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On a class of metrics related to graph layout problems

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A B S T R A C T

We examine the metrics that arise when a finite set of points is embedded in the real line, in such a way that the distance between each pair of points is at least 1. These metrics are closely related to some other known metrics in the literature, and also to a class of combinatorial optimization problems known as graph layout problems. We prove several results about the structure of these metrics. In particular, it is shown that their convex hull is not closed in general. We then show that certain linear inequalities define facets of the closure of the convex hull. Finally, we characterize the unbounded edges of the convex hull and of its closure.

1. Introduction

For a given positive integer n, let $[n]$ denote $\{1, \ldots, n\}$. A *metric* on $[n]$ is a mapping d: $[n] \times [n] \to \mathbb{R}_+$ which satisfies the following three conditions:

- $d(i, j) = d(j, i)$ for all $\{i, j\} \subset [n]$,
- $d(i, k) + d(j, k) \geqslant d(i, j)$ for all ordered triples $(i, j, k) \subset [n]$,
- $d(i, j) = 0$ if and only if $i = j$.

Metrics are a special case of *semimetrics*, which are obtained by dropping 'and only if' from the third condition. There is a huge literature on metrics and semimetrics; see for example [12]. The inequalities in the second condition are the well-known *triangle inequalities*.

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In this paper we study the metrics d on $[n]$ that arise when n points are embedded in the real line, in such a way that the distance between each pair of points is at least 1. More formally, we require that d satisfies the following two properties:

- there exist real numbers $r_1, \dots, r_n$ such that $d(i,j) = |r_i - r_j|$ for all $\{i,j\} \subset [n]$;
- $d(i,j) \geqslant 1$ for all $\{i,j\} \subset [n]$.

We remark that one could easily replace the value 1 with some arbitrary constant $\epsilon > 0$; the results in this paper would remain essentially unchanged.

We call the metrics in question '$\mathbb{R}$-embeddable 1-separated' metrics. We believe that these metrics are a natural object of study, and of interest in their own right. We have, however, two specific motives for studying them. First, they are closely related to certain well-known metrics that have appeared in the literature. Second, they are also closely related to an important class of combinatorial optimization problems, known as *graph layout problems*.

As well as studying the metrics themselves, we also study their convex hull. It turns out that the convex hull is not always closed, which leads us to study also the closure of the convex hull. Among other things, we characterize some of the $(n-1)$-dimensional faces (i.e., facets) of the closure, and some of the one-dimensional faces (i.e., edges) of both the convex hull and its closure.

The structure of the paper is as follows. In Section 2, we review some of the relevant literature on metrics and graph layout problems. In Section 3, we present various results concerned with the structure of the metrics and their convex hull. Next, in Section 4, we present some inequalities that define facets of the closure of the convex hull. In Section 5, we give a combinatorial characterization of the unbounded edges of the convex hull and of its closure. Finally, some concluding remarks are given in Section 6.

We close this section with a word on notation. To study convex geometric properties, we view metrics as points in a vector space $\mathbb{S}_n^0$. In our notation, $\mathbb{S}_n^0$ will be either the vector space of all symmetric functions $[n] \times [n] \to \mathbb{R}$ or the vector space of all real symmetric $(n \times n)$-matrices whose diagonal entries are zero, and we will switch freely between them. For the latter, the inner product is defined as usual by

$$A \bullet B := \operatorname{tr}(A^\top B) = \sum_{k=1}^{n} \sum_{l=1}^{n} A_{k,l} B_{k,l}.$$

We understand a metric both as a function and a matrix, and we will switch between the two concepts without further mentioning.

By $S(n)$ we denote the set of all permutations of $[n]$. We occasionally view $S(n)$ as a subset of $\mathbb{R}^n$ by identifying the permutation π with the point $(\pi(1), \dots, \pi(n))^\top$. Furthermore we let $\iota_n := (1, \dots, n)$ the identity permutation in $S(n)$. We omit the index n when no confusion can arise. $\mathbf{1}$ is a column vector of appropriate length consisting of ones. Similarly $\mathbf{0}$ is a vector whose entries are all zero. If appropriate, we will use a subscript $\mathbf{1}_k, \mathbf{0}_k$ to identify the length of the vectors. The symbol $\mathbb{0}$ denotes an all-zeros matrix not necessarily square, and we also use it to say "this part of the matrix consists of zeros only." By $\mathbb{1}_n$ we denote the square matrix of order n whose (k,l)-entry is 1 if $k \neq l$ and 0 otherwise. As above we will omit the index n when appropriate. We denote by $\complement U$ the complement of the set U.

2. Literature review

In this section, we review some of the relevant literature. We cover related semimetrics in Section 2.1 and graph layout problems in Section 2.2. To facilitate reading we have summarized all matrix sets discussed in Table 1.

2.1. Some related semimetrics

The following four classes of semimetrics on $[n]$, which are closely related to the $\mathbb{R}$-embeddable 1-separated metrics, have been extensively studied in the literature (see [12] for a detailed survey):

Table 1
Sets of matrices.

CUT_n	ℓ_1-embeddable semimetrics (cut cone)
HYP_n	Hypermetrics, see (1)
NEG_n	Negative-type cone, see (2)
M_n^{L2}	ℓ_2-embeddable semimetrics
M_n^R	$\mathbb{R}$-embeddable semimetrics
M_n^{R1}	$\mathbb{R}$-embeddable 1-separated metrics
Q_n	Convex hull of M_n^{R1}
$\overline{Q_n}$	Closure of Q_n
P_n	Permutation metrics polytope, see (5)

- The ℓ_1-*embeddable* semimetrics, i.e., those for which there exist a positive integer m and points $x_1, \ldots, x_n \in \mathbb{R}^m$ such that $d(i,j) = |x_i - x_j|_1 := \sum_{k=1}^m |x_{ik} - x_{jk}|$ for all $\{i,j\} \subset [n]$.
- The ℓ_2-*embeddable* semimetrics, which are defined as in the ℓ_1 case, except that $d(i,j) = |x_i - x_j|_2 := \sqrt{\sum_{k=1}^m (x_{ik} - x_{jk})^2}$.
- The $\mathbb{R}$-*embeddable* semimetrics, which are the special case of ℓ_1- (or ℓ_2-) embeddable semimetrics obtained when $m = 1$.
- The *hypermetrics*, which are semimetrics that satisfy the following *hypermetric* inequalities [10]:

$$\sum_{\{i,j\} \subset [n]} b_i b_j d(i,j) \leqslant 0 \qquad \left(\forall b \in \mathbb{Z}^n : \sum_{i=1}^n b_i = 1 \right). \tag{1}$$

It is known [4] that the set of ℓ_1-embeddable semimetrics on $[n]$ is a polyhedral cone in $\mathbb{R}^{\binom{n}{2}}$. In fact, it is nothing but the well-known *cut cone*, denoted by CUT_n. The set of all hypermetrics on $[n]$, called the *hypermetric cone* and denoted by HYP_n, is also polyhedral [11].

We will let M_n^{L2} and M_n^R denote the set of ℓ_2- and $\mathbb{R}$-embeddable semimetrics, respectively. It is known that M_n^{L2} and M_n^R are not convex (unless n is small), and that the convex hull of M_n^{L2} and M_n^R is CUT_n. It is also known [21] that a symmetric function d lies in M_n^{L2} if and only if d^2 (i.e., the symmetric function obtained by squaring each value) lies in the so-called *negative-type cone*. The negative-type cone, denoted by NEG_n, is the (non-polyhedral) cone defined by the following *negative-type* inequalities:

$$\sum_{\{i,j\} \subset [n]} b_i b_j d(i,j) \leqslant 0 \qquad \left(\forall b \in \mathbb{R}^n : \sum_{i=1}^n b_i = 0 \right). \tag{2}$$

The structure of M_n^R and related sets is studied in [5].

In recent years, there has been a stream of papers on so-called *negative-type* semimetrics (also known as ℓ_2^2-semimetrics) [2,3,9,16–18]. These are simply semimetrics that lie in NEG_n. They have been used to derive approximation algorithms for various combinatorial optimization problems, including the graph layout problems that we mention in the next section.

The following inclusions are known: $M_n^R \subset M_n^{L2} \subset \mathrm{CUT}_n \subset \mathrm{HYP}_n \subset \mathrm{NEG}_n$. Denoting the set of all $\mathbb{R}$-embeddable 1-separated metrics by M_n^{R1}, we obtain from their definition $M_n^{R1} \subset M_n^R$. We will explore the relationship between M_n^{R1}, M_n^R and CUT_n further in Section 3.1.

2.2. Graph layout problems

Given a graph $G = (V, E)$, with $V = [n]$, a *layout* is simply a permutation of $[n]$. If we view a layout $\pi \in S(n)$ as a placing of the vertices on points $1, \ldots, n$ along the real line, the quantity $|\pi(i) - \pi(j)|$ corresponds to the Euclidean distance between vertices i and j. Several important combinatorial optimization problems, collectively known as *graph layout problems*, call for a layout minimizing a function of these distances (see the survey [13]). For example, in the *Minimum Linear Arrangement*

Problem (MinLA), the objective is to minimize $\sum_{\{i,j\}\in E} |\pi(i) - \pi(j)|$. In the *Bandwidth Problem*, the objective is to minimize $\max_{\{i,j\}\in E} |\pi(i) - \pi(j)|$.

Now, let $d(i,j)$ for $\{i,j\} \subset [n]$ be a decision variable, representing the quantity $|\pi(i) - \pi(j)|$. It has been observed by several authors that interesting relaxations of graph layout problems can be formed by deriving valid linear inequalities that are satisfied by all feasible symmetric functions d. To our knowledge, the first paper of this kind was [19], which presented the following *star* inequalities:

$$\sum_{j\in S} d(i,j) \geqslant \lfloor (|S|+1)^2/4 \rfloor. \tag{3}$$

Here, $i \in [n]$ and $S \subset [n] \setminus \{i\}$ is such that every node in S is adjacent to i.

Apparently independently, Even et al. [14] defined the so-called *spreading metrics*. These are metrics that satisfy the following *spreading* inequalities:

$$\sum_{j\in S} d(i,j) \geqslant |S|\,(|S|+2)/4 \qquad (\forall i \in [n], \forall S \subseteq [n] \setminus \{i\}). \tag{4}$$

Note that the spreading inequalities are more general than the star inequalities, but have a slightly weaker right-hand side when n is odd. Spreading metrics were used in [14,20] to derive approximation algorithms for various graph layout problems.

In [8,15], it was noted that one can get a tighter relaxation of graph layout problems by requiring the spreading metrics to lie in the negative-type cone NEG_n. The authors called the resulting metrics *ℓ_2^2-spreading* metrics.

A natural way to derive further valid linear inequalities for graph layout problems is to study the following *permutation metrics polytope:*

$$P_n = \mathrm{conv}\,\{d\,|\exists \pi \in S(n):\ d(i,j) = |\pi(i) - \pi(j)|\ \ \forall \{i,j\} \subset [n]\}\ . \tag{5}$$

Surprisingly, this was not done until very recently [1]. In [1], it is shown that P_n is of dimension $\binom{n}{2} - 1$ and that its affine hull is defined by the equation $\sum_{\{i,j\}\subset[n]} d(i,j) = \binom{n+1}{3}$. It is also shown that the following four classes of inequalities define facets of P_n under mild conditions:

- *pure hypermetric* inequalities, which are simply the hypermetric inequalities (1) for which $b \in \{0, \pm 1\}^n$;
- *strengthened pure negative-type* inequalities, which are like the negative-type inequalities (2) for which $b \in \{0, \pm 1\}^n$, except that the right-hand side is increased from 0 to $\frac{1}{2}\sum_{i\in[n]} |b_i|$;
- *clique* inequalities, which take the form

  $$\sum_{\{i,j\}\subset S} d(i,j) \geqslant \binom{|S|+1}{3}, \tag{6}$$

  where $S \subset [n]$ satisfies $2 \leqslant |S| < n$;
- *strengthened star* inequalities, which take the form

  $$(|S|-1)\sum_{i\in S} d(r,i) - \sum_{\{i,j\}\subset S} d(i,j) \geqslant \left\lfloor (|S|+1)^2(|S|-1)/12 \right\rfloor, \tag{7}$$

  where $r \in V$ and $S \subseteq V \setminus \{r\}$ with $|S| \geqslant 2$.

It is pointed out in the same paper that each star inequality (3) with $|S| \geqslant 2$ is dominated by a clique inequality (6) and a strengthened star inequality (7). Therefore, very few of the star inequalities define facets of P_n.

Finally, we mention that some more valid inequalities were presented recently by Caprara et al. [7]. Some of them were proved to define facets of the *dominant* of P_n, though not of P_n itself.

We will establish an interesting connection between M_n^{R1}, CUT_n and P_n in Section 3.2.

3. On M_n^{R1} and its convex hull

3.1. On M_n^{R1} and related sets

We now study M_n^{R1} and its relationship with M_n^R, P_n and CUT_n. We will find it helpful to recall the definition of a *cut metric*:

Definition 3.1. For a set $U \subset [n]$, we let d_U be the metric which assigns to two points on different sides of the bipartition U, $\complement U$ of $[n]$ a value of 1 and to points on the same side a value of 0.

We will say that the set U *induces* the associated cut metric. In other words, if we let $D_{k,l}(x) := |x_k - x_l|$ for every vector $x \in \mathbb{R}^n$ (and identify, as promised, functions and matrices), then $d_U = D(\chi^U)$. With this notation, CUT_n is the convex cone with apex 0 in $\mathbb{S}_n^0$ generated by the points d_U, i.e.,

$$\mathrm{CUT}_n := \operatorname{cone}\left\{ d_U \;\middle|\; d_U \text{ is the cut metric for } U \subset [n] \right\}.$$

It is known [6] that each cut metric defines an extreme ray of CUT_n.

We will also need the following notation. For a given permutation $\pi \in S(n)$, let N_π be the set of $x \in \mathbb{R}^n$ which satisfy $x_{\pi(i)} \leqslant x_{\pi(i+1)}$ for $i = 1, \ldots, n-1$. Now let $M(\pi)$ denote the set of metrics d for which there exists an $x \in N_\pi$ with $d = D(x)$. Also, for a given π and for $k = 1, \ldots, n-1$, we emphasize that $D(\chi^{\pi^{-1}([k])})$ is the cut metric induced by the set $U = \{\pi^{-1}(1), \ldots, \pi^{-1}(k)\}$. (So, for example, if $n = 4$ and $\pi = \{2, 3, 1, 4\}$, then $D(\chi^{\pi^{-1}([2])})$ is the cut metric induced by the set $\{2, 3\}$.)

We have the following lemma:

Lemma 3.2. *$M(\pi)$ is a polyhedral cone of dimension $n-1$ defined by the $n-1$ cut metrics $D(\chi^{\pi^{-1}([1])}), \ldots, D(\chi^{\pi^{-1}([n-1])})$.*

Proof. Let $d^* \in M(\pi)$ and let $x_1, \ldots, x_n$ be the corresponding points in $\mathbb{R}$. One can check that:

$$d^* = \sum_{k=1}^{n-1} (x_{k+1} - x_k) D(\chi^{\pi^{-1}([k])}).$$

From the definition of $M(\pi)$, we have $x_{k+1} - x_k \geqslant 0$ for $k = 1, \ldots, n-1$. Thus, d^* is a conical combination of the $n-1$ cut metrics mentioned. This shows that $M(\pi)$ is contained in the cone mentioned. The reverse direction is similar. $\square$

This enables us to describe the structure of M_n^R.

Proposition 3.3. *M_n^R is the union of $n!/2$ polyhedral cones, each of dimension $n-1$.*

We define the *antipodal* permutation of $\pi \in S(n)$ by

$$\pi^- := (n+1) \cdot \mathbf{1} - \pi.$$

This is the permutation obtained by reversing π. A swift computation shows that $D(\pi) = D(\pi^-)$.

Proof. From the definitions, we have $M_n^R = \bigcup_{\pi \in S(n)} M(\pi)$. From the above lemma, the set $M(\pi)$ is a polyhedral cone of dimension $n-1$. Now, note that, for any $\pi \in S(n)$, we have $M(\pi) = M(\pi^-)$. Thus, the union can be taken over $n!/2$ permutations, instead of over all permutations. $\square$

We note in passing that every cut metric belongs to $M(\pi)$ for some $\pi \in S(n)$. This explains the well-known fact, mentioned in Section 2.1, that the convex hull of M_n^R is equal to CUT_n.

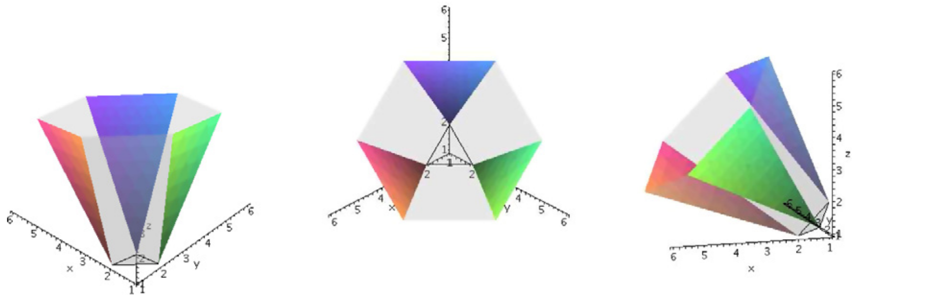

Fig. 1. The convex set Q_3.

Now, we adapt these results to the case of M_n^{R1}. We define $M^1(\pi)$ similar to $M(\pi)$: we denote by $M^1(\pi)$ the set of all metrics d which are of the form $D(x)$ for an $x \in \mathbb{R}^n$ which satisfies $x_{\pi(i)} + 1 \leqslant x_{\pi(i+1)}$ for $i = 1, \ldots, n-1$.

Note that the $D(\pi)$ are nothing but the metrics associated with feasible layouts, which by a result in [1] are the extreme points of P_n. Note also that the sets $M^1(\pi)$ are disjoint.

We have the following lemma:

Lemma 3.4. *$M^1(\pi)$ is the Minkowski sum of the point $D(\pi)$ and the cone $M(\pi)$:*

$$M^1(\pi) = D(\pi) + D(N_\pi).$$

Proof. This can be proven in the same way as Lemma 3.2. The only difference is that we decompose $d^* \in M^1(\pi)$ as:

$$d^* = D(\pi) + \sum_{k=1}^{n-1} (r_{k+1} - r_k - 1) D(\chi^{\pi^{-1}([k])}),$$

and note that $r_{k+1} - r_k - 1 \geqslant 0$ for $k = 1, \ldots, n-1$. $\square$

We can now derive an analog of Proposition 3.3.

Proposition 3.5. *M_n^{R1} is the union of $n!/2$ disjoint translated polyhedral cones, each of dimension $n-1$.*

Proof. From the definitions, we have $M_n^{R1} = \bigcup_{\pi \in S(n)} M^1(\pi)$. From Lemmas 3.2 and 3.4, each set $M^1(\pi)$ is a translated polyhedral cone of dimension $n-1$. As in the proof of Proposition 3.3, the union can be taken over only $n!/2$ permutations. $\square$

3.2. On the convex hull of M_n^{R1} and related sets

We now turn our attention to the convex hull of M_n^{R1}, which we denote by Q_n. To give some intuition, we present in Fig. 1 drawings of M_n^{R1} and Q_3 from three different angles. (Of course, the drawing is truncated, since Q_3 is unbounded.) The three co-ordinates represent $d(1,2)$, $d(1,3)$ and $d(2,3)$. The three coloured regions represent the three disjoint subsets of M_3^{R1} mentioned in Proposition 3.5.

One can see that Q_3 is a three-dimensional polyhedron, with one bounded facet, six unbounded facets, three bounded edges and six unbounded edges.

For $n \leqslant 3$, Q_n is closed (and therefore a polyhedron). We will show in Section 5, however, that Q_n is not closed for $n \geqslant 4$. Therefore, we are led to look at the closure of Q_n, which we denote by $\overline{Q_n}$.

Our next result shows that there is a close connection between the polyhedron $\overline{Q_n}$, the polytope P_n, and the cone CUT_n:

Proposition 3.6. *$\overline{Q_n}$ is the Minkowski sum of P_n and* CUT_n.

Proof. We use the same notation as in the previous section. By definition, every point in M_n^{R1} belongs to $M^1(\pi)$ for some $\pi \in S(n)$. From Lemma 3.4, every point in $M^1(\pi)$ is the sum of the point $D(\pi)$ and a point in the cut cone CUT_n. Moreover, the point $D(\pi)$ is an extreme point of P_n. Thus, every point in M_n^{R1} is the sum of an extreme point of P_n and a point in CUT_n. Since $\overline{Q_n}$ is the closure of the convex hull of M_n^{R1}, it must be contained in the Minkowski sum of P_n and CUT_n. The reverse direction is proved similarly, noting that every cut metric is of the form $D(\chi^{\pi^{-1}([k])})$ for some $\pi \in S(n)$ and some $k \in [n-1]$. $\square$

This immediately implies the following result:

Corollary 3.7. *$\overline{Q_n}$ is full-dimensional (i.e., of dimension $\binom{n}{2}$).*

We also have the following result:

Proposition 3.8. *P_n is the unique bounded facet of $\overline{Q_n}$.*

Proof. As mentioned in the previous section, all points in P_n satisfy the equation $\sum_{\{i,j\}\subset[n]} d(i,j) = \binom{n+1}{3}$. Moreover, every point in CUT_n satisfies $\sum_{\{i,j\}\subset[n]} d(i,j) > 0$. Since $\overline{Q_n}$ is the Minkowski sum of P_n and CUT_n, it follows that the inequality $\sum_{\{i,j\}\subset[n]} d(i,j) \geqslant \binom{n+1}{3}$ is valid for $\overline{Q_n}$ and that P_n is the face of $\overline{Q_n}$ exposed by this inequality. Since $\overline{Q_n}$ and P_n are of dimension $\binom{n}{2}$ and $\binom{n}{2}-1$, respectively, P_n is a facet of $\overline{Q_n}$. It must be the unique bounded facet, since all extreme points of $\overline{Q_n}$ are in P_n. $\square$

In the next section, we will explore the connection between $\overline{Q_n}$, P_n and CUT_n in more detail. To close this section, we make an observation about how the individual 'pieces' of M_n^{R1}, called the $M^1(\pi)$ in the previous section, are positioned within $\overline{Q_n}$:

Proposition 3.9. *For any $\pi \in S(n)$, the set $M^1(\pi)$ is an $(n-1)$-dimensional face of $\overline{Q_n}$.*

Proof. By definition, $\overline{Q_n}$ satisfies all triangle inequalities. Now, without loss of generality, suppose that π is the identity permutation. Every point in $M^1(\pi)$ satisfies all of the following triangle inequalities at equality:

$$d(i,j) + d(j,k) \geqslant d(i,k) \qquad (\forall 1 \leqslant i < j < k \leqslant n).$$

Moreover, no other point in M_n^{R1} does so. Thus, $M^1(\pi)$ is a face of $\overline{Q_n}$. It was shown to be $(n-1)$-dimensional in the previous section. $\square$

4. Inequalities defining facets of $\overline{Q_n}$

In this section, we study linear inequalities that define *facets* of $\overline{Q_n}$, i.e., faces of dimension $\binom{n}{2}-1$. Section 4.1 presents some general results about such inequalities, whereas Section 4.2 lists some specific inequalities.

4.1. General results on facet-defining inequalities

In this section, we prove a structural result about inequalities that define facets of $\overline{Q_n}$, and show how this can be used to construct facets of $\overline{Q_n}$ in a mechanical way from facets of either P_n or CUT_n.

We will need the following definition, taken from [1]:

Definition 4.1 (*1*)**.**

Let $\alpha^T d \geqslant \beta$ be a linear inequality, where $\alpha, d \in \mathbb{R}^{\binom{n}{2}}$. The inequality is said to be 'canonical' if:

$$\min_{\emptyset \neq S \subset [n]} \sum_{i \in S} \sum_{[n] \setminus S} \alpha_{ij} = 0. \tag{8}$$

By definition, an inequality $\alpha^T d \geqslant 0$ defines a proper face of CUT_n if and only if it is canonical. In [1], it is shown that every facet of P_n is defined by a canonical inequality. The following lemma is the analogous result for $\overline{Q_n}$:

Lemma 4.2. *Every unbounded facet of $\overline{Q_n}$ is defined by a canonical inequality.*

Proof. Suppose that the inequality $\alpha^T d \geqslant \beta$ defines an unbounded facet of $\overline{Q_n}$. Since $\overline{Q_n}$ is the Minkowski sum of P_n and CUT_n, the inequality must be valid for CUT_n. Therefore, the left-hand side of (8) must be non-negative. Moreover, since the inequality defines an unbounded facet, there must be at least one extreme ray of CUT_n satisfying $\alpha^T d = 0$. Therefore the left-hand side of (8) cannot be positive. □

We remind the reader that only one facet of $\overline{Q_n}$ is bounded (Proposition 3.8).

Now, we show how to derive facets of $\overline{Q_n}$ from facets of P_n.

Proposition 4.3. *Let F be any facet of P_n, and let $\alpha^T d \geqslant \beta$ be the canonical inequality that defines it. This inequality defines a facet of $\overline{Q_n}$ as well.*

Proof. The fact that the inequality is valid for $\overline{Q_n}$ follows from the fact that $\overline{Q_n}$ is the Minkowski sum of P_n and CUT_n. Now, since F is a facet of P_n, there exist $\binom{n}{2} - 1$ affinely-independent vertices of P_n that satisfy the inequality at equality. Moreover, since the inequality is canonical, there exists at least one extreme ray of CUT_n that satisfies $\alpha^T d = 0$. Since $\overline{Q_n}$ is the Minkowski sum of P_n and CUT_n, there exist $\binom{n}{2}$ affinely-independent points in $\overline{Q_n}$ that satisfy the inequality at equality. Thus, the inequality defines a facet of $\overline{Q_n}$. □

Now, we show how to derive facets of $\overline{Q_n}$ from facets of CUT_n:

Proposition 4.4. *Let $\alpha^T d \geqslant 0$ define a facet of CUT_n, and let β be the minimum of $\alpha^T d$ over all $d \in P_n$. Then the inequality $\alpha^T d \geqslant \beta$ define a facet of $\overline{Q_n}$.*

Proof. As before, the fact that the inequality $\alpha^T d \geqslant \beta$ is valid for $\overline{Q_n}$ follows from the fact that $\overline{Q_n}$ is the Minkowski sum of P_n and CUT_n. Now, since the inequality $\alpha^T d \geqslant 0$ defines a facet of CUT_n, there exist $\binom{n}{2} - 1$ linearly-independent extreme rays of CUT_n that satisfy $\alpha^T d = 0$. Moreover, from the definition of β, there exists at least one extreme point of P_n that satisfies $\alpha^T d = \beta$. Since $\overline{Q_n}$ is the Minkowski sum of P_n and CUT_n, there exist $\binom{n}{2}$ affinely-independent points in $\overline{Q_n}$ that satisfy $\alpha^T d = \beta$. Thus, the inequality $\alpha^T d \geqslant \beta$ defines a facet of $\overline{Q_n}$. □

4.2. Some specific facet-defining inequalities

The results in the previous section enable one to derive a wide variety of facets of $\overline{Q_n}$. In this section, we briefly examine some specific valid inequalities; namely, the inequalities mentioned in [1].

First, we deal with the clique and pure hypermetric inequalities:

Proposition 4.5. *The clique inequalities* (6) *define facets of* $\overline{Q_n}$ *for all* $S \subseteq [n]$ *with* $|S| \geqslant 2$.

Proof. It was shown in [1] that the clique inequalities define facets of P_n when S is a proper subset of $[n]$. In this case, the inequalities are canonical and so, by Proposition 4.3, they define facets of $\overline{Q_n}$ as well. The case $S = [n]$ is covered in the proof of Proposition 3.8. $\square$

Proposition 4.6. *All pure hypermetric inequalities define facets of* $\overline{Q_n}$.

Proof. It was shown in [6] that all pure hypermetric inequalities define facets of CUT_n. It was also shown in [1] that every pure hypermetric inequality is satisfied at equality by at least one extreme point of P_n. The result then follows from Proposition 4.4. $\square$

As for the strengthened pure negative-type and strengthened star inequalities, it was shown in [1] that they define facets of P_n under certain conditions. Since they are canonical, they define facets of $\overline{Q_n}$ under the same conditions. In fact, using the same proof technique used in [1], one can show the following two results:

Proposition 4.7. *All strengthened pure negative-type inequalities define facets of* $\overline{Q_n}$.

Proposition 4.8. *Strengthened star inequalities define facets of* $\overline{Q_n}$ *if and only if* $|S| \neq 4$.

We omit the proofs, for the sake of brevity.

5. Unbounded edges of Q_n and $\overline{Q_n}$

5.1. Unbounded edges of Q_n

We now investigate *how* the polyhedral cones $M^1(\pi) = D(\pi) + D(N_\pi)$ are subsets of Q_n. In Fig. 1, it can be seen that in the case $n = 3$, the three cones are faces of Q_3 (recall that Q_3 is a polyhedron, which means that we can safely speak of faces). In the following proposition, we show that this is the case for all n, and we also characterize the extremal half-lines of Q_n. This will be useful in comparing Q_n with its closure: We will characterize the unbounded edges issuing from each vertex for the polyhedron $\overline{Q_n} = P_n + \mathrm{CUT}_n$ in the following section.

We are dealing with an unbounded convex set of which we do not know whether it is closed or not. (In fact, we will show that Q_n is almost never closed). For this purpose, we supply the following fact for easy reference.

Fact 5.1. *For* $k = 1, \ldots, m$ *let* K_k *be a (closed) polyhedral cone with apex* x_k. *Suppose that the* K_k *are pairwise disjoint and define* $S := \biguplus_{k=1}^m K_k$. *Let* x, y *be vectors such that* $x + \mathbb{R}_+ y$ *is an extremal subset of* $\operatorname{conv}(S)$. *It then follows that there exists a* $\lambda_0 \in \mathbb{R}_+$ *and a* k *such that* $x + \lambda y \in K_k$ *for all* $\lambda \geqslant \lambda_0$. *Since* $x + \mathbb{R}_+ y$ *is extremal, this implies that there exists a* $\lambda_1 \in \mathbb{R}_+$ *such that* $x_k = x + \lambda_1 y$ *and* $x_k + \mathbb{R}_+ y = \{x + \lambda y | \lambda \geqslant \lambda_1\}$ *is an extreme ray of the polyhedral cone* K_k.

Definition 5.2. We say that a permutation π and a non-empty set $U \subsetneq [n]$ are *incident,* if $U = \{\pi^{-1}(1), \ldots, \pi^{-1}(k)\}$, where $k := |U|$.

Proposition 5.3

1. *For every $\pi \in S(n)$, each edge of the cone $D(\pi) + D(N_\pi)$ is an exposed subset of Q_n.*
2. *The unbounded one-dimensional extremal sets of Q_n are exactly the defining half-lines. In other words, every half-line $X + \mathbb{R}_+ Y$ which is an extremal subset of Q_n is of the form $D(\pi) + \mathbb{R}_+ D(\chi^U)$ for a $\pi \in S(n)$ and a set U incident to π. In particular, for every vertex $D(\pi)$ of Q_n, the unbounded one-dimensional extremal subsets of Q_n containing $D(\pi)$ are in bijection with the non-empty proper subsets of $[n]$ incident to π. Thus there are precisely $n-1$ of them.*

Proof. (i) By symmetry it is sufficient to treat the case $\pi = \iota := (1, \ldots, n)^\top$, the identity permutation. Consider the matrix

$$C := \begin{pmatrix} 0 & 1 & & & & & -1 \\ 1 & 0 & 1 & & & \mathbb{0} & \\ & 1 & & & & & \\ & & & \ddots & & & \\ & & & & & 1 & \\ & \mathbb{0} & & & 1 & 0 & 1 \\ -1 & & & & & 1 & 0 \end{pmatrix} \in \mathbb{S}_n^0.$$

It is easy to see that the minimum over all $C \bullet D(\pi)$, $\pi \in S(n)$, is attained only in $\pi = \iota, \iota^-$ with the value 0. Moreover, for any non-empty proper subset U of $[n]$, we have $C \bullet D(\chi^U) = 0$ if U is incident to ι and $C \bullet D(\chi^U) > 0$ otherwise. Hence, we have that $D(\iota) + D(N_\iota)$ is equal to the set of all points in Q_n which satisfy the valid inequality $C \bullet X \geqslant 0$ with equality. Out of this matrix C we will now construct a matrix C' and a right-hand side such that only some of the subsets incident to ι fulfill the inequality with equality. To do so let U_0 be a subsets of $[n]$ incident to ι. If, for each $U \subset [n]$ incident to ι but different from U_0, we increase the matrix entries $C_{\max U, \max U+1}$ and $C_{\max U+1, \max U}$ by one, we obtain an inequality $C' \bullet X \geqslant 0$ which is valid for Q_n and such that the set of all points of Q_n which are satisfied with equality is precisely the edge of $D(\iota) + D(N_\iota)$ generated by the half-lines $D(\iota) + \mathbb{R}_+ D(\chi^{U_0})$.

(ii) That the defining half-lines are extremal has just been proved in i. The converse statement follows from Fact 5.1 and the fact that the extreme points of Q_n are precisely the vertices of P_n, which are of the form $D(\pi)$, for $\pi \in S(n)$. $\square$

5.2. Unbounded edges in $\overline{Q_n}$

We have just identified some unbounded edges of $\overline{Q_n} = P_n + \mathrm{CUT}_n$ starting at a particular vertex $D(\pi)$ of this polyhedron. We now set off to characterize *all* unbounded edges of $\overline{Q_n}$. Clearly, the unbounded edges are of the form $D(\pi) + \mathbb{R}_+ D(\chi^U)$, but not all these half-lines are edges. For a permutation π and a non-empty subset $U \subsetneq [n]$, we say that $D(\pi) + \mathbb{R}_+ D(\chi^U)$ is the half-line *defined by the pair* $\pi \nearrow U$. In this section, we characterize the pairs $\pi \nearrow U$ which have the property that the half-lines they define are edges. For this, we make the following definition.

Definition 5.4. Let π be a permutation, and let U be a subset of $[n]$. We say that U is *almost incident* to π, if there exists a $k \in [n-1]$ such that $U = \pi^{-1}([k-1] \cup \{k+1\})$.

We can now state our theorem.

Theorem 5.5. *For all $n \geqslant 3$, the unbounded edges of $\overline{Q_n}$ are precisely the half-lines defined by those pairs $\pi \nearrow U$, for which neither U nor $\complement U$ is almost incident to π.*

From Theorem 5.5, we have the following consequences.

Corollary 5.6. *For $n \geqslant 4$, the number of unbounded edges issuing from a vertex of $\overline{Q_n} = P_n + C_n$ is $2^{n-1} - n$.*

Corollary 5.7. *For $n \geqslant 4$, the extremal half-lines containing an extreme point of Q_n are a proper subset of the unbounded edges issuing from the same vertex of $\overline{Q_n}$.*

Proof. We have $n - 1 < 2^{n-1} - n$ if $n \geqslant 4$. $\square$

Corollary 5.8. *The convex set Q_n is closed if and only if $n \leqslant 3$.*

Major parts of the proof of the above stated theorem work in an inductive fashion by reducing to the case when $n \in \{3, 4, 5, 6\}$. We will present the cases $n = 3$ and $n = 4$ as examples, which also helps motivating the definitions we require for the proof.

We will switch to a more "visual" notation of the subsets of $[n]$ by identifying a set U with a "word" of length n over $\{0, 1\}$ having a 1 in the jth position iff $j \in U$ – it is just the row-vector $(\chi^U)^\top$.

Example 5.9 (*Unbounded edges of $\overline{Q_3}$*).

We deal with the case $n = 3$ "visually" by regarding Fig. 1. There are two edges starting at each vertex. In fact, with some computation, it can be seen that the unbounded edges containing $D(\iota)$ are

$$M\begin{pmatrix}1\\2\\3\end{pmatrix} + \mathbb{R}_+ M\begin{pmatrix}1\\0\\0\end{pmatrix} = \begin{pmatrix}0&1&2\\1&0&1\\2&1&0\end{pmatrix} + \mathbb{R}_+\begin{pmatrix}0&1&1\\1&0&0\\1&0&0\end{pmatrix}, \quad \text{and}$$

$$M\begin{pmatrix}1\\2\\3\end{pmatrix} + \mathbb{R}_+ M\begin{pmatrix}1\\1\\0\end{pmatrix} = \begin{pmatrix}0&1&2\\1&0&1\\2&1&0\end{pmatrix} + \mathbb{R}_+\begin{pmatrix}0&0&1\\0&0&1\\1&1&0\end{pmatrix}; \quad \text{while}$$

$$M\begin{pmatrix}1\\2\\3\end{pmatrix} + \mathbb{R}_+ M\begin{pmatrix}1\\0\\1\end{pmatrix} = \begin{pmatrix}0&1&2\\1&0&1\\2&1&0\end{pmatrix} + \mathbb{R}_+\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}$$

is not an edge. This agrees with Proposition 5.3, because the sets 100 and 110 are incident to ι, while 101 and 010 are not.

Moreover, the set 101 is almost incident to ι and 010 is its complement. Thus, Theorem 5.5 is true for the special case when $\pi = \iota$. For the other permutations, the easiest thing to do is to use symmetry. We describe this in the next remark.

Remark 5.10. For every $\sigma, \pi \in S(n)$ and $U \subset [n]$ we have the following.

1. Due to symmetry the pair $\pi \nearrow U$ defines an edge of $\overline{Q_n}$ if and only if the pair $\pi \circ \sigma \nearrow \sigma^{-1}(U)$ defines an edge of $\overline{Q_n}$.
2. U is incident to π if and only if $\sigma^{-1}(U)$ is incident to $\pi \circ \sigma$.
3. U is almost incident to a permutation π if and only if $\sigma^{-1}(U)$ is almost incident $\pi \circ \sigma$.
4. $\complement U$ is almost incident to a permutation π if and only if U is almost incident to π^-.

Proof. Can be checked using the definitions of $\pi \nearrow U$ and U being incident, respectively, almost incident of π. $\square$

We now give the first general result as a step towards the proof of Theorem 5.5.

Lemma 5.11. *If $\pi \in S(n)$ and $U \subset [n]$ is almost incident π, then the half-line $D(\pi) + \mathbb{R}_+ D(\chi^U)$ defined by the pair $\pi \nearrow U$ is not an edge of $\overline{Q_n}$.*

Proof. By the above remarks on symmetry, it is sufficient to prove the claim for the identity permutation $\iota \in S(n)$. Consider a $k \in [n-1]$, and let $\pi' := \langle k, k+1 \rangle$ be the transposition exchanging k and

$k+1$, and let $U := [k-1] \cup \{k+1\}$. Then a little computation shows that $D(\chi^U)$ can be written as a conic combination of vectors defining rays issuing from $D(\iota)$ as follows:

$$D(\chi^U) = D(\chi^{[k]}) + \left(D(\pi') - D(\iota)\right).$$

Hence $D(\iota) + \mathbb{R}_+ D(\chi^U)$ is not an edge. $\square$

Note that by applying Remark 5.10, the Lemma 5.11 implies that if $\complement U$ is almost incident π, then the pair $\pi \nearrow \complement U$ does not define an edge of $\overline{Q_n}$.

Before we proceed, we note the following easy consequence of Farkas' Lemma.

Lemma 5.12. *The following are equivalent:*

1. *The half-line $D(\iota) + \mathbb{R}_+ D(\chi^U)$ defined by the pair $\iota \nearrow U$ is an edge of $\overline{Q_n}$.*
2. *There exists a matrix D satisfying the following constraints:*

$$D \bullet D(\pi) > D \bullet D(\iota) \quad \forall\, \pi \neq \iota, \iota^-, \tag{9a}$$

$$D \bullet D(\chi^{U'}) > D \bullet D(\chi^U) = 0 \quad \forall\, U' \neq U, \complement U. \tag{9b}$$

3. *There exists a matrix C satisfying*

$$C \bullet D(\pi) \geqslant C \bullet D(\iota) \quad \forall\, \pi \neq \iota, \iota^-, \tag{10a}$$

$$C \bullet D(\chi^{U'}) \geqslant 0 \quad \forall\, U' \neq U, \complement U, \tag{10b}$$

$$C \bullet D(\chi^U) < 0. \tag{10c}$$

Condition (9) is easier to check for individual matrices, but condition (10) will be needed in a proof below.

We move on to the next example which both provides some cases needed for the proof of Theorem 5.5 and motivates the following definitions.

Let U be a subset of $[n]$ and consider its representation as a word of length n. We say that a maximal sequence of consecutive 0s in this word is a *valley* of U. In other words, a valley is an inclusion-wise maximal subset $[l, l+j] \subset \complement U$. Accordingly, a maximal sequence of consecutive 1s is called a *hill*. A valley and a hill meet at a *slope*. Thus the number of slopes is the number of occurrences of the patterns 01 and 10 in the word, or in other words, the number of $k \in [n-1]$ with $k \in U$ and $k+1 \notin U$ or vice versa. If all valleys and hills of a subset U of $[n]$ consist of only one element (as for example in 10101) or, equivalently, if U has the maximal possible number $n-1$ of slopes, or, equivalently, if U consists of all odd or all even numbers in $[n]$, we speak of an *alternating* set.

Lemma 5.13. *For every set $\{W_1, \ldots, W_r\}$ of non-empty proper subsets of $[n]$ incident on π, there is a matrix C such that the minimum $C \bullet D(\sigma)$ over all $\sigma \in S(n)$ is attained solely in π and π^-, and that $C \bullet D(\chi^{U'}) \geqslant 0$ for every non-empty proper subset U' of $[n]$ where equality holds precisely for the sets W_i and their complements. This implies that $D(\pi) + \mathrm{cone}\{D(\chi^{W_1}), \ldots, D(\chi^{W_r})\}$ is a face of the polyhedron $\overline{Q_n} = P_n + \mathrm{CUT}_n$.*

Proof. Follows from Proposition 3.9. $\square$

Example 5.14 (*Unbounded edges of $\overline{Q_4}$*)**.** We consider the edges of $\overline{Q_4}$ containing $D(\iota) = D(\iota^-)$ (this is justified by Remark 5.10). We distinguish the sets U by their number of slopes. Clearly, a set U with a single slope is incident either to ι or to ι^-, and we have already dealt with that case in Lemma 5.13. The following sets have two slopes: 0100, 0110, 0010, 1011, 1001, and 1101. We only have to consider 1011, 1001, and 1101, because the others are their complements. The first one, 1011, is almost incident to ι^-, and the last one, 1101, is almost incident to ι, so we know that the pairs $\iota\nearrow 1011$ and $\iota\nearrow 1101$ do not define edges of $\overline{Q_4}$ by Lemma 5.11. For the remaining set with two slopes, 1001, the following matrix satisfies property (10) with C replaced by C^{1001} and U by 1001:

$$C^{1001} := \begin{pmatrix} 0 & 1 & -2 & 1 \\ 1 & 0 & 3 & -2 \\ -2 & 3 & 0 & 1 \\ 1 & -2 & 1 & 0 \end{pmatrix}.$$

The two alternating sets (i.e., sets with tree slopes) are 1010 and 0101, which are almost incident to ι and ι^-, respectively. This concludes the discussion of $\overline{Q_4}$.

Having settled some of the cases for small values of n, we give the result by which the reduction to smaller n is performed, which is an important ingredient for settling Theorem 5.5. The following lemma shows that unbounded edges of $\overline{Q_n}$ can be "lifted" to a larger polyhedron $\overline{Q_{n+k}}$.

Lemma 5.15. *Let U_0 be a non-empty proper subset of $[n]$ whose word has the form $a1b$ for two (possibly empty) words a, b. For any $k \geqslant 0$ define the subset U_k of $[n+k]$ by its word*

$$U_k := a\underbrace{1\dots1}_{k+1}b.$$

If the pair $\iota_n\nearrow U_0$ defines an edge of $\overline{Q_n}$, then the pair $\iota_{n+k}\nearrow U_k$ defines an edge of $\overline{Q_{n+k}}$.

Note that the lemma also applies to consecutive zeroes, by exchanging the respective set by its complement.

Proof. Let $C \in \mathbb{S}^0_n$ be a matrix satisfying conditions (10) for $U := U_0$. Fix $k \geqslant 1$ and let $n' := n + k$. We will construct a matrix $C' \in \mathbb{S}^0_{n'}$ satisfying (10) for $U := U_k$. For a "big" real number $\omega \geqslant 1$ define a matrix $B_\omega \in \mathbb{S}^0_{k+1}$ whose entries are zero except for those connecting j and $j+1$, for $j \in [k]$:

$$B_\omega := \begin{pmatrix} 0 & \omega & & & & & \\ \omega & 0 & \omega & & \mathbb{0} & & \\ & \omega & & & & & \\ & & & \ddots & & & \\ & & & & & \omega & \\ & \mathbb{0} & & & \omega & 0 & \omega \\ & & & & & \omega & 0 \end{pmatrix}.$$

We use this matrix to put a heavy weight on the "path" which we "contract."

For our second ingredient, let l_a denote the length of the word a and l_b the length of the word b (note that $l_a = 0$ and $l_b = 0$ are possible). Then we define

$$B_- := \begin{pmatrix} +1 & \dots & +1 \\ \mathbf{0}_{k-1} & \dots & \mathbf{0}_{k-1} \\ -1 & \dots & -1 \end{pmatrix} \in \mathbb{M}((k+1)\times l_a) \quad \text{and}$$

$$B_+ := \begin{pmatrix} -1 & \dots & -1 \\ \mathbf{0}_{k-1} & \dots & \mathbf{0}_{k-1} \\ +1 & \dots & +1 \end{pmatrix} \in \mathbb{M}((k+1)\times l_b),$$

where $\mathbf{0}_{k-1}$ stands for a column of $k-1$ zeros. Putting these matrices together we obtain an $n' \times n'$-matrix B:

$$B := \begin{pmatrix} \mathbb{0} & B_-^\top & \mathbb{0} \\ B_- & B_\omega & B_+ \\ \mathbb{0} & B_+^\top & \mathbb{0} \end{pmatrix}.$$

Now it is easy to check that for any $\pi' \in \pi[n']$ we have $B \bullet D(\pi') \geqslant B \bullet D(\iota)$. Moreover let $\pi' \in \pi[n']$ satisfy $B \bullet D(\pi') < B \bullet D(\iota) + 1$. By exchanging π' with π'^-, we can assume that $\pi'(1) < \pi'(n')$. It is easy to see that such a π' then has the following "coarse structure"

$$\begin{aligned} &\pi'([l_a]) \subset [l_a] \\ &\pi'([n'] \setminus [n' - l_b]) \subset [n'] \setminus [n' - l_b] \\ &\pi'(j) = j \quad \forall\, j \in \{l_a + 1, \ldots, l_a + k + 1\}. \end{aligned} \tag{11}$$

Thus the matrix B enforces that the "coarse structure" of a $\pi' \in \pi[n']$ minimizing $B \bullet D(\pi')$ coincides with ι. We now modify the matrix C to take care of the "fine structure". For this, we split C into matrices $C_{11} \in \mathbb{S}^0_{l_a}$, $C_{22} \in \mathbb{S}^0_{l_b}$, $C_{12} \in \mathbb{M}(l_a \times l_b)$, $C_{21} = C_{12}^\top \in \mathbb{M}(l_b \times l_a)$, and vectors $c \in \mathbb{R}^{l_a}$, $d \in \mathbb{R}^{l_b}$ as follows:

$$C = \begin{pmatrix} C_{11} & c & C_{12} \\ c^\top & 0 & d^\top \\ C_{21} & d & C_{22} \end{pmatrix}.$$

Then we define the "stretched" matrix $\check{C} \in \mathbb{S}^0_{n'}$ by

$$\check{C} := \begin{pmatrix} C_{11} & c & \mathbb{0} & \mathbf{0} & C_{12} \\ c^\top & 0 & & 0 & \mathbf{0}^\top \\ & & & & \\ \mathbb{0} & & \mathbb{0} & & \mathbb{0} \\ & & & & \\ \mathbf{0}^\top & 0 & & 0 & d^\top \\ C_{21} & \mathbf{0} & \mathbb{0} & d & C_{22} \end{pmatrix}$$

where the middle $\mathbb{0}$ has dimensions $(k-1) \times (k-1)$. Finally we let $C' := B + \varepsilon \check{C}$, where $\varepsilon > 0$ is small. We show that C' satisfies (10).

We first consider $C' \bullet D(\chi^{U'})$ for non-empty subsets $U' \subsetneq [n']$. Note that, if U' contains $\{l_a + 1, \ldots, l_a + k + 1\}$, then for $U := U' \setminus \{l_a + 1, \ldots, l_a + k + 1\}$, we have $C' \bullet D(\chi^{U'}) = C \bullet D(\chi^{U})$. Thus we have $C' \bullet D(\chi^{U_k}) = C \bullet D(\chi^{U_0}) < 0$ proving (10c) for C' and U_k. For every other U' with $C' \bullet D(\chi^{U'}) < 0$, if ω is big enough, then either U' or $\complement U'$ contains $\{l_a + 1, \ldots, l_a + k + 1\}$, and w.l.o.g. we assume that U' does. By (10b) applied to C and U, we know that this implies $U = U_0$ or $U = \complement U_0$ and hence $U' = U_k$ or $\complement U' = U_k$. Thus, (10b) holds for C' and U_k.

Second, we address the permutations. To show (10a), let $\pi' \in S(n)$ be given which minimizes $C' \bullet D(\pi')$. Again, by replacing π' by π'^- if necessary, we assume $\pi'(1) < \pi'(n')$ w.l.o.g. If ε is small enough, we know that π' has the coarse structure displayed in (11). This implies that we can define a permutation $\pi \in S(n)$ by letting

$$\pi(j) := \begin{cases} \pi'(j) & \text{if } j \in [l_a], \\ \pi'(j) = j & \text{if } j = l_a + 1, \\ \pi'(j-k) + k & \text{if } j \in [n] \setminus [l_a + 1]. \end{cases}$$

An easy but lengthy computation (see [22] for the details) shows that

$$\begin{aligned} C' \bullet D(\pi') - C' \bullet D(\iota_{n'}) &\geqslant \varepsilon \left[C \bullet D(\pi) + k \cdot C \bullet \begin{pmatrix} \mathbb{0}_{l_a \times l_a} & \mathbb{1} \\ \mathbb{1} & \mathbb{0}_{l_b \times l_b} \end{pmatrix} \right. \\ &\quad \left. - \left(C \bullet D(\iota_n) + k \cdot C \bullet \begin{pmatrix} \mathbb{0}_{l_a \times l_a} & \mathbb{1} \\ \mathbb{1} & \mathbb{0}_{l_b \times l_b} \end{pmatrix} \right) \right] \\ &= \varepsilon \left[C \bullet D(\pi) - C \bullet D(\iota_n) \right] \geqslant 0. \end{aligned}$$

Thus (10a) holds. $\square$

Example 5.16. We give an example for the application of Lemma 5.15.

For $n = 5$, consider the half-line defined by the pair $\iota \nearrow 11001$. The set 11001 can be reduced to 1001 by contracting the hill 1–2. To do so we set

$$C^{11001} := \varepsilon \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 1 & 0 & 3 & -2 \\ 0 & -2 & 3 & 0 & 1 \\ 0 & 1 & -2 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & \omega & -1 & -1 & -1 \\ \omega & 0 & 1 & 1 & 1 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \end{pmatrix}$$

for a small $\varepsilon > 0$ and a big $\omega \geqslant 1$.

After these preparations we can tackle the proof of the theorem.

Proof of Theorem 5.5. By Remark 5.10, we only need to consider $\pi = \iota$. We distinguish the sets U by their numbers of slopes.

One slope. This is equivalent to U or $\complement U$ being incident to ι. We have treated this case in Lemma 5.13.

Two slopes. The complete list of all possibilities, up to complements, and how they are dealt with is summarized in Table 2. In this table, 0 stands for a valley consisting of a single zero while $0\ldots0$

Table 2
List of all sets with two slopes (up to complement).

Word			Edge?	Why?
Hill 1	Valley	Hill 2		
1	0	1	No	Almost incident to ι
1	0	$1\ldots1$	No	Almost incident to ι^-
1	$0\ldots0$	1	Yes	Reduce to $n = 4$, 1001, by Lemma 5.15
1	$0\ldots0$	$1\ldots1$	Yes	Reduce to $n = 4$, 1001, by Lemma 5.15
$1\ldots1$	0	1	No	Almost incident to ι
$1\ldots1$	0	$1\ldots1$	Yes	Reduce to $n = 5$, 11011, by Lemma 5.15
$1\ldots1$	$0\ldots0$	1	Yes	Reduce to $n = 4$, 1001, by Lemma 5.15
$1\ldots1$	$0\ldots0$	$1\ldots1$	Yes	Reduce to $n = 5$, 11011, by Lemma 5.15

Table 3
List of all sets with three slopes (up to complement).

Word				Edge?	Why?
Hill 1	Valley 1	Hill 2	Valley 2		
1	0	1	0	No	Almost incident to ι
1	0	1	$0\ldots0$	No	Almost incident to ι
1	0	$1\ldots1$	0	Yes	Reduce to $n = 5$, 10110, by Lemma 5.15
1	0	$1\ldots1$	$0\ldots0$	Yes	Reduce to $n = 5$, 10110, by Lemma 5.15
1	$0\ldots0$	1	0	Yes	Reduce to $n = 5$, 10010, by Lemma 5.15
1	$0\ldots0$	1	$0\ldots0$	Yes	Reduce to $n = 5$, 10010, by Lemma 5.15
1	$0\ldots0$	$1\ldots1$	0	Yes	Reduce to $n = 5$, 10010, by Lemma 5.15
1	$0\ldots0$	$1\ldots1$	$0\ldots0$	Yes	Reduce to $n = 5$, 10110, by Lemma 5.15
$1\ldots1$	0	1	0	No	Almost incident to ι
$1\ldots1$	0	1	$0\ldots0$	No	Almost incident to ι
$1\ldots1$	0	$1\ldots1$	0	Yes	Reduce to $n = 5$, 10110, by Lemma 5.15
$1\ldots1$	0	$1\ldots1$	$0\ldots0$	Yes	Reduce to $n = 5$, 10110, by Lemma 5.15
$1\ldots1$	$0\ldots0$	1	0	Yes	Reduce to $n = 5$, 10010, by Lemma 5.15
$1\ldots1$	$0\ldots0$	1	$0\ldots0$	Yes	Reduce to $n = 5$, 10010, by Lemma 5.15
$1\ldots1$	$0\ldots0$	$1\ldots1$	0	Yes	Reduce to $n = 5$, 10010, by Lemma 5.15
$1\ldots1$	$0\ldots0$	$1\ldots1$	$0\ldots0$	Yes	Reduce to $n = 5$, 10010, by Lemma 5.15

Table 4
Matrices certifying unbounded edges of Q_n.

n	Slopes	Matrix
4	2	$C^{1001} := \begin{pmatrix} 0 & 1 & -2 & 1 \\ 1 & 0 & 3 & -2 \\ -2 & 3 & 0 & 1 \\ 1 & -2 & 1 & 0 \end{pmatrix}$
5	2	$C^{11011} := \begin{pmatrix} 0 & 8 & -6 & -1 & -1 \\ 8 & 0 & 2 & 9 & -3 \\ -6 & 2 & 0 & 5 & -7 \\ -1 & 9 & 5 & 0 & 11 \\ -1 & -3 & -7 & 11 & 0 \end{pmatrix}$
5	3	$C^{10110} := \begin{pmatrix} 0 & 2 & 2 & 1 & -3 \\ 2 & 0 & 0 & -2 & 2 \\ -2 & 0 & 0 & 2 & 0 \\ 1 & -2 & 2 & 0 & 1 \\ -3 & 2 & 0 & 1 & 0 \end{pmatrix}$
5	3	$C^{10010} := \begin{pmatrix} 0 & 2 & -2 & 2 & -2 \\ 2 & 0 & 4 & -3 & 1 \\ -2 & 4 & 0 & 1 & 1 \\ 2 & -3 & 1 & 0 & 1 \\ -2 & 1 & 1 & 1 & 0 \end{pmatrix}$
5	4	$C^{10101} := \begin{pmatrix} 0 & 0 & 3 & -2 & -1 \\ 0 & 0 & 1 & 1 & -2 \\ 3 & 1 & 0 & 1 & 3 \\ -2 & 1 & 1 & 0 & 0 \\ -1 & -2 & 3 & 0 & 0 \end{pmatrix}$
6	5	$C^{101010} := \begin{pmatrix} 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 & -2 & 0 \\ 1 & 1 & 0 & 1 & 3 & -2 \\ -1 & 1 & 1 & 0 & 0 & 1 \\ 0 & -2 & 3 & 0 & 0 & 1 \\ 0 & 0 & -2 & 1 & 1 & 0 \end{pmatrix}$

stands for a valley consisting of at least two zeros (the same with hills). The matrices for the reduced words satisfying (10) can be found in Table 4. The condition (10) can be verified by some case distinctions.

Three slopes. This case can be tackled using the same methods we applied in the case above. Table 3 gives the results.

$s \geqslant 4$ *slopes.* Using Lemma 5.15, we reduce such a set to an alternating set with s slopes showing that for all these sets U the pair $\imath \nearrow U$ defines an edge of $\overline{Q_n}$. This is in accordance with the statement of the theorem because sets which are almost incident to $\imath$ can have at most three slopes. The statement for alternating sets is proven by induction on n in Lemma 5.17 below. Note that the starts of the inductions in the proof of that lemma are $n = 5$ and $n = 6$ for even or odd s, respectively.

This concludes the proof of the theorem. □

We now present the inductive construction which we need for the case of an even number of $s \geqslant 4$ slopes.

Lemma 5.17. *For an integer $n \geqslant 5$ let U be an alternating subset of $[n]$. The pair $\imath \nearrow U$ defines an edge of $\overline{Q_n}$.*

Proof. We first prove the case when n is odd.

The proof is by induction over n. For the start of the induction we consider $n = 5$ and offer the matrix $C^{10101} \in \mathbb{S}_5^0$ in Table 4 of the appendix satisfying (9).

We will need this matrix in the inductive construction.

Now set $E^5 := C^{10101}$ and assume that the pair $\iota \nearrow U^-$ defines an edge of $\overline{Q_n}$ where U^- is an alternating subset of $[n]$. W.l.o.g., we assume that $U^- = 10\ldots01$. There exists a matrix $E^- \in \mathbb{S}_n^0$ for which (9) holds. We will construct a matrix $E \in \mathbb{S}_{n+2}^0$ satisfying (9) for $U := 010\ldots010$.

We extend E^- to a $(n+2) \times (n+2)$-Matrix

$$\widehat{E} := \begin{pmatrix} E^- & \mathbf{0} & \mathbf{0} \\ & & \\ \mathbf{0}^\top & 0 & 0 \\ \mathbf{0}^\top & 0 & 0 \end{pmatrix}.$$

We do the same with E^5, except on the other side:

$$\widehat{E^5} := \begin{pmatrix} 0 & 0 & \mathbf{0}^\top \\ 0 & 0 & \mathbf{0}^\top \\ & & \\ \mathbf{0} & \mathbf{0} & E^5 \end{pmatrix}.$$

Now we let $E := \widehat{E} + \widehat{E^5}$ and check the conditions (9) on E. These are now easily verified.

For the even case we guarantee the start of induction investigating $n = 6$. We give a matrix C^{101010} satisfying (9) in Table 4 in the appendix. (Note that 101010 is the only set which is not incident to ι, is not almost incident to ι or ι^-, cannot be reduced by Lemma 5.15 and is no complement of sets of any of these three types.) The induction is proved in the same way by using the matrix $E^6 := C^{101010}$. $\square$

6. Concluding remarks

The $\mathbb{R}$-embeddable 1-separated metrics are a natural and fascinating class of metrics, which are also of some practical importance due to their connection with graph layout problems. We have established some fundamental properties of such metrics, and also initiated a study of their convex hull and its closure.

There are several possible avenues for future research. First, one could search for new valid or facet-defining inequalities. Second, one could study the complexity of the separation problems associated with various families of inequalities, which would be essential if one wished to use the inequalities within a cutting-plane algorithm. Third, it would be interesting to know whether the *bounded* edges of the convex hull, or its closure, have a simple combinatorial interpretation.

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