t_1, \dots, t_r\}$ be the simplices whose inequality constraints are tight at the optimal solution $\boldsymbol{f}^*$, and we assume (without loss of generality) that $(\partial_{k-1} \cdot \boldsymbol{e}_{t_i})^T \cdot \boldsymbol{f} = d(t_i)$ for $i \in [r]$. Since $\boldsymbol{f}^*$ is an (optimal) solution to the linear program, the coefficient vector $\partial_{k-1} \cdot \boldsymbol{e}_t$ in the linear program must be in the cone of vectors of the tight constraint. That is, there are non-negative $\beta_1, \dots, \beta_r$ such that,

$$
\partial_{k-1} \cdot \boldsymbol{e}_t = \sum_{i=1}^{r} \beta_i \cdot (\partial_{k-1} \cdot \boldsymbol{e}_{t_i}) = \partial_{k-1} \cdot \left(\sum_{i=1}^{r} \beta_i \boldsymbol{e}_{t_i} \right) \ . \tag{1}
$$

From that, we show

$$
\sum_{i=1}^{r} \beta_i \cdot d(t_i) \geq d(t) \geq (\partial_{k-1} \cdot \boldsymbol{e}_t)^T \boldsymbol{f}^* = \sum_{i=1}^{r} \beta_i \cdot d(t_i).
$$

---

[7] We note that all ℓ_p norms are equivalent in one dimension. I.e., for scalars $x \in \mathbb{R}$ and $p, q \in [1, \infty]$ we have that $\|x\|_p = \|x\|_q = |x|$. Because of this, $\mathcal{C}^1_{k,\infty} = \mathcal{C}^1_{k,|\cdot|}$.

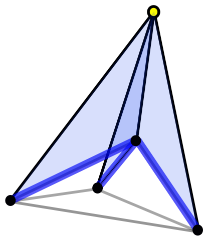

Figure 3 A visualization of apex extension. The initial metric is the coboundary (pseudo) 2-metric induced by the black vertices, which are 0-simplices. It has value one on the bold blue edges and zero on other edges. By including the apex vertex (shown at the top in yellow), this is transformed into a coboundary 3-metric that has value one on the shaded blue triangles and zero on all other triangles.

The first inequality uses the strong simplex inequality (the condition holds by Equation (1)), and the second holds since the coboundary metric induced by $\boldsymbol{f}^*$ is non-expanding. Therefore, we have that $d(t) = (\partial_{k-1} \cdot \boldsymbol{e}_t)^T \boldsymbol{f}^*$, as desired. We also remark that we crucially used the fact that (X, d) was a *strong* (pseudo) k-metric space, which we believe is good motivation for our definition of strong k-metrics.

1.1.4 Other ℓ_p Metrics are Not as Powerful

Other ℓ_p metrics are not as expressive as ℓ_∞. Indeed, for any $p \neq \infty$, there is a finite metric space (X, d) that is not an ℓ_p metric. In this work, we show the analogous result for coboundary metrics. Specifically, we show that for any $p \neq \infty$ there is a strong pseudo k-metric that is not in $\mathcal{C}_{k,p}$.

Apex extension. In order to prove this, we use a simple but powerful technique called *apex extension* for constructing a $(k+1)$-metric space from a k-metric space in such a way that the new space shares certain properties of the original space. Somewhat more specifically, given a k-metric (X, d), apex extension builds a point set X' and a function $d' : (X')^{k+1} \to \mathbb{R}$ such that (X, d) is in $\mathcal{C}_{k,p}$ if and only if (X', d') is in $\mathcal{C}_{k+1,p}$. We can then combine this technique with examples of non-ℓ_p-metric spaces (i.e., examples of finite metric spaces not isometrically embeddable into ℓ_p) to construct strong k-metric spaces that do not belong to $\mathcal{C}_{k,p}$ for all $k \geq 3$. See Figure 3 for an illustration of apex extension.

Let (X, d) be a k-metric, and let a be an element not in X that we call ***apex***. Now, let $X' = X \cup \{a\}$, and let d' be a function on $(k+1)$-tuples of X' defined as follows.

(i) For any $x_1, \ldots, x_{k+1} \in X'$, if $x_1, \ldots, x_{k+1}$ are not distinct or do not include a, $d'(x_1, \ldots, x_{k+1}) = 0$.

(ii) Otherwise, if $x_i = a$ for some i, $d'(x_1, \ldots, x_{k+1}) = d(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_{k+1})$.

We call (X', d') the ***apex extension*** of (X, d). In addition to the fact that (X', d') is a weak $(k+1)$-metric, we show that (X', d') is in $\mathcal{C}_{k+1,\|\cdot\|}$ for any $k \geq 2$ and any norm if any only if (X, d) is in $\mathcal{C}_{k,\|\cdot\|}$. Since $\mathcal{S}_k = \mathcal{C}_{k,\infty}$, the statement above in particular implies that (X', d') is a strong pseudo $(k+1)$-metric if and only if (X, d) is a strong pseudo k-metric. We use this fact to build pseudo k-metrics that are not strong pseudo k-metrics for $k > 3$ from an explicit 3-metric that is not a strong 3-metric.

1.1.5 Other Generalizations of Embedding Results

We also generalize several other well-known results from the study of metric embeddings. First, we give a "meta" result for converting linear norm embedding results to results for coboundary metrics. From this, we get two corollaries: (1) a generalization of the Johnson-Lindenstrauss lemma [20] for dimension reduction in ℓ_2 and (2) a generalization of embedding ℓ_2 into ℓ_p nearly isometrically, which is (a strengthening of a special case of) Dvoretzky's theorem [10, 12]. Specifically, we show any n-point k-metric in $\mathcal{C}_{k,2}^m$ is ε-close to (1) a k-metric $\mathcal{C}_{k,2}^{O(k \log n/\varepsilon^2)}$, and (2) a k-metric in $\mathcal{C}_{k,p}^{m'}$ for $p \in [1, \infty)$ and $m' = \mathrm{poly}(m, n)$.

Second, we show the generalization of the fact that all tree metrics are ℓ_1-metrics (see, e.g., [25, Chapter 1, Exercise 4]). We start by defining a higher-order analog of tree metrics called *hypertree k-metrics*, the family of which we denote by $\mathcal{T}_k$. We then show that $\mathcal{T}_k \subseteq \mathcal{C}_{k,1}$. Hypertree k-metrics are a special case of minimum bounding chain k-metrics where the underlying complex K is a $(k-1)$-hypertree, that is, K does not have any $(k-1)$-cycles and all of its $(k-2)$-cycles are boundaries of $(k-1)$-chains. [8] In particular, 1-trees are "standard" trees from graph theory, i.e., they are acyclic and connected graphs.

1.1.6 Volume k-metrics

We conclude by studying what is likely the most natural generalization of Euclidean distance to k points instead of 2: the $(k-1)$-dimensional volume of the simplex spanned by the k points (i.e., the volume of the convex hull of the points). For points $x_1, \ldots, x_k$, we denote this volume by $\mathrm{vol}_{k-1}(x_1, \ldots, x_k)$. More formally, we study the spaces (X, d) where $X \subsetneq \mathbb{R}^m$ is a finite set and $d : X^k \to \mathbb{R}$ is the function that assigns to each k-tuple $(x_1, \ldots, x_k)$ the $(k-1)$-dimensional volume of the simplex with vertices $x_1, \ldots, x_k$. We denote the family of all such metrics by $\mathcal{V}_k^m$, and the family of all volume k-metrics (in any dimension) by $\mathcal{V}_k = \bigcup_{m \in \mathbb{Z}^+} \mathcal{V}_k^m$.

As volume k-metrics ($\mathcal{V}_k$ spaces) and coboundary k-metrics with respect to the Euclidean norm ($\mathcal{C}_{k,2}$ spaces) are both generalizations of Euclidean distance, it is natural to compare them with each other. To that end, we show that for all $k \geq 3$, $\mathcal{V}_k \subsetneq \mathcal{C}_{k,2}$, and thus coboundary k-metrics are (strictly) richer. (We note that this result stands in contrast to the situation for $k = 2$: $\mathcal{C}_{2,2} = \mathcal{V}_2$.)

We prove that $\mathcal{V}_k \subsetneq \mathcal{C}_{k,2}$ in two parts. First, we show that for any $m \in \mathbb{Z}^+$, $\mathcal{V}_k^m \subseteq \mathcal{C}_{k,2}^{m'}$, where $m' = \binom{m}{k-1}$. Second, we show that for every $k \geq 3$, there exists a k-metric in $C_{2,k}^m$, with $m = \binom{3k-5}{k-1}$ that is not in $\mathcal{V}_k$.

We also complement our second result by showing that there exists a $\mathcal{C}_{3,2}^1$ metric that is not even *approximately* captured by a low-dimensional volume metric. More precisely, we give n-point $\mathcal{C}_{3,2}^1$ spaces that do not embed into $\mathcal{V}_3^m$ spaces with any constant distortion and $m = o(\log n)$ dimensions.

We now summarize the proofs of the first two of these results.

Volume k-metrics are coboundary k-metrics with respect to the ℓ_2 norm. We sketch the proof of $\mathcal{V}_k^m \subseteq \mathcal{C}_{k,2}^{m'}$, $m' = \binom{m}{k-1}$ for the special case of $k = 3$. The Cauchy-Binet theorem implies that the area of any triangle with vertices in $\mathbb{R}^m$ equals the ℓ_2 norm of the vector of the areas of its $\binom{m}{2}$ projections into axis-aligned planes; see the left image in Figure 4 for an illustration of these projections when $m = 3$. This allows us to reduce showing that $\mathcal{V}_3^m \subseteq \mathcal{C}_{3,2}^{m'}$ ($m' = \binom{m}{k-1} = \binom{m}{2}$) to showing that $\mathcal{V}_3^2 \subseteq \mathcal{C}_{3,2}^1 = \mathcal{C}_{3,|\cdot|}^1$.

---

[8] A $(k-1)$-cycle is a non-zero $(k-1)$-chain with no boundary. In particular, 1-cycles are circulations in a graph, i.e., flows that have net value zero on every vertex.

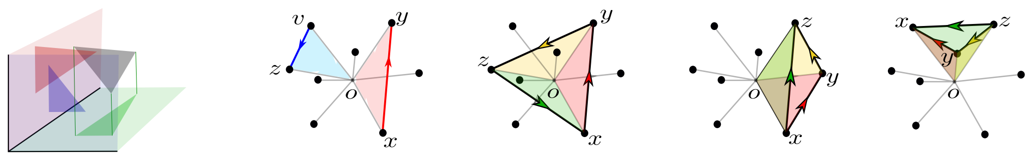

Figure 4 Left: a triangle in $\mathbb{R}^3$ and its projection onto the $\binom{3}{2}$ axis-aligned planes in $\mathbb{R}^3$. Middle-left: $f(x, y)$ equals the area of the red triangle, $f(v, z)$ is the area of the blue triangle, $f(y, x) = -f(x, y)$, and $f(v, z) = -f(z, v)$. Middle: the coboundary 3-metric at (x, y, z) is $f(x, y) + f(y, z) + f(z, x)$, which is the area of the triangle (x, y, z). Middle-right: the coboundary 3-metric at (x, y, z) is $f(x, y) + f(y, z) - f(z, x)$, which is the area of the triangle (x, y, z). Right: the coboundary 3-metric at (x, y, z) is $-f(x, y) - f(y, z) + f(z, x)$, which is the area of the triangle (x, y, z).

To this end, we define the 1-chain f on the edges of the complete 2-complex K with vertex set X as $f(x, x')$ is the signed area of the triangle (o, x, x'), where o is the origin. The *signed area* of a triangle is the area of the triangle times 1 if the (o, x, x') is counter clockwise and -1 otherwise. See the middle-left image in Figure 4 for an example.

We then show that the coboundary 3-metric $|\delta_1 \cdot \boldsymbol{f}|$ is the vector of areas of the triangles, which is what we need (here $|\cdot|$ denotes element-wise absolute value). Specifically, we show the area of any triangle t equals $|\boldsymbol{e}_t^T \cdot \delta_1 \cdot \boldsymbol{f}|$. See the middle, middle-right, and right images of Figure 4 for illustration of different cases.

Not all coboundary k-metrics are volume k-metrics. We next show that for any $k \geq 3$, $\mathcal{C}_{k,2} \nsubseteq \mathcal{V}_k$, by showing an $O(k)$-point, $2^{O(k)}$-dimensional k-coboundary pseudometric with respect to the Euclidean norm that is not a volume k-metric (in particular, $\mathcal{V}_k \subsetneq C_{k,2}$.

For this, we start by showing that for $k \geq 2$, the "all-ones" (discrete) k-metric (X, d) (that assigns a 1 to every k-tuple of distinct points) with $n := |X| = \Omega(k)$ is an example of a high-dimensional volume k-metric (and hence also coboundary k-metric) that is not a $\mathcal{V}_k^{k-1}$ metric.

We then construct $\mathcal{C}_{k,2}$ spaces that are not $\mathcal{V}_k$ spaces for $k \geq 3$ as follows. We start with an all-ones $\mathcal{V}_{k-1}$ space (X, d) that is not a $\mathcal{V}_{k-1}^{k-2}$ space (as described above), and take its apex extension to get a $\mathcal{C}_{k,2}$ space $(X \cup \{a\}, d')$. We then suppose for the sake of contradiction that $(X \cup \{a\}, d')$ is a $\mathcal{V}_k$ space. Specifically, suppose that there exists an embedding $f : (X \cup \{a\}) \to \mathbb{R}^m$ for some m such that $d'(y_1, \ldots, y_k) = \mathrm{vol}_{k-1}(f(y_1), \ldots, f(y_k))$ for all $y_1, \ldots, y_k \in X \cup \{a\}$.

By the definition of apex extension, $d'(x_{i_1}, \ldots, x_{i_k}) = 0$ for any points $x_{i_1}, \ldots, x_{i_k} \in X$, and so $f(X)$ must be contained in a $(k-2)$-dimensional hyperplane H. On the other hand, for any points $x_{i_1}, \ldots, x_{i_{k-1}} \in X$, $d'(x_{i_1}, \ldots, x_{i_{k-1}}, a) = d(x_{i_1}, \ldots, x_{i_{k-1}})$ is proportional to $h \cdot \mathrm{vol}_{k-2}(f(x_{i_1}), \ldots, f(x_{i_{k-1}}))$, where h is the distance between H and $f(a)$. Therefore, $d(x_{i_1}, \ldots, x_{i_{k-1}})$ is also proportional to $\mathrm{vol}_{k-2}(f(x_{i_1}), \ldots, f(x_{i_{k-1}}))$, which, because $f(X) \subset H$, implies that $(X, d) \in \mathcal{V}_{k-1}^{k-2}$. This is a contradiction.

1.2 Related Work

As we have already discussed, prior work on k-metrics is closely related to this work. See, e.g., [17, 18, 8, 9, 27]. We also again note that according to [8], around 1990 Gähler collected a bibliography of over a hundred works related to k-metrics, and it seems that a substantial amount of additional work has been done since then (e.g., [27]). We do not attempt to summarize this extensive body of work, but note that, to the best of our knowledge, none of it has defined or studied our topological (i.e., strong) k-metrics.

Past that, the large body of work on (finite) metric spaces and (algorithmic applications of) metric embeddings is related to this paper. We refer the interested reader to the books and surveys [25, 19, 23] for summaries of this body of work. Indeed, we have provided higher-order analogs of most of the standard concepts in metric spaces, and it will be interesting to see which results on metric embeddings can be adapted to these higher-order analogs and what algorithmic applications these results have.

Additionally, we note two other notions of "higher-order metrics" besides k-metrics. First, we note the work of Feige [11], which defines a notion of "volume" for finite metric spaces in terms of embeddings into Euclidean space and studies volume-preserving embeddings. More specifically, Feige defines the volume of k points in a finite metric space (X, d) to be the maximum volume of the convex hull of their images for any non-expanding embedding f into Euclidean space (i.e., embedding f such that $\|f(x) - f(y)\| \leq d(x, y)$ for all $x, y \in X$). Then, he uses embeddings that (nearly) preserve this notion of volume to design an approximation algorithm for the minimum bandwidth problem. While our work is not directly related to this type of (nearly) volume-preserving embedding, we pose as an open question whether Feige's notion of volume is a (strong) k-metric.

Second, we note the work of Bryant and Tupper [6, 7] on *diversities*. Diversities are spaces (X, d) where d is a function from (finite) subsets $S \subseteq X$ to the non-negative reals that satisfies the "triangle inequality" condition $d(A \cup C) \leq d(A \cup B) + d(B \cup C)$ for all finite subsets $A, B, C \subseteq X$ with B non-empty. They note that the restriction of d to subsets S of size 2 induces a "standard" metric, and so one can view diversities as a different generalization of metrics from (strong) k-metrics. Indeed, we note that diversities are substantially different from (strong) k-metrics. In particular, the d in diversities is defined on sets of elements of different sizes, and the "triangle inequality" in diversities upper bounds a given evaluation of d as the sum of two other evaluations of d (as with the "standard" triangle inequality) as opposed to k other evaluations of d in the (weak) simplex inequality. A primary goal of Bryant and Tupper's work on diversities is to extend graph algorithms based on metric embeddings to hypergraph algorithms based on diversity embeddings. Their definition and techniques indeed seem well-suited to hypergraph problems, however, our definition is better suited to problems in computational topology (i.e., problems on simplicial complexes) like the topological sparsest cut problem and the minimum bounding chain problem.

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