

## ON THE EXTREME RAYS OF THE METRIC CONE

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**Introduction.** A classical result in the theory of convex polyhedra is that every bounded polyhedral convex set can be expressed either as the intersection of half-spaces or as a convex combination of extreme points. It is becoming increasingly apparent that a full understanding of a class of convex polyhedra requires the knowledge of both of these characterizations.

Perhaps the earliest and neatest example of this is the class of doubly stochastic matrices. This polyhedron can be defined by the system of equations

$$P: \sum_{j=1}^n x_{ij} = 1, \quad i = 1, 2, \dots, n \\ x_{ij} \geq 0, \quad i, j = 1, 2, \dots, n.$$

Birkhoff [2] and Von Neuman have shown that the extreme points of this bounded polyhedron are just the  $n \times n$  permutation matrices. The importance of this result for mathematical programming is that it tells us that the maximum of any linear form over  $P$  will occur for a permutation matrix  $X$ . In the assignment problem a matrix  $C$  of weights is given and the permutation matrix  $X$  is sought that maximizes

$$\sum_{1 \leq i, j \leq n} c_{ij} x_{ij}.$$

Therefore we can apply a simplex procedure to the polyhedron  $P$  and be assured of an integral solution. Since both methods of describing  $P$  are straightforward, it is perhaps not surprising that efficient methods exist for solving the assignment problem.

Recently, many research investigations have sought similar results for apparently much more complicated polyhedra. In integer programming, the integral extreme points are usually known and a characterization of the system of intersecting half spaces is sought. The solution of the matching problem by Edmonds [4] is a particularly successful result here. For a systematic treatment of this and many interesting examples, the reader is referred to Chvátal [3].

An example of the converse procedure is given by Veinott [8] for the Leontief substitution systems. These are matrices  $A$  with exactly one positive element in each column, and the additional property that

$$X(b) = \{x: Ax = b, x \geq 0\}$$

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is nonempty for some positive vector  $b$ . It is shown in [8] that the extreme points of the sets  $X(b)$  have a particular form and this has application in the solution of certain inventory models.

The polyhedra that will be examined in this paper are related to finite metric spaces. The  $\binom{n}{2} = {}_nC_2$  distances between  $n$  points can be represented as a vector  $\mathbf{R}_+^{nC_2}$ , after a suitable ordering of the distances has been established. The set of all such vectors is a pointed cone in which the facets are triangle inequalities. The major problem addressed is to determine the extreme rays of this cone.

Section 1 provides the necessary definitions and notation from the theory of metric spaces and finite graphs. The second section contains a proof that the complete bi-partite graph  $K_{3,2}$  induces an extreme ray. This proof is generalized to provide a means of showing that a large class of graphs induce extreme rays. These graphs are the topic of Section 3. The large class of dense multi-partite graphs are shown to induce extreme rays. Then it is shown that "almost all" sufficiently large graphs of medium density induce extreme rays. The complexity of the set of extreme rays is demonstrated at the end of this section, where it is shown that extreme rays can be found with arbitrary local structure. Section 4 deals with non-graphical extreme rays. These can be easily produced by including zero distances but this does not produce genuinely "new" extreme rays. A "union" operation for metric spaces is given here that can be used to generate non-trivial non-graphical extreme rays.

**1. Preliminaries.** In this section we group most of the terms and notation used throughout the paper. We will frequently use vectors contained in the positive orthant of Euclidean  ${}_nC_2$ -space, denoted  $\mathbf{R}_+^{nC_2}$ . Depending on the context, it will be convenient to use different subscripting methods for these vectors. For a vector  $d \in \mathbf{R}_+^{nC_2}$  we use the following subscripts interchangeably:

- (i)  $d = (d_1, d_2, \dots, d_{nC_2})$
- (ii)  $d = (d_{(1,2)}, d_{(1,3)}, \dots, d_{(1,n)}, d_{(2,3)} \dots d_{(n-1,n)})$
- (iii)  $d = (d_{12}, d_{13}, \dots, d_{n-1,n})$ .

It will occasionally be necessary to refer to the matrix  $D \in \mathbf{R}^{n \times n}$  defined by

$$D_{ij} = \begin{cases} d_{ij} & i < j \\ 0 & i = j \\ d_{ji} & i > j. \end{cases}$$

Such a vector  $d$  is called a *metric* on  $n$  points if it satisfies the triangle inequalities

$$(1) \quad d_{ij} + d_{jk} \geq d_{ik}, \quad 1 \leq i, j, k \leq n.$$

The set of all metrics on  $n$  points is denoted  $M_n$ . The notation  $[x]$  denotes the

greatest integer less than or equal to  $x$ ;  $\lceil x \rceil$  denotes the least integer greater than  $x$ .

We require some standard terminology from the theory of polyhedral convex sets. Brief definitions are given here; the reader is referred to [7] for details. A (*convex*) *polyhedron* is the solution set of a finite system of linear inequalities. Let  $K$  be any convex set. A convex subset  $W$  of  $K$  is an *extreme subset* of  $K$  if none of its points are contained in an open line segment spanned by two points of  $K$  which are not both in  $W$ . A one-dimensional extreme subset is called an *extreme ray*. We frequently refer to an extreme ray as a vector; unless specified explicitly, the vector is any nonzero point on the ray.  $K$  is a *convex cone* if positive combinations of points in  $K$  are again in  $K$ . A *facet* of  $K$  is an extreme subset with dimension one less than that of  $K$ .

The following proposition summarizes some facts about  $M_n$ .

PROPOSITION 1.1.  $M_n$  is an  ${}_nC_2$ -dimensional convex cone with facets given by

$$d_{ij} + d_{jk} - d_{ik} = 0, \quad 1 \leq i, j, k \leq n.$$

Further,  $M_n$  is generated by a finite set of extreme rays.

The first statement follows easily from the definition of  $M_n$  and the second is the finite basis theorem, applied to this cone.

Graphs appear in various places throughout this paper and some basic definitions are given here. The notation used is normally that of [6], which should be consulted by the reader wishing more detail. A *graph*  $G = (V, E)$  consists of a finite set  $V$  of *vertices* and a set  $E$  of unordered pairs of vertices called *edges*. The *order* of  $G$  is the number of vertices in  $G$  and is denoted  $|G|$ . The number of edges of  $G$  is denoted  $\|G\|$ . By a *path* in  $G$ , we mean a sequence of distinct vertices  $v_1v_2 \dots v_{m+1}$  such that  $v_iv_{i+1}$  is an edge for all  $i = 1, 2, \dots, m$ . Such a path is called a  $v_1v_{m+1}$  path and has *length*  $m$ . A graph is *connected* if there exists at least one path between each pair of vertices of  $V$ . Unless otherwise stated, all graphs considered in this paper are connected. A subset of vertices of  $V$  is *independent* if no two are adjacent.

Each graph  $G$  induces a metric denoted  $d_G$ , where  $d_G(i, j)$  is the length of the shortest path in  $G$  between vertices  $i$  and  $j$ . It is easily verified that  $d_G$  satisfies the triangle inequalities. If  $G$  induces an extreme ray of  $M_n$ , then  $G$  is called an *extreme ray graph*.

Two special graphs will occur frequently. The *complete graph* of order  $n$ , denoted  $K_n$ , contains all possible  ${}_nC_2$  edges. A *bi-partite* graph is a graph in which the vertex set can be partitioned into two non-empty independent sets. The *complete bi-partite graph*,  $K_{m,n}$ , contains  $m + n$  vertices partitioned into independent sets of size  $m$  and  $n$  with all other  $mn$  possible edges between these sets.

The vector  $d$  is a *graphical metric space* if there exists a graph  $G$  and a positive

constant  $a$  such that  $d = a \cdot d_G$ .  $F = (V_1, E_1)$  is a subgraph of  $G = (V, E)$  if  $V_1 \subset V$  and  $E_1 \subset E$ .  $F$  is an *isometric subgraph* of  $G$  if

$$d_F(i, j) = d_G(i, j) \quad \text{for all } i, j \in V_1.$$

**2. A proof technique.** In the first part of this section we show that the metric induced by  $K_{3,2}$  (Figure 2.1) is an extreme ray of  $M_5$ . This argument is generalized to give an easy method for proving that a large class of graphs induces extreme rays.

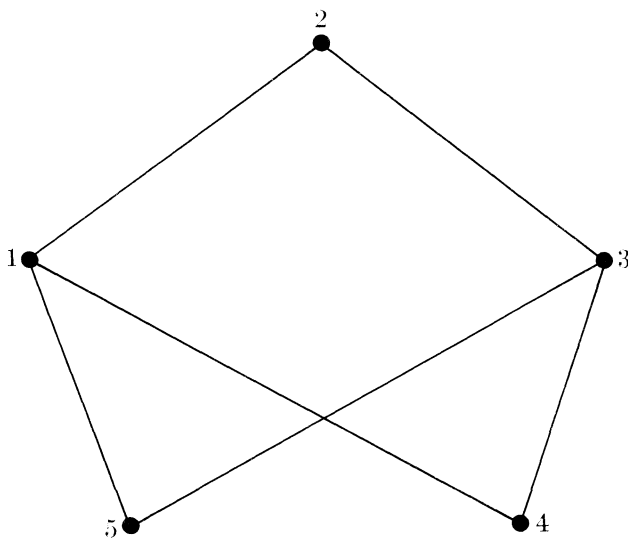


FIGURE 2.1.  $K_{3,2}$

Suppose we have  $x, y \in M_5$  and  $\lambda$  in the open interval  $(0, 1)$ , such that

$$(1) \quad d \triangleq d_G = \lambda x + (1 - \lambda)y.$$

Observe that  $d_{13} = d_{12} + d_{23}$ . Substituting for  $d$  we get

$$(2) \quad \lambda x_{13} + (1 - \lambda)y_{13} = \lambda x_{12} + (1 - \lambda)y_{12} + \lambda x_{23} + (1 - \lambda)y_{23}.$$

But since  $x, y \in M_5$  we have

$$(3) \quad x_{13} \leq x_{12} + x_{23} \quad \text{and} \quad y_{13} \leq y_{12} + y_{23}.$$

Therefore the equality (2) implies that in fact equalities hold in (3). These equations are examples of *light constraints* and we have just seen that  $x$  and  $y$  must have the same tight constraints as  $d$ . Geometrically, this is the observation that  $x$  and  $y$  must be contained in any facet that contains  $d$ .

Let us consider the subgraph  $F$  induced by the vertices  $\{1, 2, 3, 4\}$ . This is

an isometric subgraph since it preserves the distances of  $K_{3,2}$ .  $F$  is a cycle of length 4 denoted  $C_4$ .

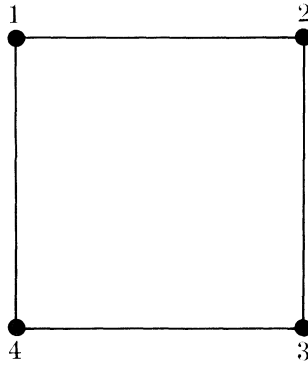


FIGURE 2.2.  $C_4$

The tight constraints for this graph are

$$\begin{aligned} d_{13} &= d_{12} + d_{23} & d_{13} &= d_{14} + d_{34} \\ d_{24} &= d_{12} + d_{14} & d_{24} &= d_{23} + d_{34}. \end{aligned}$$

Solving this system we have

$$(4) \quad d_{12} = d_{34} \quad \text{and} \quad d_{23} = d_{14}.$$

Since we are dealing with an isometric subgraph, the conclusions are valid for the distances in the original graph  $K_{3,2}$ . By the earlier remarks we see that (4) must hold with  $d$  replaced by  $x$  or  $y$ . We have thus proved

**LEMMA 2.1.** *Let  $G$  be a graph with an induced subgraph isomorphic to  $C_4$ . If  $x \in M_n$  has the same tight constraints as  $d_G$  then*

$$x_{12} = x_{34} \quad \text{and} \quad x_{23} = x_{14}.$$

(We have assumed that the vertices of the cycle were labelled sequentially 1, 2, 3, 4.)

Returning to our example, repeated application of the lemma yields

$$\begin{aligned} x_{12} &= x_{34} & x_{34} &= x_{15} & x_{15} &= x_{23} \\ x_{23} &= x_{14} & x_{14} &= x_{35} & x_{35} &= x_{12}. \end{aligned}$$

Hence all of the above distances are equal to some constant  $a > 0$ . We now claim that  $x = a \cdot d$ . First note that distances between points  $u$  and  $v$  in  $G$  that are not adjacent are determined by summing the distances (all equal to one) along a shortest  $uv$ -path. Since  $x$  must satisfy the same tight constraints as  $d$ , the distance  $x(u, v)$  must be determined by the same ‘‘edges’’ as determined  $d(u, v)$ . Since each of these edges corresponds to a distance of  $a$ ,  $x(u, v) = a \cdot d(u, v)$ . This proves

LEMMA 2.2. Let  $G$  be a graph of order  $n$  and let  $x \in M_n$  be defined as in (1). If all distances in  $x$  corresponding to edges of  $G$  are equal to some constant  $a$ , then  $x = a \cdot d_G$ .

This lemma shows that  $K_{3,2}$  induces an extreme ray of  $M_5$ . The proof was given in detail as it generalizes to provide a powerful method of proving that certain graphs induce extreme rays. The next lemma gives a generalization of Lemma 2.1.

LEMMA 2.3. Let  $G$  be a graph of order  $n$  with an induced isometric cycle of length  $2k$ ,  $k \geq 2$  (denoted  $C_{2k}$ ), and let  $x \in M_n$  have the same tight constraints as  $d_G$ . If  $ab$  and  $cd$  are opposite edges of the cycle then  $x_{ab} = x_{cd}$ .

*Proof.* We assume the vertices of the cycle have been labelled sequentially  $1, 2, \dots, 2k$  around the cycle. Consider the two opposite edges  $(1, 2)$  and  $(k+1, k+2)$ . Since  $x$  has the same tight constraints as  $d_G$  we have

$$\begin{aligned} x(1, k+1) &= x(1, k+2) + x(k+1, k+2) \\ x(1, k+1) &= x(1, 2) + x(2, k+1) \\ x(2, k+2) &= x(1, 2) + x(1, k+2) \\ x(2, k+2) &= x(2, k+1) + x(k+1, k+2). \end{aligned}$$

Hence  $x(1, k+1) = x(2, k+2)$  and  $x(1, 2) = x(k+1, k+2)$ .

We now define an equivalence relation on the edges of a graph  $G$ . Two edges  $uv$  and  $ab$  are equivalent if and only if every metric  $X$  with the same tight constraints as  $d_G$  must also satisfy  $x(u, v) = x(a, b)$ . The equivalence classes will be denoted by colors so that all equivalent edges receive the same color. An isometric cycle coloring (ic-coloring) of  $G$  is defined by the following procedure:

(i) Initially all edges of  $G$  are uncolored. Pick any edge and give it color 1, set  $k = 1$ .

(ii) Find an uncolored edge that is opposite an edge colored  $k$  in some even isometric cycle of  $G$ . If there is no such edge go to step (iii), otherwise color the edge  $k$  and repeat step (ii).

(iii) If  $G$  is not completely colored, pick any uncolored edge, give it color  $k+1$ , set  $k \leftarrow k+1$  and go to step (ii).

A graph is  $k$ -ic-colorable if exactly  $k$  colors are used in the above procedure. It is easy to see that the procedure will produce the same color classes, regardless of how the uncolored edges are chosen. It is also clear that all edges in the same color class will be in the same equivalence class, as defined earlier.

THEOREM 2.4. If  $G$  is 1-ic-colorable then  $d_G$  is an extreme ray of  $M_n$ .

*Proof.* Assume  $d_G = \lambda x + (1 - \lambda)y$ . The preceding discussion and Lemma 2.2 shows that  $d_G = a \cdot x = b \cdot y$  for positive constants  $a$  and  $b$ .

Unfortunately the converse to this theorem is false. The graph in Figure 2.3 is 2-ic-colorable, the color classes denoted by the heavy and light edges. It is also an extreme ray. Indeed, if  $x$  is any metric with the same tight constraints as  $d_G$  then  $x$  must also satisfy

$$x_{uv} = x_{us} + x_{sv} = 2x_{us}$$

$$x_{uv} = x_{ut} + x_{tv} = 2x_{ut}$$

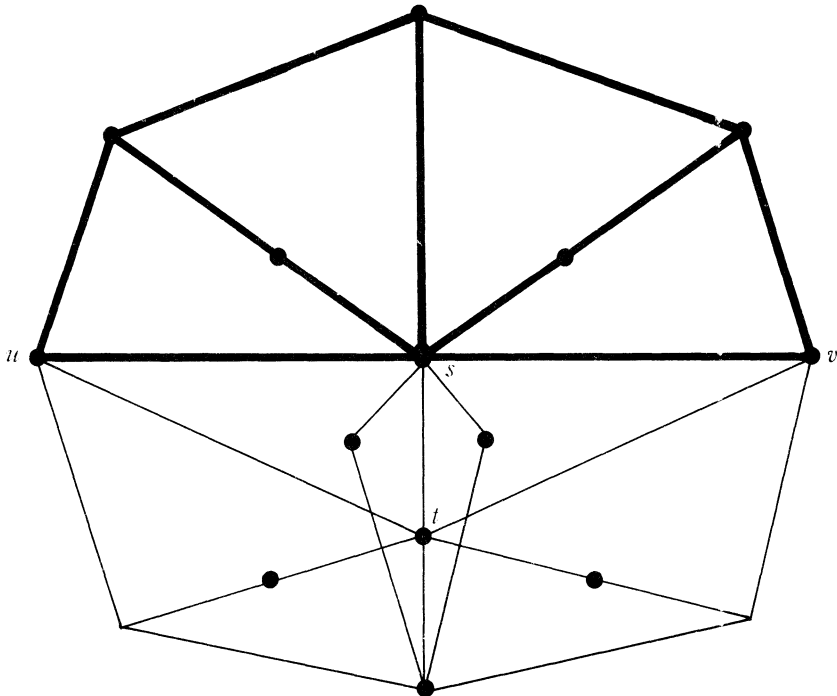


FIGURE 2.3. A 2-ic-colorable extreme ray

Therefore  $x_{us} = x_{ut}$  and  $G$  induces an extreme ray. This suggests adding a step (iv) to the ic-coloring procedure:

(iv) If  $G$  is 1-ic-colorable stop. Otherwise for each pair of vertices  $uv$  examine the shortest  $uv$ -paths. Merge the color classes of all such paths that use exactly one color.

It is clear that Theorem 2.4 holds for the four step coloring procedure. Will this modified procedure always succeed? The answer is still no; an example can be constructed that terminates with the configuration of Figure 2.4. Again the color classes denoted by the heavy and light lines can be merged. This case could also be handled by a modified step (iv), but it is beginning to

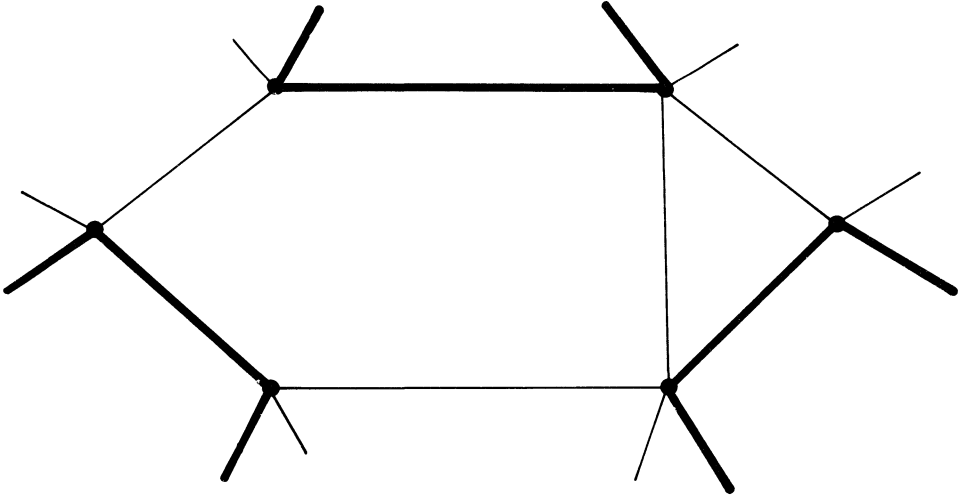


FIGURE 2.4

look like we are back to solving the original system of tight constraints. Although ic-coloring a graph is not a practical method of determining whether it induces an extreme ray, it will come in very useful in the next section for proving that large classes of graphs induce extreme rays.

**3. Graphical extreme rays.** In this section we use ic-coloring to identify a large class of graphical extreme rays. It will also be shown that “almost all” sufficiently large graphs with medium density induce extreme rays. Finally a construction will be given for producing extreme rays with arbitrary local structure.

By a *dense  $m$ -partite* graph  $G$  we mean a graph in which the vertex set can be partitioned into independent sets  $V_1, V_2, \dots, V_m$  with the properties:

- (i)  $|V_m| \geq |V_{m-1}| \geq \dots \geq |V_1| \geq 3$
- (ii)  $\|V_i \cup V_j\| \geq |V_i| |V_j| - \max\{|V_i|, |V_j|\} + 2$ , for  $1 \leq i < j \leq m$ .

Roughly speaking, a dense  $m$ -partite graph is a complete  $m$ -partite graph, possibly missing a “few” edges, with each part containing at least three vertices.

A graph will be called a *dense multipartite* graph if the decomposition (i) and (ii) is possible for some  $m \geq 2$ . We now show that the dense multipartite graphs induce extreme rays.

**LEMMA 3.1.** *If  $G$  is a dense bi-partite graph of order  $n$ , then  $d_G$  is an extreme ray of  $M_n$ .*

*Proof.* Let  $s = |V_1|$  and  $t = |V_2|$ . Then we claim that



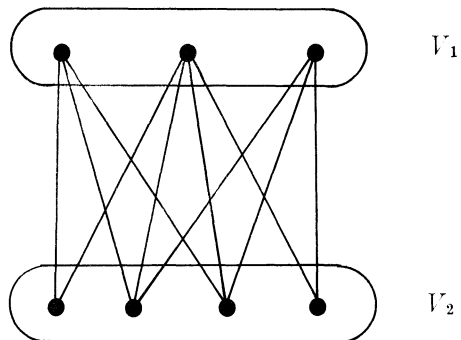


FIGURE 3.1. A dense bi-partite graph

- (i) there exist  $u, v \in V_2$  such that  $V_1 \cup \{u, v\}$  induces  $K_{s,2}$ ,
- (ii) the minimum degree of  $G$  is two.

To prove (i), note that if it failed, the number of edges in  $G$  would be at most

$$s + (t - 1)(s - 1) = st - t + 1,$$

a contradiction. Similarly for (ii), we have

$$\text{min degree of } G \geq \|G\|/t = s - (t - 1)/t \geq s - 1 \geq 2.$$

We now show that (i) and (ii) imply that  $d_G$  is an extreme ray. In an  $i$ -coloring of  $G$ , all of the edges in the induced  $K_{s,2}$  will be colored the same color, say red. Consider some other vertex  $w$  in  $V_2$ . By (ii) it must be adjacent to at least two vertices of  $V_1$ , say  $a$  and  $b$  (Figure 3.2).

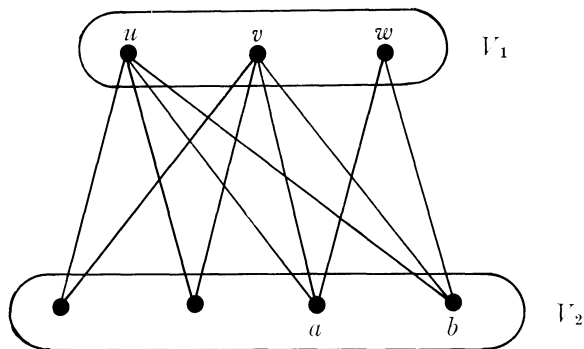


FIGURE 3.2

Then  $uawb$  is an induced cycle of length 4 and so  $aw$  and  $bw$  must be colored red. The same argument applies to all edges from  $w$ , and to all other vertices in  $V_2$ . The lemma then follows from Theorem 2.4.

It is apparent from the proof of Lemma 2.1 that weaker conditions can be found that depend more on the structure of  $G$ . These are the weakest conditions stated merely in terms of the number of edges of  $G$ .

**THEOREM 3.2.** *If  $G$  is a dense  $m$ -partite graph of order  $n$  then  $d_G$  is an extreme ray of  $M_n$ .*

*Proof.* Let  $G$  be ic-colored and consider the  ${}_m C_2$  pairs of vertex sets  $V_i, V_j$ . By the argument of Lemma 3.1, each pair will end up with all mutual edges in one color class, say  $c_{ij}$ . Each pair can be treated independently because the argument in the lemma uses only induced cycles of length 4 and these will be isometric in the original graph  $G$ . Note that it is not true that  $V_i \cup V_j$  induces an isometric subgraph of  $G$ .

Pick any three parts  $V_i, V_j, V_k$  with cardinalities  $r, s$  and  $t$  respectively. Assume  $r \leq s \leq t$ . Since  $\|V_j \cup V_k\| \geq st - t + 2$ , each point in  $V_k$  is adjacent to at least  $s - 1$  vertices in  $V_j$ . Similarly, each point in  $V_k$  is adjacent to at least  $r - 1$  vertices in  $V_i$ . Let  $u$  and  $v$  be two vertices in  $V_k$ . By the previous remarks and the fact that  $3 \leq r \leq s$ , there must exist common neighbors,  $x \in V_i$  and  $y \in V_j$ , of  $u, v$  (Figure 3.3). Since this induces a  $C_4$ , color classes

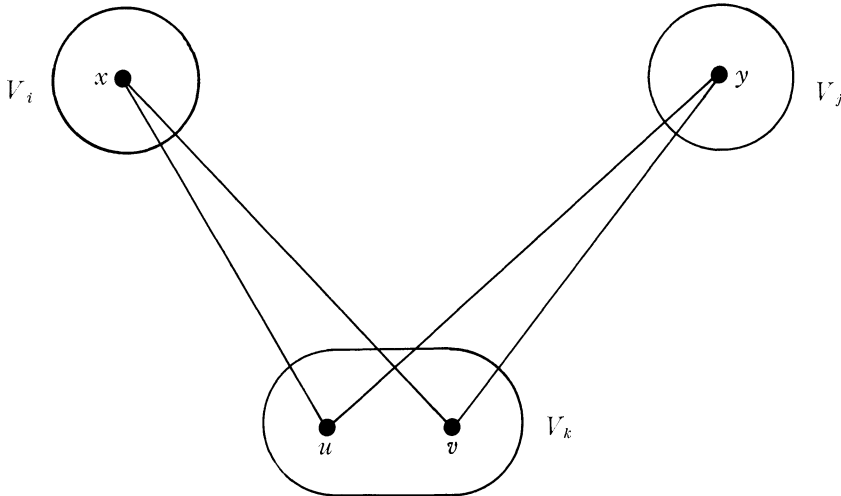


FIGURE 3.3

$c_{ik}$  and  $c_{jk}$  must be identical. Now pick two neighbors  $s$  and  $t$  of  $u$  in  $V_j$ . Again  $s$  and  $t$  must have some common neighbor  $z$  in  $V_i$  (Figure 3.4). Thus color classes  $c_{ij}$  and  $c_{jk}$  must be identical. Since the three parts were chosen arbitrarily, the theorem follows.

This theorem gives an easy way to construct a large number of extreme rays. If we restrict attention to those multipartite graphs with 3 vertices in

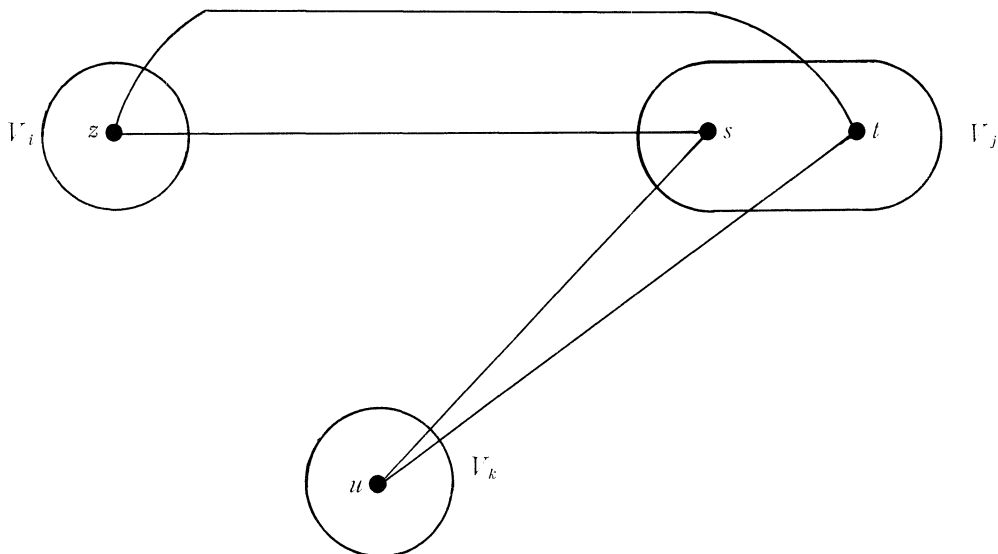


FIGURE 3.4

each part, the conditions of the theorem state that between each pair at most one edge can be dropped. It is easily seen that there are exactly  $10^{nC_2}$  such labeled graphs on  $3n$  points, each inducing an extreme ray of  $M_{3n}$ .

We now prove nonconstructively that “almost all” graphs of medium density induce extreme rays. To make this precise we use the concept of *random graph* due to Erdős and Spencer [5]. The symbol  $G_{n,p}$  denotes a random variable of which the values are graphs on  $n$  points with edge probability  $p$  ( $0 < p < 1$ ). That is, for each edge  $ij$ ,

$$\text{Prob}(ij \in G_{n,p}) = p,$$

and these probabilities are independent for each edge.

**THEOREM 3.3.** *For any  $\epsilon$  and  $p$  satisfying*

- (1)  $0 < \epsilon < 1/5$  and
- (2)  $n^{-1/5+\epsilon} \leq p(n, \epsilon) \leq 1 - n^{-1/4+\epsilon}$

$$\text{Prob}(G_{n,p} \text{ induces an extreme ray}) = 1 - o(1).$$

*Proof.* We begin by showing that the probability that  $G_{n,p}$  contains any isolated points is  $o(1)$ . Indeed,

$$\begin{aligned} \text{Prob}(G_{n,p} \text{ contains an isolate}) &\leq n(1-p)^{n-1} \leq ne^{-p(n-1)} \\ &\leq n \exp\{-(n-1)n^{-1/5+\epsilon}\} = o(1), \end{aligned}$$

over the range (2). We can therefore restrict attention to those random graphs that have no isolated points.

We proceed by obtaining an upper bound on the probability that  $G_{n,p}$  does not induce an extreme ray. This will be denoted  $\text{Prob}(G_{n,p} \text{ not ex.})$ . Observe that by Theorem 2.4,  $G_{n,p}$  will be an extreme ray if

- (i)  $G_{n,p}$  has no isolates, and
- (ii) for every pair of edges  $st$  and  $uv$  of  $G_{n,p}$ , the configuration of Figure 3.5 occurs.

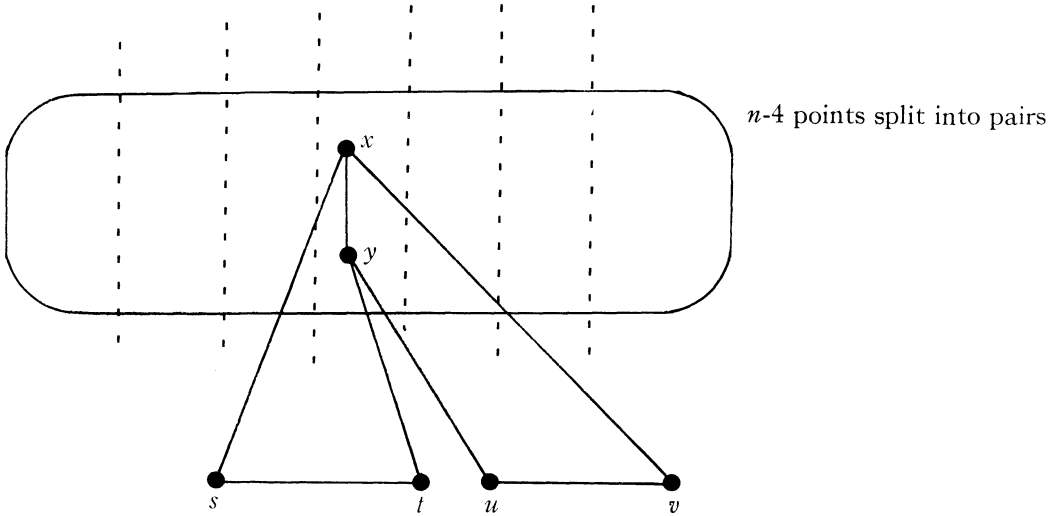


FIGURE 3.5

In Figure 3.5 we have divided the remaining  $n - 4$  points into  $\lfloor (n - 4)/2 \rfloor$  pairs that can each be treated independently. The subgraph induced by  $s, t, u, v, x$  and  $y$  shown in Figure 3.5 has probability  $p^5(1 - p)^4$ . There are at most  $3_n C_4$  possible choices for  $st$  and  $uv$ . Therefore,

$$\begin{aligned} \text{Prob}(G \text{ not ex.}) &\leq 3 \cdot \binom{n}{4} (1 - p^5(1 - p)^4)^{\lfloor (n-4)/2 \rfloor} + o(1) \\ &\leq 3 \cdot \binom{n}{4} \exp \{ -p^5(1 - p)^4(n - 5)/2 \} + o(1). \end{aligned}$$

The theorem now follows for any constant value of  $p$  in the open interval  $(0, 1)$ . Let  $f$  be defined by

$$f(p, n) = p^5(1 - p)^4(n - 5)/2.$$

We now show that  $f$  is bounded below by a polynomial in  $n$  for  $p$  in the range (2). Indeed, for  $p = n^{-1/5+\epsilon}$  we have

$$f(p, n) \geq n^\epsilon(1 - 4n^{-1/5+\epsilon})(1 - 5n^{-1})/2 \geq c_1 n^\epsilon$$

for some  $c_1 > 0$  and  $n \geq 4^5$ . For  $p = 1 - n^{-1/4\epsilon}$  we have

$$f(p, n) \geq n^\epsilon(1 - 5n^{-1/4+\epsilon})(1 - 5n^{-1})/2 \geq c_2 n^\epsilon$$

for some  $c_2 > 0$  and  $n \geq 5^4$ . To complete the proof we note that

$$\begin{aligned} \partial f / \partial p &= (5p^4(1-p)^4 - 4p^5(1-p)^3)(n-5)/2, \\ \partial f / \partial p &\begin{cases} \geq 0 & 0 \leq p \leq 5/9 \\ \leq 0 & 5/9 < p \leq 1. \end{cases} \end{aligned}$$

Therefore  $f(p, n) \geq cn^\epsilon$  for some constant  $c \geq 0$  and all  $n \geq 4^5$ , over the range (2). The theorem follows.

Applying the theorem with  $p = 1/2$  we can easily see that “most” graphs induce extreme rays. Indeed, in this case all graphs are equally likely and so the theorem shows that there are  $2^{n^{c_2}}(1 - o(1))$  distinct extreme rays.

We conclude this section by constructively showing that extreme rays of  $M_n$  can have arbitrary local structure. A metric is *rational* if all the distances are rational numbers. Given any rational metric  $x$  we construct a metric  $y$  that includes  $x$  as a submetric and is an extreme ray of the metric cone of appropriate dimension. We begin by embedding a graph in a larger extreme ray graph.

For any graph  $G$  construct the graph  $F(G)$  as follows:

- (i) Make two copies  $G_1$  and  $G_2$  of  $G$  and join each vertex in  $G_1$  to its twin in  $G_2$ .
- (ii) For each edge  $u_1v_1$  of  $G_1$  with  $u_1 < v_1$  and its twin  $u_2v_2$  of  $G_2$  with  $u_2 < v_2$ , insert a new vertex  $x$  and connect it to  $u_1$  and  $v_2$ .

Observe that  $|F| = 2|G| + \|G\|$ . Figure 3.6 contains an example of the construction.

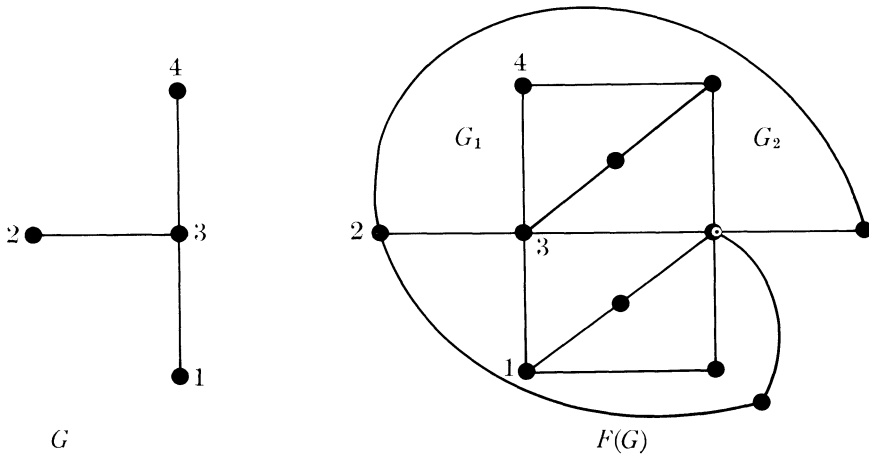


FIGURE 3.6. Example of an isometric embedding

LEMMA 3.4.  $F(G)$  includes  $G$  as an isometric subgraph and induces an extreme ray  $d_{F(G)}$ .

*Proof.*  $G$  is an isometric subgraph of  $F(G)$  since if  $u_1, v_1 \in G_1$ , the shortest  $u_1v_1$  path outside of  $G_1$  has length

$$2 + d_{G_2}(u_2, v_2) = 2 + d_{G_1}(u_1, v_1).$$

Now assume  $F(G)$  has been ic-colored. Choose an edge  $u_1v_1$  in  $G_1$ , and consider its twin  $u_2v_2$  in  $G_2$ , and the interconnecting vertex  $x$ . By construction  $\{x, u_1, v_1, u_2, v_2\}$  induce  $K_{3,2}$  which is always an isometric subgraph. Therefore all the edges of this subgraph will be 1-colored. A repetition of this argument together with the assumption that  $G$  is connected completes the proof.

A rational metric  $d$  on  $n$  points can always be embedded in a graph  $G$  so that  $d(u, v) = d_G(u, v)/k$ , where  $k$  is the smallest integer that makes  $k \cdot d$  integral. Simply construct a path of length  $k \cdot d(i, j)$  between each pair of points  $i$  and  $j$  (Figure 3.7).

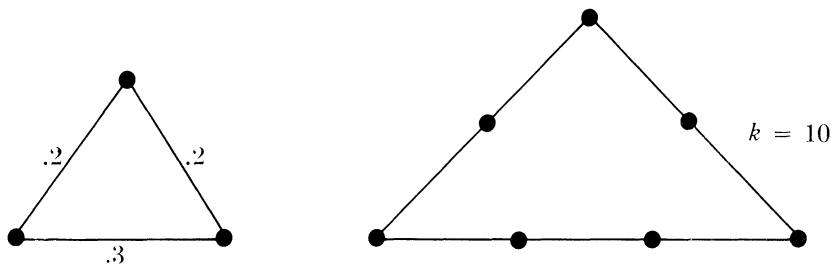


FIGURE 3.7. Embedding a rational metric in a graph

If  $x$  is a metric on  $n$  points and  $m < n$ , then the symbol  $x|_m$  denotes the metric induced by  $x$  on the points  $\{1, 2, \dots, m\}$ . The above observation and lemma 3.4 may be combined to yield the following theorem.

**THEOREM 3.5.** *If  $x$  is a rational metric on  $m$  points, there exists an integer  $n$  and an extreme ray  $d \in M_n$  so that  $d|_m = x$ .*

**4. Non-graphical extreme rays.** In this section we discuss extreme rays that are not induced by graphs. These are rays,  $x$ , such that there does not exist a graph  $G$  and a constant  $a$  satisfying  $d_G = a \cdot x$ . The easiest way to obtain such rays is to include zero distances. The first part of this section shows that the inclusion of zero distances does not lead to “new” rays. In the second part of this section a method of “patching” together extreme rays is given that generates non-graphical extreme rays.

We define the *zero-distance graph*  $Z(d)$  of a metric  $d$  on  $n$  points. The vertices of  $Z(d)$  are the  $n$  points and two vertices are joined if and only if the corresponding distance in  $d$  is zero.

**LEMMA 4.1.** *Every zero-distance graph  $Z(d)$  is a collection of isolated complete*

subgraphs (cliques)  $C_1, C_2, \dots, C_m$ . Further if  $i, j \in C_l$  and  $k$  is any point, then  $d_{ik} = d_{jk}$ .

*Proof.* From the triangle inequality, for any points  $i, j, k$  of  $d$ ,  $d_{ij} = 0$  and  $d_{jk} = 0$  imply that  $d_{ik} = 0$ . This proves the first statement. If  $i, j \in C_l$  and  $k$  is any point then

$$d_{ik} \leq d_{jk} + d_{ij} \leq d_{ik} + 2d_{ij} = d_{ik},$$

so  $d_{ik} = d_{jk}$ .

For a metric  $d$  on  $n$  points we define the *zero-distance contraction*  $d_0$  by picking one point from each of the  $m$  cliques in  $Z(d)$ . If  $S_0$  is the distinguished set, then Lemma 4.1 gives  $d_0 = d|_{S_0}$ .

**THEOREM 4.2.**  *$d$  is an extreme ray if and only if  $d_0$  is an extreme ray.*

*Proof.* Suppose  $d$  is an extreme ray and  $d_0$  is not. Then there exists a constant  $\lambda$  and metrics  $x_0$  and  $y_0$  such that

$$(1) \quad d_0 = \lambda x_0 + (1 - \lambda)y_0, \quad 0 < \lambda < 1,$$

and  $x_0 \neq a \cdot d_0$  for any constant  $a > 0$ . Now extend  $x_0$  and  $y_0$  to  $x$  and  $y$  in  $\mathbf{R}_+^{nC_2}$  by adding zero distances. Then

$$(2) \quad d = \lambda x + (1 - \lambda)y, \quad 0 < \lambda < 1 \quad \text{and} \quad x \neq a \cdot d,$$

a contradiction. Conversely, suppose that (2) holds for suitable metrics  $x, y$  and constant  $a$ . If  $d_{ij} = 0$  then  $x_{ij} = y_{ij} = 0$ . Hence the zero distance contractions of  $x$  and  $y$  are metrics and satisfy (1).

Theorem 4.2 tells us that when looking for new classes of extreme rays, zero distances can be ignored. There is, however, an important class of extreme rays that have exactly two cliques in the corresponding zero-distance graphs. These are called *Hamming extreme rays* and the cone they span is called the *Hamming cone*. This cone is the subject of [1].

A restricted union operation will now be described between certain metric spaces. It will be necessary to distinguish the point sets of different metrics. A *metric space* will be denoted by the ordered pair  $(S, d)$  where  $S$  is a set of  $n$  points and  $d$  is a metric. Two metric spaces  $(S_1, d_1)$  and  $(S_2, d_2)$  *overlap* if

$$|S_1 \cap S_2| \geq 2 \quad \text{and} \quad d_1|_{S_1 \cap S_2} = d_2|_{S_1 \cap S_2}.$$

The union  $(S, d)$  of two overlapping spaces is defined by

$$S = S_1 \cup S_2 \quad d(x, y) = \begin{cases} d_1(x, y) & x, y \in S_1 \\ d_2(x, y) & x, y \in S_2 \\ \min_{z \in S_1 \cap S_2} [d_1(x, z) + d_2(z, y)] & x \in S_1 - S_2 \\ & y \in S_2 - S_1 \end{cases}$$

The metric spaces in Figure 4.1 overlap and their union is shown. The weights

on the edges of the graphs denote the corresponding distances in the metric space. Distances between nonadjacent points are given by the weight of the shortest path in the weighted graph.

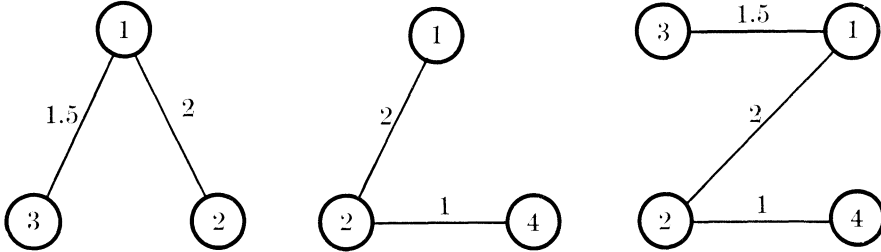


FIGURE 4.1. Example of the union operation

LEMMA 4.3. *The union of two overlapping metric spaces is a metric space.*

*Proof.* It suffices to check the triangle inequality for  $x, y \in S_1$  and  $z \in S_2 - S_1$ , since the other cases are obvious. By the definition of  $d$  there exist  $s, t \in S_1 \cap S_2$  with

$$d(x, z) = d_1(x, s) + d_2(s, z) \quad \text{and} \quad d(y, z) = d_1(y, t) + d_2(t, z).$$

Therefore,

$$\begin{aligned} d(x, z) &\leq d_1(x, t) + d_2(t, z) \leq d_1(x, y) + d_1(y, t) + d_2(t, z) \\ &= d(x, y) + d(y, z), \\ d(x, y) &\leq d_1(x, s) + d_1(s, t) + d_1(t, y) \leq d_1(x, s) + d_2(s, z) \\ &\quad + d_2(z, t) + d_1(t, y) = d(x, z) + d(y, z). \end{aligned}$$

THEOREM 4.4. *The union of two overlapping extreme rays is again an extreme ray.*

*Proof.* Let  $(S_1, d_1)$ ,  $(S_2, d_2)$  and  $(S, d)$  be as in the definitions above with  $n_1 = |S_1|$  and  $n_2 = |S_2|$ .  $d_1$  and  $d_2$  are extreme rays. Suppose  $d$  is not an extreme ray of  $M_{n_1+n_2}$ . Then there exists  $\lambda$  and metrics  $x$  and  $y$  satisfying

$$\begin{aligned} d &= \lambda x + (1 - \lambda)y, \quad 0 < \lambda < 1 \quad \text{and} \\ x &\neq a \cdot d \quad \text{for any } a > 0. \end{aligned}$$

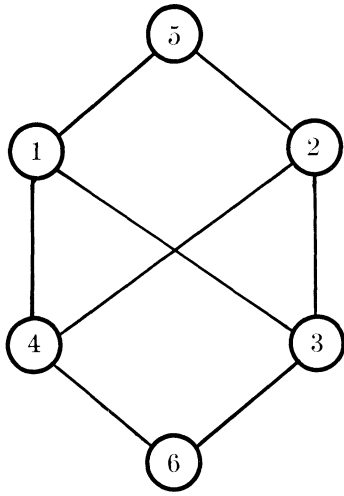
But by the definition of  $d$ ,

$$\begin{aligned} d|_{S_1} &= d_1 = \lambda x|_{S_1} + (1 - \lambda)y|_{S_1} \quad \text{and} \\ d|_{S_2} &= d_2 = \lambda x|_{S_2} + (1 - \lambda)y|_{S_2}. \end{aligned}$$

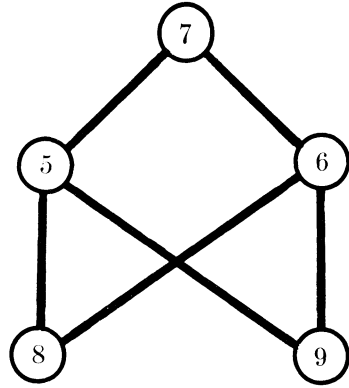
Since  $d_1$  and  $d_2$  are extreme rays there must exist constants  $a, b > 0$  such that

$$d|_{S_1} = a \cdot x|_{S_1} \quad \text{and} \quad d|_{S_2} = b \cdot x|_{S_2}.$$

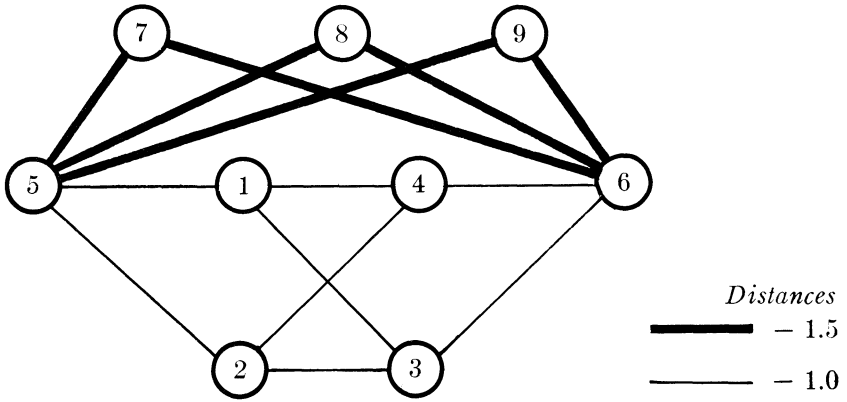




(a)  $(S_1, d_1)$



(b)  $(S_2, d_2)$



(c)  $(S, d)$

*Distances*  
**—** — 1.5  
 — — 1.0

FIGURE 4.2. A nongraphical extreme ray

Since  $(S_1, d_1)$  and  $(S_2, d_2)$  overlap,  $a = b$ . Pick  $u \in S_1 - S_2$  and  $v \in S_2 - S_1$ . Then

$$\begin{aligned} d(u, v) &= \min_{z \in S_1 \cap S_2} [d_1(u, z) + d_2(z, v)] = d_1(u, t) + d_2(t, v) \\ &= a(x(u, t) + x(t, v)) = a \cdot x(u, v) \end{aligned}$$

where  $t$  was chosen as the minimizing index. This shows that  $d = a \cdot x$ , a contradiction.

**COROLLARY.** *There exist nongraphical extreme rays that do not use zero-distances.*

*Proof.* Consider the metric spaces (a) and (b) of Figure 4.2. These were shown to be extreme rays in Section 3. The metric spaces overlap, and by Theorem 4.4 their union is an extreme ray. In a graphical metric space, all distances must be an integral multiple of the minimum distance of the metric. Therefore  $d$  is nongraphical.

**5. Conclusions.** We have seen that the extreme rays of the metric cone have a complicated local structure and have given both constructive and probabilistic lower bounds of  $2^{cn^2}$  on their number. Apart from the mathematical interest in these lower bounds, they relate to a problem in computer science. Indeed, in [9], Yao and Rivest give a procedure for developing a lower bound on the decision tree complexity of the all pairs shortest paths problem from the number of extreme rays. They show that the minimum depth of such a tree is at least a constant times the logarithm of the number of extreme rays. The bounds given in this paper thus yield just the trivial  $O(n^2)$  bound for the all pairs shortest paths problem. The question is thus the following: can the lower bounds given in this paper be improved to achieve a non-trivial lower bound for the all pairs shortest paths problem. This question has recently been answered negatively in [10] where an upper bound on the number of extreme rays of  $2^{2.72n^2}$  is demonstrated.

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