Embeddings of Graphs

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LIENS - 94 - 6

April 1994

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Abstract

In this paper, we survey the metric properties of isometric subgraphs of hypercubes and, more generally, of ℓ_1-graphs. An ℓ_1-graph is a graph which is hypercube embeddable, up to scale. In particular, we present several characterizations for hypercube embeddable graphs and a combinatorial algorithm (from [Shp93]) permitting to recognize ℓ_1-graphs in polynomial time. The link with the metric representation of graphs as Cartesian products (from [GW85]) is also described. In particular, we see how a well known equivalence relation of Djokovic [Djo73], leading to the notion of isometric dimension of a graph, plays a central and unifying role between the various embeddability concepts.

1 Introduction

In this paper, we survey various embeddability properties of graphs. A metric space can be attached to any connected graph in the following way. Let $G = (V, E)$ be a connected graph. Its **path metric** d_G is the metric defined on V by letting $d_G(a, b)$ denote the length of a shortest path joining a to b in G, for all nodes $a, b \in V$. Then, (V, d_G) is a metric space, called the **graphic metric space** associated with G. The **distance matrix** of G is the matrix $D_G := (d_G(a, b))_{a,b \in V}$.

There exists a hierarchy of metric properties that a given distance space may enjoy, in particular, isometric embeddability into the hypercube, into the Banach ℓ_1-, ℓ_2-spaces, hypermetricity, or the negative type condition. We study here what are the classes of graphs whose path metric enjoys some of these properties. Accordingly, a graph G is called an

ℓ_1-graph, a **hypercube embeddable graph**, a **hypermetric graph**, a **graph of negative type**, if its path metric d_G is isometrically ℓ_1-embeddable, hypercube embeddable, hypermetric, of negative type, respectively.

Given two connected graphs G and H, we write

$$G \hookrightarrow H$$

and say that G is an **isometric subgraph** (or, **distance-preserving** subgraph) of H if there exists a mapping

$$\sigma : V(G) \longrightarrow V(H)$$

such that

$$d_H(\sigma(a), \sigma(b)) = d_G(a, b)$$

for all nodes $a, b \in V(G)$. We will consider here in particular the cases when the host graph H is a hypercube (see Section 2), a Hamming graph or, more generally, a cartesian product of irreducible graphs (see Section 3).

Several other weaker types of embeddings of graphs have been considered in the literature. For instance, one may consider the graphs G that can be embedded into H as an induced subgraph; such embeddings are called **topological embeddings** and will not be considered here. An even weaker notion of embedding consists of asking which graphs G can be embedded into H as a (partial) subgraph, i.e., requiring only that the edges be preserved; see Remark 2.19 where the case of the hypercube as host graph H is briefly discussed.

The theory of isometric embeddings of graphs is a rich theory, with many applications. The main goal is to try to embed graphs isometrically into some other simpler graphs. The research in this area was probably motivated by a problem in communication theory posed by Pierce [Pie72]. In a telephone network one wishes to be able to establish a connection between two terminals A and B without B knowing that a message is on its way. The idea is to let the message be preceded by some "address" of B, permitting to decide at each node of the network in which direction the message should proceed. Namely, the message will proceed to the next node if its Hamming distance to the destination node B is shorter. The most natural way of devising such a scheme is by labeling the nodes by binary strings, which amounts to try to embed the graph in a hypercube. Unfortunately, not all graphs can be embedded into hypercubes. We study in detail in Section 2 the hypercube embeddable graphs. We present their basic structural characterization, due to Djokovic (Theorem 2.2), and some other equivalent characterizations (Theorems 2.7,2.11, and 2.14).

The notion of isometric embedding into hypercubes can be relaxed in several ways.

First, one may consider isometric embeddings into squashed hypercubes [GP71]. Namely, one tries to label the nodes by sequences using the symbols "$0, 1, *$", with the distance between $x, y \in \{0, 1, *\}$ being equal to 1 if $\{x, y\} = \{0, 1\}$ and to 0 otherwise. It turns out that every connected graph on n nodes can be isometrically embedded into the squashed hypercube of dimension $n - 1$ [Win83]. (Note that the squashed hypercube is not a semimetric space.)

One may also consider isometric embeddings into arbitrary cartesian products. In fact, every connected graph admits a unique canonical isometric embedding into a cartesian product whose factors are irreducible [GW85]. This result together with some applications is presented in Section 3.

Another way of relaxing isometric embeddings into hypercubes is to look for isometric embeddings into hypercubes up to scale, i.e., to consider ℓ_1-graphs; such embeddings were first considered in [BG73]. We present results on ℓ_1-graphs in Section 4; they come essentially from [Shp93].

Finally, we group in Section 5 some additional results related to the metric structure of graphs.

We now introduce some notions, leading to the definition of the isometric dimension of a graph, which will play a central role in this paper.

Let $G = (V, E)$ be a graph. Each edge (a, b) of G induces a partition of the node set V of G into

$$V = G(a,b) \cup G(b,a) \cup G_=(a,b),$$

where

$$\left\{ \begin{array}{l} G(a,b) = \{x \in V : d_G(x,a) < d_G(x,b)\}, \\ G(b,a) = \{x \in V : d_G(x,b) < d_G(x,a)\}, \\ G_=(a,b) = \{x \in V : d_G(x,a) = d_G(x,b)\}. \end{array} \right. \tag{1.1}$$

Clearly, if G is a bipartite graph, then $G_=(a,b) = \emptyset$ for each edge (a,b) of G.

The following relation θ, defined on the edge set of a graph, was first introduced in [Djo73]. It plays a crucial role in the theory of isometric embeddings of graphs. Given two edges $e = (a,b)$ and $e' = (a',b')$ of G, set

$$e\theta e' \quad \text{if} \quad d_G(a',a) - d_G(a',b) \neq d_G(b',a) - d_G(b',b). \tag{1.2}$$

In other words, e' is in relation by θ with e if the edge e' "cuts" the partition $V = G(a,b) \cup G(b,a) \cup G_=(a,b)$ induced by the edge e, i.e., the endpoints of e' belong to distinct sets in this partition. The relation θ is clearly reflexive and symmetric, but not transitive in general. For instance, θ is not transitive if G is the complete bipartite graph $K_{2,3}$. Actually, the relation θ is transitive precisely when the graph G can be isometrically embedded into $(K_3)^m$ for some $m \geq 1$ (see Corollary 3.3). The transitive closure of θ is denoted by θ^*. The number of equivalence classes of θ^* is called the **isometric dimension** of G and denoted by $dim_I(G)$. As will be seen in Section 3, each connected graph G can be embedded in a canonical way in a cartesian product of $dim_I(G)$ irreducible graphs.

We recall some preliminaries needed for the paper. Given two sequences $x = (x_1, \ldots, x_m)$, $y = (y_1, \ldots, y_m) \in \mathbb{R}^m$, their **Hamming distance** $d_H(x,y)$ is defined by

$$d_H(x,y) = |\{i \in \{1, \ldots, m\} : x_i \neq y_i\}|.$$

Given two graphs G and H, their **cartesian product** is the graph $G \times H$ with node set $V(G) \times V(H)$ and whose edges are the pairs $((a,x),(b,y))$ with $a, b \in V(G)$, $x, y \in V(H)$ and, either $(a,b) \in E(G)$ and $x = y$, or $a = b$ and $(x,y) \in E(H)$. A **Hamming graph** is a cartesian product of complete graphs, i.e., of the form $\prod_{j=1}^{m} K_{q_j}$ for some integers $q_1, \ldots, q_m, m \geq 1$. Note that the graphic space of $\prod_{j=1}^{m} K_{q_j}$ coincides with the distance space

$(\prod_{j=1}^{m}\{0,1,\ldots,q_j-1\},d_H)$. The m-**hypercube graph** is the graph $H(m,2)$ with node set $\{0,1\}^m$ and whose edges are the pairs $(x,y)\in\{0,1\}^m\times\{0,1\}^m$ with $d_H(x,y)=1$. Hence, $H(m,2)$ is isomorphic to the Hamming graph $(K_2)^m$ and its graphic metric space coincides with the space $(\{0,1\}^m,d_H)$. Equivalently, given a finite set Ω, the $|\Omega|$-hypercube, also denoted as $H(\Omega)$, can be defined as the graph whose node set is the set of all subsets of Ω and whose edges are the pairs (A,B) of subsets of Ω such that $|A\triangle B|=1$. The **half-cube graph** $\frac{1}{2}H(m,2)$ is the graph whose node set is the set of all subsets of even cardinality of $\{1,\ldots,m\}$ and with edges the pairs (A,B) such that $|A\triangle B|=2$. The **cocktail-party graph** $K_{m\times 2}$ is the complete multipartite graph with m parts, each of size 2. Hence, $K_{m\times 2}$ is the graph on $2m$ nodes $v_1,\ldots,v_{2m}$ whose edges are all pairs of nodes except the m pairs (v_i,v_{i+m}) for $i=1,\ldots,m$.

A connected graph G is said to be **hypercube embeddable** if its nodes can be labeled by binary vectors in such a way that the distance between two nodes coincides with the Hamming distance between their labels. In other words, G is hypercube embeddable if G is an isometric subgraph of $(K_2)^m$ for some $m\geq 1$. Then, the smallest integer m such that G can be isometrically embedded into $H(m,2)$ is denoted by $m_h(G)$.

The graph G is an ℓ_1**-graph** if its path metric d_G is ℓ_1-embeddable, i.e., if the nodes of G can be labeled by vectors (not necessarily binary) in such a way that the distance between two nodes coincides with the Hamming distance between their labels. Equivalently, G is an ℓ_1-graph if ηd_G is hypercube embeddable for some integer η. The smallest integer η such that ηd_G is hypercube embeddable is called the **minimum scale** of G. G is an ℓ_1**-rigid graph** if its path metric d_G is ℓ_1-rigid, i.e., admits an essentially unique ℓ_1-embedding. It can be checked that the cartesian product $G\times H$ is an ℓ_1-rigid graph if and only if both graphs G,H are ℓ_1-rigid.

Given a subset S of $V_n:=\{1,\ldots,n\}$, the **cut semimetric** $\delta(S)$ is the vector of $\mathbb{R}^{\binom{n}{2}}$ defined by $\delta(S)(i,j)=1$ if $|S\cap\{i,j\}|=1$ and $\delta(S)(i,j)=0$ otherwise, for $1\leq i<j\leq n$. Then, the cone in $\mathbb{R}^{\binom{n}{2}}$ generated by the cut semimetrics $\delta(S)$ for $S\subseteq V_n$ is called the **cut cone** and is denoted by CUT_n. More generally, if $(S_1,\ldots,S_t)$ is a partition of V_n, then the **multicut semimetric** $\delta(S_1,\ldots,S_t)$ is the vector of $\mathbb{R}^{\binom{n}{2}}$ defined by $\delta(S_1,\ldots,S_t)(i,j)=0$ if $i,j\in S_h$ for some $1\leq h\leq t$ and $\delta(S_1,\ldots,S_t)(i,j)=1$ otherwise.

It is well known (see, e.g., the survey [DL93a]) that a graph $G=(V,E)$ is an ℓ_1-graph if and only if its path metric d_G can be decomposed as

$$d_G=\sum_{S\subseteq V}\lambda_S\delta(S) \tag{1.3}$$

with $\lambda_S\geq 0$ for all S. Note that G is ℓ_1-rigid if and only if d_G lies on a simplex face of the cut cone. (A simplex face of the cut cone is a face F such that the nonzero cut semimetrics belonging to F are linearly independent.) Moreover, G is hypercube embedable if and only if d_G can be decomposed as (1.3) with $\lambda_S\in\mathbb{Z}_+$ for all S. More generally, G is an isometric subgraph of a Hamming graph if and only if d_G can be decomposed as a nonnegative integer combination of multicut semimetrics. Note that, if $(S_1,\ldots,S_t)$ is a partition of V_n, then the multicut semimetric $\delta(S_1,\ldots,S_t)$ can be decomposed as

$$\delta(S_1,\ldots,S_t)=\frac{1}{2}\sum_{1\leq i\leq t}\delta(S_i).$$

This implies that, for every isometric subgraph G of a Hamming graph, $2d_G$ is a non-negative integer combination of cut semimetrics, i.e., $2d_G$ is hypercube embeddable. In other words, every isometric subgraph of a Hamming graph is an ℓ_1-graph with scale 2 or, equivalently, is an isometric subgraph of a half-cube graph. We summarize in the figure below the links existing between the various embeddings we just discussed.

G is hypercube embeddable
$\Longrightarrow$ G is an isometric subgraph of a Hamming graph
$\Longrightarrow$ G is an isometric subgraph of a half-cube graph
$\Longrightarrow$ G is an ℓ_1-graph

Consider the inequality:

$$\sum_{1\leq i<j\leq n} b_i b_j x_{ij} \leq 0 \tag{1.4}$$

where $b_1, \ldots, b_n \in \mathbb{Z}$. If $\sum_{1\leq i\leq n} b_i = 1$, then the inequality (1.4) is called a **hypermetric inequality** and, if $\sum_{1\leq i\leq n} b_i = 0$, then it is called a **negative type inequality**. If $\sum_{1\leq i\leq n} |b_i| = 2k+1$, then (1.4) is called a $(2k+1)$**-gonal inequality**. A graph G is said to be **hypermetric** (resp. **of negative type**) if its path metric d_G satisfies all hypermetric inequalities (resp. all negative type inequalities). The hypermetric and negative type inequalities are valid for the cut cone CUT_n. Hence, each ℓ_1-graph is hypermetric and of negative type.

We refer, for instance, to [DL93a] for a survey on ℓ_1-metrics and hypercube embeddable metrics and the link with cut polyhedra.

2 Isometric embeddings of graphs into hypercubes

We study in this section the graphs that can be isometrically embedded into hypercubes. We give several equivalent characterizations for these graphs in Theorems 2.2, 2.7, 2.11, and 2.14. As an application, one can recognize in polynomial time whether a graph can be isometrically embedded in a hypercube. Hypercube embeddable graphs admit, in fact, an essentially unique embedding in a hypercube; two formulations for the dimension of this hypercube are given in Propositions 2.3 and 2.16.

We start with a definition.

Definition 2.1. *A subset U of the node set V of G is said to be* **convex** *if, for all $x, y \in U$, $z \in V$, $d_G(x,z) + d_G(z,y) = d_G(x,y)$ implies that $z \in U$.*

We now state the main result of this section, which is a structural characterization of the hypercube embeddable graphs, due to Djokovic [Djo73]. Recall the definition of the set $G(a,b)$ from relation (1.1).

Theorem 2.2. [Djo73] *Let G be a connected graph. The following assertions are equivalent.*
(i) G can be isometrically embedded into a hypercube.
(ii) G is bipartite and $G(a,b)$ is convex for each edge (a,b) of G.

PROOF. $(i) \Longrightarrow (ii)$ If G is hypercube embeddable, then its path metric d_G satisfies

$$d_G(a,b) + d_G(a,c) + d_G(b,c) \equiv 0 \pmod 2$$

for all nodes a, b, c of G, which means that G is bipartite. Let us now check the convexity of $G(a,b)$ for all adjacent nodes a, b. Let (a,b) be an edge of G and let $x, y \in G(a,b)$ and $z \in V$ lying on a shortest path from x to y. Consider a hypercube embedding of G in which node a is labeled by $\emptyset$, node b is labeled by a singleton $\{1\}$, and nodes x, y, z are labeled by the sets X, Y, Z. Then, $1 \notin X, Y$ since $x, y \in G(a,b)$, and $|X \triangle Y| = |X \triangle Z| + |Y \triangle Z|$ since $d_G(x,y) = d_G(x,z) + d_G(z,y)$. This implies that $1 \notin Z$, i.e., $z \in G(a,b)$. This shows that the set $G(a,b)$ is convex.
$(ii) \Longrightarrow (i)$ We first show that, given two edges $e = (a,b), e' = (a',b')$ of G, $e\theta e'$ if and only if the two bipartitions of V into $G(a,b) \cup G(b,a)$ and $G(a',b') \cup G(b',a')$ are identical. Suppose, for instance, that $a' \in G(a,b)$ and $b' \in G(b,a)$. We show that $G(a,b) = G(a',b')$. For this, it suffices to check that $G(a,b) \subseteq G(a',b')$. Let $x \in G(a,b)$. If $x \in G(b',a')$, then b' lies on a shortest path from x to a'. By convexity of $G(a,b)$, this implies that $b' \in G(a,b)$, yielding a contradiction. Therefore, the relation θ is transitive. Let $\overline{E} := E/\theta$ denote the set of equivalence classes of the relation θ. For $e \in E$, let $\overline{e}$ denote the equivalence class of e in $\overline{E}$. So, all edges (a,b) of a common equivalence class correspond to the same bipartition $G(a,b) \cup G(b,a)$ of V. Fix a node x_0 of G. For each node $x \in V$, let $A(x)$ denote the set of all $\overline{e} \in \overline{E}$ for which x and x_0 belong to distinct sets of the bipartition $V = G(a,b) \cup G(b,a)$, if (a,b) is an edge of $\overline{e}$. In particular, $A(x_0) = \emptyset$. We show that this labeling provides a hypercube embedding of G, i.e., that

$$|A(x) \triangle A(y)| = d_G(x,y)$$

holds for all nodes $x, y \in V$. Let $x, y \in V$ and $m := d_G(x,y)$. Let $P := (x_0 = x, x_1, \ldots, x_m = y)$ be a shortest path in G from x to y, with edges $e_i = (x_{i-1}, x_i)$ for $i = 1, \ldots, m$. We claim that

$$A(x) \triangle A(y) = \{\overline{e}_1, \ldots, \overline{e}_m\}.$$

Clearly, each $\overline{e}_i$ belongs to $A(x) \triangle A(y)$. Indeed if, for instance, $x_0 \in G(x_{i-1}, x_i)$, then $\overline{e}_i \in A(y) \setminus A(x)$ since $x \in G(x_{i-1}, x_i)$ and $y \in G(x_i, x_{i-1})$. Conversely, let $e = (a,b) \in E$ such that $\overline{e} \in A(x) \triangle A(y)$. We can suppose, for instance, that $\overline{e} \in A(y) \setminus A(x)$ with $x_0, x \in G(a,b)$ and $y \in G(b,a)$. Let i be the largest index from $\{1, \ldots, p\}$ for which $x_{i-1} \in G(a,b)$. Then, $e_i \theta e$, which shows that $\overline{e} = \overline{e}_i$.
Therefore, we have shown that $|A(x) \triangle A(y)| = d_G(x,y)$ holds for all nodes $x, y \in V$. This shows that G can be isometrically embedded into the hypercube of dimension $dim_I(G) := |\overline{E}|$. ∎

The following result will also be a consequence of Theorem 3.9.

PROPOSITION 2.3. [DL94a] *If G is hypercube embeddable, then G is ℓ_1-rigid; in particular, G has a unique (up to equivalence) isometric embedding into a hypercube and*

$m_h(G) = dim_I(G)$.

PROOF. Suppose that G is hypercube embeddable. We show that G is ℓ_1-rigid. Then, this implies that G has a unique hypercube embedding and, therefore, $m_h(G) = dim_I(G)$. We keep the notation from the proof of Theorem 2.2. For each $\overline{e} \in \overline{E}$ with $e = (a, b)$, let $S_{\overline{e}}$ denote the one of the two sets $G(a, b)$ and $G(b, a)$ that does not contain the fixed node x_0. From the fact that $d_G(x, y) = |A(x) \triangle A(y)|$ for all nodes $x, y \in V$, we deduce that d_G can be decomposed as

$$d_G = \sum_{\overline{e} \in \overline{E}} \delta(S_{\overline{e}}).$$

Let F_G denote the smallest face of the cut cone CUT_n (n is the number of nodes of G) that contains d_G. We claim that F_G is a simplex face of CUT_n of dimension $dim_I(G)$. Clearly, the cut semimetrics $\delta(S_{\overline{e}})$ belong to F_G and they are linearly independent. We show that every cut semimetric $\delta(S)$ lying on F_G is of the form $\delta(S_{\overline{e}})$ for some $\overline{e} \in \overline{E}$. If this is the case, then we have indeed shown that F_G is a simplex face of CUT_n of dimension $|\overline{E}| = dim_I(G)$. Let S be a subset of V such that $\delta(S) \in F_G$. Then, $\delta(S)$ satisfies the same triangle equalities as d_G. As the graph G is connected, we can find an edge $e = (a, b)$ such that $a \in S$ and $b \in V \setminus S$. Suppose, for instance, that $x_0 \in G(b, a)$, i.e., $S_{\overline{e}} = G(a, b)$. As d_G satisfies the triangle equality $d_G(x_0, a) = d_G(x_0, b) + d_G(a, b)$, we deduce that $\delta(S)$ satisfies the equality $\delta(S)(x_0, a) = \delta(S)(x_0, b) + \delta(S)(a, b)$, which implies that $x_0 \in V \setminus S$. We claim that $S = G(a, b)$ holds. If $x \in G(a, b)$, then $d_G(x, b) = d_G(x, a) + d_G(a, b)$ from which we deduce that $\delta(S)(x, b) = \delta(S)(x, a) + \delta(S)(a, b)$, implying that $x \in S$. In the same way, $G(b, a)$ is contained in $V \setminus S$, which implies that $S = G(a, b)$. ∎

REMARK 2.4. An immediate consequence of Theorem 2.2 is that one can test in polynomial time whether a graph G is hypercube embeddable. Note that the minimum dimension $m_h(G)$ of a hypercube containing G as an isometric subgraph can also be computed in polynomial time, since it coincides with the isometric dimension $m_I(G)$ of G (by Proposition 2.3). ∎

EXAMPLE 2.5. **Case of trees.**
Let T be a tree on n nodes. Then, T embeds isometrically into the $(n-1)$-hypercube, i.e., $dim_I(T) = n - 1$. The hypercube embedding of T can be easily constructed, as follows from the proof of Theorem 2.2. Namely, choose a node x_0 in T and label each node x of T by the set $A(x)$ consisting of the edges of T lying on the path from x_0 to x. We give in Figure 2.6 an example of a tree together with its hypercube embedding.

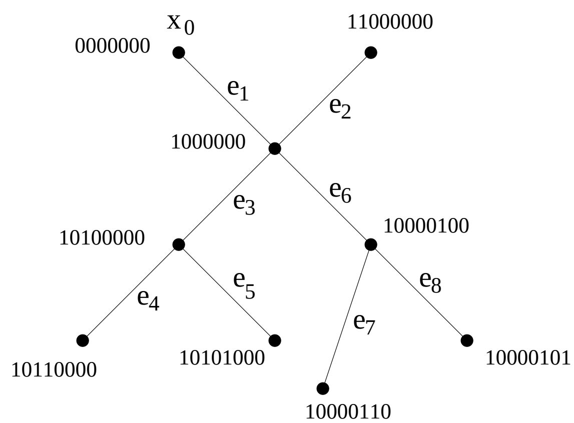


Figure 2.6

The distance matrix of a tree has some remarkable properties. In particular, its determinant depends only on the number of nodes of the tree. Namely, let T be a tree on n nodes with distance matrix D_T. Then, $det(D_T) = (-1)^{n-1}(n-1)2^{n-2}$ ([GP71]). (To see it, label the nodes of T as $a_1, \ldots, a_n$ in such a way that a_n is adjacent only to a_{n-1}. In the matrix D_T, substract the $(n-1)$-column to the n-th one and the $(n-1)$-row to the n-th one. Iterating this process brings D_T into the form of an $n \times n$ symmetric matrix having all entries equal to 0 except the $(1,i)$- and $(i,1)$ entries equal to 1 and the (i,i)-entries equal to -2, for $i = 2, \ldots, n$.) Graham and Lovász [GL78] show, more generally, how the coefficients of the characteristic polynomial of D_T can be expressed in terms of the number of occurrences of certain forests in T. ∎

We now state two further characterizations of hypercube embeddable graphs that follow from Djokovic's result.

THEOREM 2.7. [Avi81] *Let G be a connected graph. Then, G is hypercube embeddable if and only if G is bipartite and d_G satisfies the following 5-gonal inequality:*

$$d(i_1,i_2) + d(i_1,i_3) + d(i_2,i_3) + d(i_4,i_5) - \sum_{\substack{h=1,2,3 \\ k=4,5}} d(i_h,i_k) \leq 0 \tag{2.8}$$

for all nodes $i_1, \ldots, i_5 \in V$.

PROOF. If G is hypercube embeddable, then its path metric d_G is ℓ_1-embeddable and, therefore, satisfies the 5-gonal inequality. Suppose now that G is bipartite and not hypercube embeddable. Then, by Theorem 2.2, there exists an edge (a,b) of G for which the set $G(a,b)$ is not convex. Hence, there exist $x,y \in G(a,b)$ and $z \in G(b,a)$ such that $d_G(x,z) + d_G(z,y) = d_G(x,y)$. Consider the inequality (2.8) for the nodes $i_1 = x, i_2 = y, i_3 = b, i_4 = a$, and $i_5 = z$. One computes easily that the left hand side of (2.8) takes the value 2, which shows that d_G violates some 5-gonal inequality. ∎

	x	y	a	b	s
x	0	1	$n+1$	n	1
y	1	0	n	$n+1$	2
a	$n+1$	n	0	1	n
b	n	$n+1$	1	0	$n+1$
s	1	2	n	$n+1$	0

Figure 2.9: The distance space $A(n)$ on the 5 points of $\{x, y, a, b, s\}$

	x	y	a	b	r	s
x	0	1	$m+1$	m	p	$p+1$
y	1	0	m	$m+1$	$p+1$	$p+2$
a	$m+1$	m	0	1	$n+1$	n
b	m	$m+1$	1	0	n	$n+1$
r	p	$p+1$	$n+1$	n	0	1
s	$p+1$	$p+2$	n	$n+1$	1	0

Figure 2.10: The distance space $B(m, n, p)$ on the 6 points of $\{x, y, a, b, r, s\}$

THEOREM 2.11. [RW86] *Let G be a connected bipartite graph. Then, G is hypercube embeddable if and only if the space (V, d_G) does not contain as an isometric subspace any of the spaces $A(n)$ or $B(m, n, p)$, whose distance matrices are shown in Figures* 2.9 *and* 2.10*, respectively.*

PROOF. Suppose that G is not hypercube embeddable. Then, by Theorem 2.2, there exists an edge (a, b) of G for which $G(a, b)$ is not closed. Let P be an isometric path in G connecting two nodes of $G(a, b)$ such that P meets $G(b, a)$ and P has minimal length with respect to these properties. Say, $P = (y, x, z_1, \ldots, z_k, r, s)$, where $y, s \in G(a, b)$ and $x, r \in G(b, a)$. Set $m = d_G(x, b)$, $n = d_G(r, b)$ and $p = d_G(x, r)$ (hence, $p = k + 3$). One can check that the distances between the points a, b, x, y, r, s are entirely determined by the parameters m, n, p. Namely, if both points x and r coincide, then $p = 0$, $m = n$, and the 5-point subspace $(\{x, y, a, b, s\}, d_G)$ of (V, d_G) coincides with the space $A(n)$, whose distance matrix is shown in Figure 2.9. If the points x and r are distinct, then the 6-point subspace $(\{x, y, a, b, r, s\}, d_G)$ coincides with the space $B(m, n, p)$, whose distance matrix is shown in Figure 2.10.
Conversely, if (V, d_G) contains $A(n)$ or $B(m, n, p)$ as an isometric subspace, then G is not hypercube embeddable, by Theorem 2.7. Indeed, both $A(n)$ and $B(m, n, p)$ violate the 5-gonal inequality; namely, they violate the inequality (2.8) for $\{i_1, i_2, i_3\} = \{b, y, s\}$ and $\{i_4, i_5\} = \{x, a\}$. ∎

Recall that, for a finite distance space (X, d), the following chain of implications holds; see, e.g., [DL93a].

(X,d) is hypercube embeddable
$\Longrightarrow$ (X,d) is ℓ_1-embeddable
$\Longrightarrow$ (X,d) is hypermetric
$\Longrightarrow$ (X,d) is of negative type
$\Longrightarrow$ the distance matrix of (X,d) has exactly one positive eigenvalue.

Figure 2.12: The metric hierarchy

We recall also the following equivalences, due to Schoenberg [Sch38].

(X,d) is of negative type
$\Longleftrightarrow$ $(X,\sqrt{d})$ is ℓ_2-embeddable
$\Longleftrightarrow$ the matrix $(d(x,x_0)+d(y,x_0)-d(x,y))_{x,y\in X\setminus\{x_0\}}$ is positive semidefinite, where x_0 is a given element of X.

Figure 2.13

In fact, for the graphic spaces of bipartite graphs, the metric hierarchy from Figure 2.12 collapses. Blake and Gilchrist [BG73] proved already that connected bipartite ℓ_1-graphs are hypercube embeddable.

THEOREM 2.14. [RW86] *Let G be a connected bipartite graph. The following assertions are equivalent.*
(i) G is hypercube embeddable.
(ii) G is an ℓ_1-graph.
(iii) G is hypermetric.
(iv) G is of negative type.
(v) The distance matrix of G has exactly one positive eigenvalue.

PROOF. It suffices to show that, if G is not hypercube embeddable, then its distance matrix D_G has at least two positive eigenvalues. Suppose that G is not hypercube embedable. By Theorem 2.11, (V,d_G) contains as an isometric subspace a space C which is one of the forbidden subspaces $A(n)$ or $B(m,n,p)$. In other words, the distance matrix D_C of C is a principal submatrix of D_G. Clearly, D_C has at least one positive eigenvalue since its trace is equal to 0. We show below that D_C is nonsingular and has at least two positive eigenvalues. Then, as the number of positive eigenvalues of D_G is greater than or equal to the number of positive eigenvalues of D_C, we deduce that D_G has at least two positive eigenvalues.
Consider first the case when C is of the form $A(n)$. One can check that the determinant of D_C is equal to $-8n(n+1)$. Hence, D_C is nonsingular and has at least two positive eigenvalues (indeed, if D_C would have only one positive eigenvalue, then its determinant would be positive).
Suppose now that C is of the form $B(m,n,p)$. One can check that the determinant of D_C is equal to

$$4(4mnp+2mp+2np+2mn-m^2-n^2-p^2),$$

which can be rewritten as

$$16mnp+4(n+p-m)(p+m-n)+4(p+m-n)(m+n-p)+4(m+n-p)(n+p-m).$$

As m, n, p are the distances between pairs of nodes of G, we deduce from the triangle inequality that each of the quantities into parentheses in the above expression is nonnegative. Hence, the determinant of D_C is positive. This implies that D_C is nonsingular and has at least two positive eigenvalues (else, its determinant would be negative). ∎

REMARK 2.15. All the implications of the metric hierarchy from Figure 2.12 are strict for general (nonbipartite) graphs. The following unified set of counterexamples was proposed in [AM90].
• The path metrics of $K_4 - P_3$, $K_5 - P_3$, and $K_6 - P_3$ are ℓ_1-embeddable (since $2d_G$ is hypercube embeddable), but not hypercube embeddable (since they contain three points at pairwise distances one).
• The path metrics of $K_7 - P_3$, $K_8 - P_3$ are hypermetric, but not ℓ_1-embeddable.
(Hint: The inequality

$$5x_{12} + 5x_{13} + 3x_{23} - 3\sum_{j=4,5,6,7} x_{1j} - 2\sum_{j=4,5,6,7}(x_{2j} + x_{3j}) + \sum_{4\le i<j\le 7} x_{ij} \le 0$$

is valid for the cut cone CUT_7 (see [DL92]). But, the path metric of $K_7 - P_3$ violates this inequality if P_3 is the path $(2, 1, 3)$ in the complete graph K_7 on the nodes 1,2,3,4,5,6,7. Hence, $K_7 - P_3$ is not an ℓ_1-graph.)
• The path metrics of $K_9 - P_3$, $K_{10} - P_3$ are of negative type, but not hypermetric.
(Hint: The path metric of $K_9 - P_3$ violates the hypermetric inequality (1.4) for $b := (3, 2, 2, -1, -1, -1, -1, -1, -1)$ if P_3 is the path $(2, 1, 3)$.)
• The distance matrix of $K_{11} - P_3$ has exactly one positive eigenvalue, but $K_{11} - P_3$ is not of negative type; the distance matrix of $K_n - P_3$ has two positive eigenvalues for all $n \ge 12$. (Hint: $K_{11} - P_3$ is not of negative type since it violates the negative type inequality (1.4) for $b := (\frac{24}{7}, \frac{16}{7}, \frac{16}{7}, -1, -1, -1, -1, -1, -1, -1, -1)$ if P_3 is the path $(2, 1, 3)$.) Another example of a graph which is not of negative type but whose distance matrix has one positive eigenvalue is given in Example 5.2. ∎

Finally, let us mention another formulation for the isometric dimension of a hypercube embeddable graph, in terms of the number of negative eigenvalues of its distance matrix.

PROPOSITION 2.16. [GW85] *Let G be a graph with distance matrix D_G and let $n_+(D_G)$, $n_-(D_G)$ denote the number of positive and negative eigenvalues of D_G. If G is hypercube embeddable, then $dim_I(G) = n_-(D_G)$ and $n_+(D_G) = 1$ hold.*

PROOF. Suppose that G embeds isometrically into the k-hypercube, i.e., $dim_I(G) = k$. Denote by $\alpha(a) = (a_1, \ldots, a_k) \in \{0,1\}^k$ the image of each node $a \in V$ under this embedding. For $h = 1, \ldots, k$, set

$$X_h = \{a \in V : a_h = 0\},\ Y_h = \{a \in V : a_h = 1\} = V \setminus X_h.$$

Then,

$$\begin{aligned}\sum_{a,b\in V} d_G(a,b)x_ax_b &= \sum_{a,b\in V}(\sum_{1\le h\le k}|a_h-b_h|)x_ax_b = \sum_{1\le h\le k}(\sum_{a\in X_h}x_a)(\sum_{b\in Y_h}x_a)\\ &= \tfrac{k}{4}(\sum_{a\in V}x_a)^2 - \frac{1}{4}\sum_{1\le h\le k}(\sum_{a\in X_h}x_a-\sum_{b\in Y_h}x_b)^2\end{aligned}$$

(where the last equality is obtained using the identity $xy=\frac{1}{4}((x+y)^2-(x-y)^2)))$. Hence, the quadratic form

$$\sum_{a,b\in V} d_G(a,b)x_ax_b$$

can be written as the sum of one "positive" square and k "negative" squares. By Sylvester's law of inertia, this implies that $n_+(D_G)\le 1$ and $n_-(D_G)\le k$. On the other hand, $n_+(D_G)\ge 1$ since D_G has trace zero. Hence, $n_+(D_G)=1$ and the rank of D_G satisfies $rank(D_G)=n_+(D_G)+n_-(D_G)\le k+1$. We show that $rank(D_G)=k+1$. This will imply that $n_-(D_G)=k$, thus stating the result.

We can suppose without loss of generality that a given node $a^{(0)}$ of G receives the label $\alpha(a^{(0)})=(0,\ldots,0)$ in the hypercube embedding. We claim that there exist k nodes $a^{(1)},\ldots,a^{(k)}$ of G whose labels $\alpha(a^{(1)}),\ldots,\alpha(a^{(k)})$ are linearly independent. For this, it suffices to check that the system $\{\alpha(a): a\in V\}\subseteq\{0,1\}^k$ has full dimension k. Suppose for contradiction that, say, the k-th coordinate can be expressed in terms of the others, i.e., there exist scalars $\lambda_1,\ldots,\lambda_{k-1}$ such that $a_k=\sum_{1\le j\le k-1}\lambda_ja_j$ for all $a\in V$. Then, $a_k=b_k$ holds for any two adjacent nodes a,b in G. This implies that $a_k=0$ holds for each node $a\in V$, by considering a shortest path from $a^{(0)}$ to a. So, one could have embedded G into the $(k-1)$-hypercube, contradicting the fact that $dim_I(G)=k$. We now claim that the submatrix

$$M:=(d_G(a^{(i)},a^{(j)}))_{i,j=0,\ldots,k}$$

is nonsingular. This will imply that $rank(D_G)\ge k+1$ and, therefore, $rank(D_G)=k+1$. For $i=0,1,\ldots,k$, set

$$u^{(i)}=2\alpha(a^{(i)})-e,$$

where $e=(1,\ldots,1)$. As the vectors $u^{(i)}$ are ±1-valued, we have

$$\begin{aligned}d_G(a^{(i)},a^{(j)}) &= \sum_{1\le h\le k}|a_h^{(i)}-a_h^{(j)}| = \frac{1}{2}\sum_{1\le h\le k}|u_h^{(i)}-u_h^{(j)}|\\ &= \tfrac{1}{2}\sum_{1\le h\le k}(1-u_h^{(i)}u_h^{(j)}) = \frac{k}{2}-\frac{1}{2}(u^{(i)})^Tu^{(j)}.\end{aligned}$$

Therefore,

$$M=\frac{k}{2}J-\frac{1}{2}Gram(u^{(0)},u^{(1)},\ldots,u^{(k)}),$$

where J denotes the all ones matrix and $Gram(u^{(0)},u^{(1)},\ldots,u^{(k)})$ denotes the Gram matrix of the vectors $u^{(0)},u^{(1)},\ldots,u^{(k)}$. One can easily check that

$$\begin{aligned}\det(M)= \; & (-2)^{-(k+1)}\Big(\det(Gram(u^{(0)},u^{(1)},\ldots,u^{(k)}))\\ & -k\ \det(Gram(u^{(1)}-u^{(0)},u^{(2)}-u^{(0)},\ldots,u^{(k)}-u^{(0)}))\Big).\end{aligned}$$

But, $\det(Gram(u^{(0)},u^{(1)},\ldots,u^{(k)}))=0$ since the vectors $u^{(0)},u^{(1)},\ldots,u^{(k)}$ are linearly dependent, and $\det(Gram(u^{(1)}-u^{(0)},u^{(2)}-u^{(0)},\ldots,u^{(k)}-u^{(0)}))\neq 0$ since the vectors $u^{(1)}-u^{(0)},u^{(2)}-u^{(0)},\ldots,u^{(k)}-u^{(0)}$ are linearly independent. Therefore, $\det(M)\neq 0$. ∎

The next result gives an example of application of hypercube embeddable graphs within the context of oriented matroids (see [FH93] for definitions).

THEOREM 2.17. [FH93] *A graph G is isomorphic to the tope graph of an oriented matroid of rank at most three if and only if G is planar, hypercube embeddable, and antipodal (i.e., for each node u of G, there is a unique node u^* which is not closer to u than any neighboor of u^*).*

We conclude this section with some remarks on two possible relaxations of the notion of isometric embeddability into the hypercube. First, one may consider isometric embeddings into the squashed hypercube; second, one may consider embeddings as a subgraph (not necessarily isometric) into the hypercube.

REMARK 2.18. **Isometric embedding into squashed hypercubes.**
As we just saw, not every graph can be isometrically embedded into a hypercube. For this reason, Graham and Pollak [GP71] considered isometric embeddings into squashed hypercubes. Let d_* denote the distance defined on the set $B_* = \{0, 1, *\}$ by setting

$$d_*(x, y) = \begin{cases} 1 \text{ if } \{x, y\} = \{0, 1\} \\ 0 \text{ otherwise} \end{cases}$$

for $x, y \in B_*$. Hence, the symbol $*$ is at distance 0 from the other symbols; it is also called the "don't care" symbol. The distance d_* can be extended to B_*^m by setting

$$d_*((x_1, \ldots, x_m), (y_1, \ldots, y_m)) = \sum_{1 \le i \le m} d_*(x_i, y_i).$$

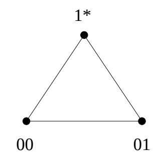
The distance space (B_*^m, d_*) is called the **squashed m-hypercube**. It contains the usual m-hypercube as a subspace. Each element $(x_1, \ldots, x_m) \in B_*^m$ can be thought of as representing a face of the m-dimensional hypercube, namely, the face consisting of all $y \in \{0, 1\}^m$ such that $y_i = x_i$ for all i such that $x_i \in \{0, 1\}$. A nice property of squashed hypercubes is that every connected graph can be isometrically embedded in some squashed hypercube. Indeed, let G be a connected graph with node set $\{1, \ldots, n\}$. Set

$$m := \sum_{1 \le i < j \le n} d_G(i, j).$$

For $1 \le i < j \le n$, let D_{ij} be pairwise disjoint subsets of $\{1, \ldots, m\}$ with $|D_{ij}| = d_G(i, j)$. Label each node i by the m-tuple $(i_1, \ldots, i_m) \in B_*^m$ by setting

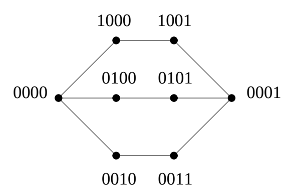
$$i_k = \begin{cases} 0 \text{ if } k \in \bigcup_{h=i+1}^{n} D_{ih} \\ 1 \text{ if } k \in \bigcup_{h=1}^{i-1} D_{ih} \\ \ \text{otherwise.} \end{cases}$$

Then, $d_*((i_1, \ldots, i_m), (j_1, \ldots, j_m)) = |D_{ij}| = d_G(i, j)$. This shows that G can be isometrically embedded into the squashed m-hypercube. Let $r(G)$ denote the smallest dimension of a squashed hypercube in which G can be embedded. Winkler [Win83] showed that $r(G) \le n - 1$ for each graph on n nodes. On the other hand, $r(G) \ge \max(n_+(D_G), n_-(D_G))$, where $n_+(D_G), n_-(D_G)$ denote the number of positive and negative eigenvalues of the distance matrix D_G of G [GP72]. For instance, $r(K_n) = n - 1$ since $n_-(D_{K_n}) = n - 1$. The next picture shows the embedding of K_3 into the squashed 2-hypercube.



∎

REMARK 2.19. **Nonisometric embedding of graphs into hypercubes.**
Another relaxation of the notion of hypercube embeddable graphs is that of cubical graphs. A graph G is said to be **cubical** if G is a subgraph of some hypercube $H(m,2)$, i.e., there exists an injective mapping from the node set of G to the node set of $H(m,2)$ which maps edges of G to edges of $H(m,2)$. Clearly, every cubical graph is bipartite and every hypercube embeddable graph is cubical. We show below an example of a graph which is cubical but not hypercube embeddable.



The structure of the minimal noncubical graphs has been studied in [GG75], where some constructions of such graphs are presented. For instance, $K_{2,3}$ and odd cycles are minimal noncubical graphs. Recall from Remark 2.4 that one can check in polynomial time whether a graph G is hypercube embeddable and, moreover, the minimum dimension $m_h(G)$ of a hypercube containing G as an isometric subgraph can be computed in polynomial time. On the other hand, it has been proved that deciding whether a graph G is cubical is an NP-complete problem ([APP85, APP89], [KVC86]). Moreover, for G cubical, computing the minimum dimension of a hypercube containing G as a subgraph is also a difficult problem. For instance, each tree is cubical (in fact, a tree on n nodes can be isometrically embeded into an $(n-1)$-hypercube). But, given a tree T and an integer m, it is NP-complete to decide whether T is a subgraph of the m-hypercube [WC90]. The problem of determining the minimum dimension of a hypercube containing a tree has been long studied (see, e.g., [HL72, HL73]). Along the same lines, given a graph G and integers m, k, it is NP-complete to decide whether G is a subgraph of $(K_m)^k$ [WC]. ∎

3 Isometric embeddings of graphs into cartesian products

We have characterized in the previous Section 2 the graphs that can be isometrically embedded into a hypercube. The hypercube is the simplest example of a cartesian product of graphs; namely, the m-hypercube is nothing but $(K_2)^m$. We consider here isometric embeddings of graphs into arbitrary cartesian products. It turns out that every graph can be isometrically embedded in a canonical way into a cartesian product whose factors are "irreducible", i.e., cannot be further embedded into cartesian products. We present two applications of this result, for finding the prime factorization of a graph, and for showing that the path metric of every bipartite graph can decomposed in a unique way as a nonnegative combination of primitive semimetrics.

3.1 The canonical metric representation of a graph

Let G, H be two graphs. Their **cartesian product** is the graph $G \times H$ with node set $V(G) \times V(H)$ and whose edges are the pairs $((a,x),(b,y))$ with $a, b \in V(G)$, $x, y \in V(H)$ and such that, either $(a,b) \in E(G)$ and $x = y$, or $a = b$ and $(x,y) \in E(H)$. The cartesian product $H_1 \times \ldots \times H_k$ of k graphs $H_1, \ldots, H_k$ is also denoted as $\prod_{1 \leq h \leq k} H_h$. An isometric embedding of a graph G into the cartesian product $\prod_{1 \leq i \leq k} H_i$ is said to be **iredundant** if each factor H_h is a connected graph on at least two nodes, and each vertex of every factor H_h appears as a coordinate in the image of at least one node of G. Clearly, any isometric embedding into a cartesian product can be made irredundant by discarding the factors consisting of an isolated node and the unused nodes in each factor. An irredundant isometric embedding of G into a cartesian product is also called a **metric representation** of G. Two isometric embeddings of G into cartesian products are said to be **equivalent** if there is a bijection between the factors of one and the factors of the other, together with isomorphisms between the corresponding factors for which the obvious diagram commutes. A graph G is said to be **irreducible** if all its metric representations are equivalent to the trivial embedding of G into itself.

We can now state the main result of this section. It is due to Graham and Winkler [GW85]; see, also, [Win87b, Gra88].

THEOREM 3.1. *Every connected graph G has a unique metric representation*

$$G \hookrightarrow \prod_{1 \leq h \leq k} G_h$$

in which each factor G_h is irreducible; it is called the **canonical metric representation** *of G. Moreover, $k = dim_I(G)$ and, if*

$$G \hookrightarrow \prod_{1 \leq i \leq m} H_i$$

is another metric representation of G, then there exist a partition $(S_1, \ldots, S_m)$ of $\{1, \ldots, k\}$ and metric representations

$$H_i \hookrightarrow \prod_{h \in S_i} G_h,$$

for $i \in \{1, \ldots, m\}$, for which the obvious diagram commutes.

An essential tool for the proof of Theorem 3.1 is the following Lemma 3.2.

LEMMA 3.2. *Let $E_1, \ldots, E_k$ denote the equivalence classes of the transitive closure θ^* of the relation θ, defined in relation* (1.2). *Given two nodes a, b of G, let P be a shortest path from a to b, and let Q be another path joining a to b in G. Then, for all $h = 1, \ldots, k$,*

$$|E(P) \cap E_h| \leq |E(Q) \cap E_h|.$$

PROOF. Set $P = (x_0 = a, x_1, \ldots, x_p = b)$. For any index $h \in \{1, \ldots, k\}$ and any node x of G, set

$$f_h(x) := \sum_{i \in \{1,\ldots,p\} | (x_{i-1}, x_i) \in E_h} (d_G(x, x_i) - d_G(x, x_{i-1})).$$

Hence, $f_h(a) = |E(P) \cap E_h|$ and $f_h(b) = -|E(P) \cap E_h|$. Let (x, y) be an edge of G. We claim

$$f_h(x) = f_h(y) \ \text{ if } \ (x, y) \notin E_h.$$

Indeed, $f_h(x) - f_h(y) = \sum_{i:(x_{i-1},x_i) \in E_h} (d_G(x, x_i) - d_G(y, x_i)) - (d_G(x, x_{i-1}) - d_G(y, x_{i-1})) = 0$, since the edge (x, y) is not in relation by θ with any of the edges of E_h. On the other hand,

$$|f_h(x) - f_h(y)| \leq 2 \ \text{ if } \ (x, y) \in E_h.$$

Indeed, by the above argument, we have

$$\begin{aligned} |f_h(x) - f_h(y)| &= |\sum_{1 \leq j \leq k} (f_j(x) - f_j(y))| \\ &= |(d_G(x, b) - d_G(x, a)) - (d_G(y, b) - d_G(y, a))| \\ &\leq |d_G(x, b) - d_G(x, a)| + |d_G(y, b) - d_G(y, a)| \\ &\leq 2. \end{aligned}$$

As $f_h(a) = |E(P) \cap E_h|$ and $f_h(b) = -|E(P) \cap E_h|$, when moving along the nodes of the path Q, the function $f_h(.)$ changes in absolute value by $2|E(P) \cap E_h|$. But, on an edge of $E \setminus E_h$, the function $f_h(.)$ remains unchanged and, on an edge of E_h, $f_h(.)$ increases by at most 2. This implies that the path Q must contain at least $|E(P) \cap E_h|$ edges from E_h. ∎

PROOF OF THEOREM 3.1. As in Lemma 3.2, let $E_1, \ldots, E_k$ denote the equivalence classes of the transitive closure θ^* of the relation θ. For each $h = 1, \ldots, k$, let G_h denote the graph obtained from G by contracting the edges of $E \setminus E_h$. In other words, for constructing G_h, one identifies any two nodes of G that are joined by a path containing no edge from E_h. This defines a surjective mapping σ_h from $V(G)$ to $V(G_h)$ and a mapping $\sigma : V(G) \longrightarrow \prod_{1 \leq h \leq k} V(G_h)$ by setting $\sigma(v) = (\sigma_1(v), \ldots, \sigma_k(v))$ for each node v of G. We show that the mapping σ provides the required metric representation of G. For this, we have to check that σ is an irredundant isometric embedding and that each factor G_h is irreducible. Take two nodes a, b of G and a shortest path P from a to b in G. We show

$$d_G(a, b) = \sum_{1 \leq h \leq k} d_{G_h}(\sigma_h(a), \sigma_h(b)).$$

Indeed, for each h, $d_{G_h}(\sigma_h(a), \sigma_h(b))$ is the minimum value of $|E(Q) \cap E_h|$ over all paths Q joining a and b; hence, by Lemma 3.2, $d_{G_h}(\sigma_h(a), \sigma_h(b)) = |E(P) \cap E_h|$. Therefore,

$$\sum_{1 \leq h \leq k} d_{G_h}(\sigma_h(a), \sigma_h(b)) = \sum_{1 \leq h \leq k} |E(P) \cap E_h| = |E(P)| = d_G(a, b).$$

This shows that σ is an isometric embedding of G into $\prod_{1 \leq h \leq k} G_h$. Moreover, by Lemma 3.2 again, the endpoints of an edge of E_h are not identified when constructing G_h. Hence, each factor G_h has at least two nodes. Therefore, the embedding σ is irredundant since the mappings σ_h are surjective.

Consider now another metric representation

$$G \hookrightarrow \prod_{1 \leq j \leq m} H_j$$

of G and denote by $(x_1, \ldots, x_m)$ the image of a node x of G. If $e = (x, y)$ is an edge of G corresponding to an edge in the j-th factor H_j, i.e., $(x_j, y_j) \in E(H_j)$ and $x_i = y_i$ for all $i \in \{1, \ldots, m\} \setminus \{j\}$, then each edge f in relation by θ with e is also an edge in H_j. Therefore, each factor H_j "contains" exactly the edges of $\bigcup_{i \in J} E_i$ for some nonempty set J of indices. In particular, $m \leq k$ holds. This implies that each factor G_h is irreducible (else, one would have a metric representation of G with more than k factors). Therefore, $G \hookrightarrow G_1 \times \ldots \times G_k$ is the canonical metric representation of G. This concludes the proof. ∎

Corollary 3.3. *Let G be a connected graph.*
(i) G is irreducible if and only if $dim_I(G) = 1$.
(ii) If G has n nodes, then $dim_I(G) \leq n - 1$, with equality if and only if G is a tree.
(iii) G embeds isometricaly into $(K_3)^m$ for some $m \geq 1$ if and only if the relation θ is transitive.
(iv) G embeds isometrically into $(K_2)^m$ for some $m \geq 1$ if and only if G is bipartite and θ is transitive.

Proof. (i) follows immediately from Theorem 3.1.
(ii) Set $k := dim_I(G)$ and let T be a spanning tree in G. We claim that T contains at least one edge from each equivalence class E_h. Indeed, if e is an edge from $E \setminus E(T)$ belonging to the class E_h then, by Lemma 3.2, T must contain at least one edge from E_h. Therefore, $n - 1 = |E(T)| \geq k$ holds. If there are two edges $e, f \in E$ in relation by θ, let T be a spanning tree containing both e and f; then, $k \leq n - 2$ holds. This shows that equality $k = n - 1$ holds only if G is a tree.
(iii) Note that G embeds isometrically into $(K_3)^m$ if and only if each factor G_h in the canonical representation of G is K_2 or K_3 (see Remark 3.7). On the other hand, G_h is K_2 or K_3 if and only if E_h consists of all the edges that are cut by the partition of V into $G(a, b) \cup G(b, a) \cup G_=(a, b)$, where $(a, b) \in E_h$, in which case θ is transitive.
(iv) follows from (iii) since $G_=(a, b) = \emptyset$ for each edge (a, b) when G is bipartite. ∎

One can easily check that, for G bipartite, the relation θ is transitive if and only if $G(a, b)$ is convex for all adjacent nodes a, b of G. Hence, Corollary 3.3 (iv) implies the characterization of hypercube embeddable graphs stated in Theorem 2.2. In particular, if G is hypercube embeddable with isometric dimension $dim_I(G) = k$, then $G \hookrightarrow (K_2)^k$ is the canonical metric representation of G. Lomonossov and Sebö give the following additional information.

Proposition 3.4. [LS93] *If G is a bipartite graph, then the factors $G_1, \ldots, G_k$ of its canonical metric representation are all bipartite graphs.*

Proof. Suppose, for contradiction, that a factor G_h of the canonical metric representation of G is not bipartite. Then, there exists a cycle C of G such that $|E(C) \cap E_h|$ is odd. Choose such a cycle C of minimal length. As G is bipartite, C has even length, say $C = (a_1, a_1, \ldots, a_{2m})$. Consider the pairs (a_i, a_{m+i}) (where the indices are taken modulo m) of diametrally opposed nodes of C. If $d_G(a_i, a_{m+i}) = d_G(a_{i+1}, a_{m+i+1}) = m$, then $d_G(a_{m+i}, a_{i+1}) - d_G(a_{m+i}, a_i) = -1$ and $d_G(a_{m+i+1}, a_{i+1}) - d_G(a_{m+i+1}, a_i) = 1$, which implies that the edges (a_i, a_{i+1}) and (a_{m+i}, a_{m+i+1}) are in relation by θ. Hence, there exists a pair (a_i, a_{m+i}) for which $d_G(a_i, a_{m+i}) < m$ (otherwise, any two oposite edges of C are in relation by θ, implying that $|E(C) \cap E_h|$ is even). Let P be a shortest path from a_i to a_{m+i} in G. Suppose that only the endnodes of P are on C. The endnodes of P partition C into two paths which, together with P, form two cycles C_1 and C_2. As C_1 and C_2 have smaller length than C, we deduce that both $|E(C_1) \cap E_h|$ and $|E(C_2) \cap E_h|$ are even. This implies that $|E(C) \cap E_h|$ is even, yielding a contradiction. The reasoning is the same if P meets C in other nodes than its endnodes. ∎

Examples of irreducible graphs include: the complete graph K_n $(n \geq 2)$, odd cycles C_{2n+1} $(n \geq 1)$, the half-cube $\frac{1}{2}H(n,2)$ $(n \geq 2)$, the cocktail-party graph $K_{n\times 2}$ $(n \geq 3)$, the Petersen graph, the Gosset graph G_{56}, the Schläfli graph G_{27}, etc... Actually, it is observed in [GW85] that the probability that a random graph (with edge probability 1/2) on n nodes is irreducible goes to 1 as $n \longrightarrow \infty$.

The canonical metric representation $G \hookrightarrow G_1 \times \ldots \times G_k$ of a graph G can be found in polynomial time. Indeed, it can be obtained in the following way:
- Compute the relation θ.
- Determine the equivalence classes $E_1, \ldots, E_k$ of the transitive closure θ^* of θ.
- For each $h = 1, \ldots, k$, construct the graph G_h from G by contracting the edges of $E \setminus E_h$.

Hence, if G has n nodes and m edges, then its canonical metric representation can be obtained in $O(m^2)$ steps. Feder [Fed92] shows how to construct it in $O(mn)$ steps using $O(m)$ space.

The following rules can be applied for determining the equivalence classes of θ^*:
- Any two edges on an odd isometric cycle are in relation by θ.
- Let $C = (a_1, \ldots, a_{2m})$ be an even cycle. Call the two edges $e_i := (a_i, a_{i+1})$ and $e_{m+i} := (a_{m+i}, a_{m+i+1})$ (where the indices are taken modulo m) **opposite** on C if $d_G(a_i, a_{m+i}) = d_G(a_{i+1}, a_{m+i+1}) = m$. Clearly, if e_i and e_{m+i} are opposite on C, then e_i and e_{m+i} are in relation by θ.

It is observed in [LS93] that, if G is a bipartite graph, then two edges are in relation by θ if and only if they are opposite on some even cycle of G. A similar characterization of the relation θ is given for arbitrary graphs in [LS93].

We now illustrate the method on an example.

Example 3.5. Let G be the graph from Figure 3.6. The relation θ^* has three equivalence classes:

$$E_1 = \{12, 13, 23, 45, 46, 56\},\ E_2 = \{17, 39, 48, 5\ 10\},$$

$$E_3 = \{14, 35, 78, 9\ 10\}$$

(where we denote an edge (i,j) by the string ij). The edges of E_1,E_2,E_3 are represented by plain, dotted, and dark edges, respectively. Hence, $G \hookrightarrow G_1 \times G_2 \times G_3$ is the canonical metric representation of G, where G_1, G_2, G_3 are the graphs indicated in Figure 3.6. (The set asociated to each node in the factor G_h is the set of nodes of G that have been identified during the construction of G_h.) ∎

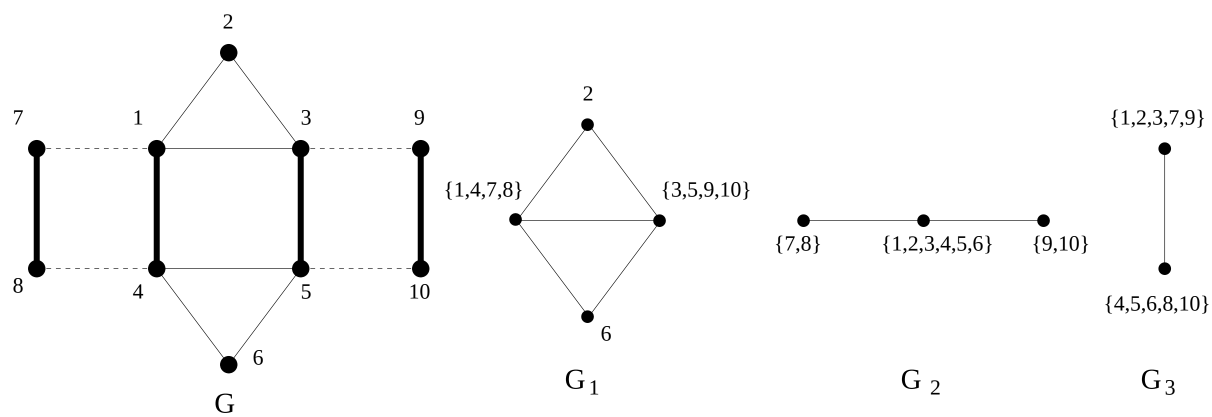


Figure 3.6

REMARK 3.7. **Isometric embedding into Hamming graphs.**
We recall that a graph can be isometrically embedded into a Hamming graph (i.e., a cartesian product of complete graphs) if its nodes can be labeled by sequences of nonnegative integers in such a way that the distance between two nodes coincides with the Hamming distance between the corresponding sequences. It follows from Theorem 3.1 that a graph G embeds isometrically into a Hamming graph if and only if each factor G_h in the canonical metric representation of G is a complete graph. (Indeed, let $\alpha : G \hookrightarrow \prod_{1\leq i\leq m} K_{q_i}$ be an isometric embedding of G into a Hamming graph. We may assume that α is irredundant since deleting a node from a complete graph yields another complete graph. Therefore, as complete graphs are irreducible, α is the canonical metric representation of G.) In particular, the embedding into a Hamming graph is unique [Win84]. One can recognize isometric subgraphs of Hamming graphs in polynomial time. An algorithm running in $O(mn)$ time and using $O(m)$ space is given in [IK93]. Wilkeit [Wil90] proposes an algorithm with running time $O(n^3)$, which yields moreover a structural characterization for isometric subgraphs of Hamming graphs.

As an example, consider the graph H from Figure 3.8 (taken from [Wil90]). The relation θ^* has three equivalences classes:

$$E_1 = \{12, 34, 35, 45\},$$

$$E_2 = \{28, 37, 56\}, \text{ and } E_3 = \{14, 23, 78\}.$$

Hence, $H \hookrightarrow K_3 \times K_2 \times K_2$ is the canonical metric representation of H. We also indicate for the graph H in Figure 3.8 the sequences from $\{0,1,2\} \times \{0,1\}^2$ providing the correct labeling of the nodes of H. Equivalently, the path metric of H can be decomposed as an integer sum of multicut semimetrics, namely,

$$d_H = \delta(\{1,4\},\{2,3,7,8\},\{5,6\}) + \delta(\{1,2,3,4,5\},\{6,7,8\}) + \delta(\{1,2,8\},\{3,4,5,6,7\}).$$

∎

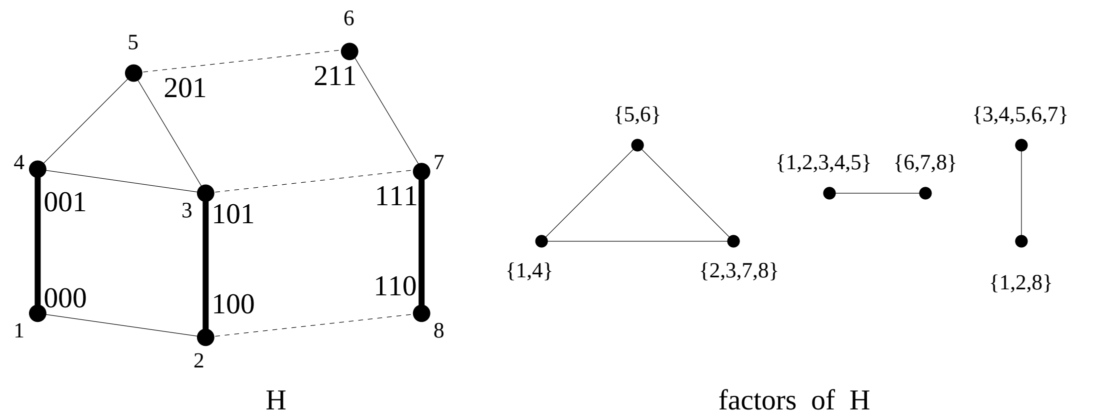


Figure 3.8

3.2 The prime factorization of a graph

Let G be a connected graph. A **factorization** of G is a metric representation which is an isomorphism. G is said to be **prime** if G cannot be decomposed as the cartesian product of two other graphs (each having at least two nodes). Sabidussi [Sab60] proved that every connected graph admits a unique prime factorization. Unicity is lost for disconnected graphs (see [Zar65]). The **Graph Factoring problem** can be stated as follows.

Instance. A connected graph G.
Question. Is G prime and, if not, find the prime factorization of G.

This problem can be solved in time polynomial in the number of nodes [FHS85, Win87a]. We restrict ourselves to connected graphs since the Graph Factoring problem for disconnected graphs is at least as hard as the Graph Isomorphism problem. (Indeed, one can determine whether two graphs G and H are isomorphic by checking whether the graph consisting of two isolated nodes is a factor of the disjoint union of G and H.) The algorithm proposed in [FHS85] is rather difficult and based on Sabidussi's original proof; it runs in $O(n^{4.5})$. Winkler [Win87a] proposes an algorithm which is based on the canonical metric representation of graphs presented in Section 3.1; it runs in $O(n^4)$. We describe briefly the main ideas of the algorithm.

Let G be the connected graph whose prime factorization is to be found. Let

$$\sigma : V(G) \longrightarrow \prod_{1 \le h \le k} V(G_h)$$

denote the canonical metric representation of G and set

$$\sigma(a) = (\sigma_1(a), \ldots, \sigma_k(a))$$

for each node $a \in V$. Set $S := \{1, \ldots, k\}$. For a subset T of S, let σ_T denote the mapping from V to $\prod_{h \in T} V(G_h)$ defined by

$$\sigma_T(a) = (\sigma_h(a) : h \in T)$$

for $a \in V$. A partition $(S_1, \ldots, S_m)$ of S is said to be "**good**" if

$$\sigma(V) = \prod_{1 \leq i \leq m} \sigma_{S_i}(V).$$

If this is the case, then

$$G = \prod_{1 \leq i \leq m} \sigma_{S_i}(G)$$

gives a factoring of G. In particular, the prime factorization of G corresponds to a good partition of S. A subset T of S is said to be **complete** if

$$\sigma_T(V) = \prod_{h \in T} V(G_h).$$

A subset $T \subseteq S$ can be checked for completeness in polynomial time. If S is itself is complete, then $G = G_1 \times \ldots \times G_k$ is the prime factorization of G. Otherwise, S is not complete. One can find a minimum incomplete subset T of S in polynomial time. (Indeed, check whether all $(k-1)$-subsets of S are complete. If yes, then S is minimal incomplete. Else, let T be an incomplete $(k-1)$-subset of S. Check all $(k-2)$-subsets of T, and so on.) The crucial fact is that, if T is minimal incomplete and if $(S_1, \ldots, S_m)$ is a good partition of S, then $T \subseteq S_i$ for some $i \in \{1, \ldots, m\}$. (If not, then $T \cap S_1, \ldots, T \cap S_m$ are complete, from which one deduces that T itself is complete.) Now, $\sigma_T(G)$ cannot be split in a factorization of G. Hence, we may consider the metric representation

$$G \hookrightarrow \sigma_T(G) \times \prod_{h \in S \setminus T} G_h$$

instead of the initial representation $G \hookrightarrow \prod_{1 \leq h \leq k} G_h$. The new representation has at most $k-1$ factors (since $|T| \geq 2$, as singletons are complete). We repeat the process with this new representation until we find a representation whose index set is complete. This final representation is the prime factorization of G.

Feder [Fed92] shows how this algorithm can be performed in $O(mn)$ steps using $O(m)$ space; another algorithm running in $O(m \log n)$ time and using $O(m)$ space is proposed in [AHI90].

3.3 Metric decomposition of bipartite graphs

We recall that the semimetric cone MET_n is defined by

$$\mathrm{MET}_n := \{x \in \mathbb{R}^{\binom{n}{2}} : x_{ij} - x_{ik} - x_{jk} \leq 0 \text{ for all } i, j, k \in \{1, \ldots, n\}\}.$$

In other words, MET_n consists of all semimetrics on n points. A semimetric $d \in \mathrm{MET}_n$ is said to be **primitive** if d lies on an extreme ray of MET_n, i.e., $d = d_1 + d_2$ with

$d_1, d_2 \in \mathrm{MET}_n$ implies that $d_1 = \alpha_1 d$, $d_2 = \alpha_2 d$ for some $\alpha_1, \alpha_2 \geq 0$. For $d \in \mathrm{MET}_n$, one can define its **0-lifting** $d' \in \mathrm{MET}_{n+1}$ by setting

$$\begin{cases} d'_{1,n+1} = 0 & \\ d'_{i,n+1} = d_{1,i} & \text{for } i = 2, \ldots, n \\ d'_{ij} = d_{ij} & \text{for } 1 \leq i < j \leq n. \end{cases}$$

Given $d \in \mathrm{MET}_n$, let $F(d)$ denote the smallest face of MET_n that contains d. Hence, $F(d)$ consists of all vectors $y \in \mathrm{MET}_n$ that satisfy the same triangle equalities as d, i.e., such that $y_{ij} - y_{ik} - y_{jk} = 0$ whenever $d_{ij} - d_{ik} - d_{jk} = 0$. One checks easily that $F(d)$ is a simplex, i.e., the primitive semimetrics lying on $F(d)$ are linearly independent, if and only if d admits a unique decomposition as a sum of primitive semimetrics.

Let G be a connected graph on n nodes. Its path metric d_G belongs to the semimetric cone MET_n. Hence, a natural question to ask is what are the possible decompositions of d_G as a sum of primitive semimetrics. It is shown below that, if G is a bipartite graph, then d_G admits a unique such decomposition, i.e., d_G lies on a simplex face of MET_n. In fact, the primitive semimetrics entering the decomposition of d_G are the 0-liftings of the path metrics of the factors of the canonical metric representation of G.

THEOREM 3.9. [LS93] *Let G be a connected bipartite graph on n nodes with isometric dimension $dim_I(G) = k$. Let $F(d_G)$ denote the smallest face of the semimetric cone MET_n that contains d_G. Then, $F(d_G)$ is a simplex face of MET_n of dimension k.*

PROOF. Let $E_1, \ldots, E_k$ denote the equivalence classes of the relation θ^* and let

$$G \hookrightarrow \prod_{1 \leq h \leq k} G_h$$

denote the associated canonical metric representation of G. For a node $a \in V$, denote by $(a_1, \ldots, a_k)$ its image under the canonical embedding. For $h = 1, \ldots, k$, let d_h denote the semimetric on V defined by

$$d_h(a, b) = d_{G_h}(a_h, b_h)$$

for $a, b \in V$. Then, d can be decomposed as

$$d = \sum_{1 \leq h \leq k} d_h.$$

The semimetrics $d_1, \ldots, d_k$ are clearly linearly independent and they belong to the face F_G. We show that $F(d_G)$ is generated by $\{d_1, \ldots, d_k\}$. For this, we show that each $x \in F_G$ is of the form $x = \sum_{1 \leq h \leq k} \alpha_h d_h$ for some scalars $\alpha_h \geq 0$. Let $x \in F_G$. By definition, this means that every triangle inequality which is satisfied at equality by d_G is also satisfied at equality by x. We claim that, if $e = (a, b)$ and $e' = (a', b')$ are edges of G, then

$$e \theta e' \implies x(a, b) = x(a', b').$$

Indeed, as G is bipartite, we can suppose that $a' \in G(a, b)$ and $b' \in G(b, a)$. One can easily check that d_G satisfies the following four triangle equalities:

$$d_G(a', b) = d_G(a', a) + d_G(a, b), \; d_G(a, b') = d_G(a, b) + d_G(b, b'),$$

$$d_G(a',b) = d_G(a',b') + d_G(b,b'), \text{ and } d_G(a,b') = d_G(a,a') + d_G(a',b').$$

Hence, x satisfies these four triangle equalities too. From the first two equalities, we obtain

$$x(a',b) - x(a,b') = x(a',a) - x(b,b'),$$

and the last two imply

$$x(a',b) - x(a,b') = x(b,b') - x(a,a').$$

Therefore, $x(a,a') = x(b,b')$ and $x(a,b') = x(a',b)$ which imply that $x(a,b) = x(a',b')$. Hence, there exist scalars $\alpha_1, \ldots, \alpha_k \geq 0$ such that $x(a,b) = \alpha_h$ for each edge (a,b) in the class E_h. We show

$$x = \sum_{1 \leq h \leq k} \alpha_h d_h.$$

Let $a, b \in V$ and let $P := (a_0 = a, a_1, \ldots, a_p = b)$ be a shortest path from a to b in G. Set $N_h = |E(P) \cap E_h|$ for $h = 1, \ldots, k$. Using the triangle equalities along P, one obtains that $x(a,b) = \sum_{1 \leq i \leq p} x(a_{i-1}, a_i) = \sum_{1 \leq h \leq k} \alpha_h N_h$. As P contains N_h edges from E_h, by contracting the other edges of P, we obtain in the graph G_h a path from a_h to b_h of length N_h. This shows that $d_{G_h}(a_h, b_h) \leq N_h$. Let Q' be a shortest path from a_h to b_h in G_h. So, Q' arises from a path Q joining a to b in G. By Lemma 3.2, Q contains at least N_h edges from E_h. Therefore, $|Q'| \geq N_h$, implying that $d_{G_h}(a_h, b_h) = N_h$. Hence, we have $\sum_{1 \leq h \leq k} \alpha_h d_h(a,b) = \sum_{1 \leq h \leq k} \alpha_h N_h = x(a,b)$.
So, we have shown that $F(d_G)$ is generated by $\{d_1, \ldots, d_k\}$. Therefore, $F(d_G)$ is a simplex face of dimension k of MET_n. ∎

COROLLARY 3.10. *Let G be a connected bipartite graph. Then, its path metric d_G lies on an extreme ray of the semimetric cone MET_n if and only if $dim_I(G) = 1$, i.e., G is irreducible.* ∎

Corollary 3.10 is not valid for nonbipartite graphs. For instance, K_3 is irreducible, but its path metric lies in the interior of the semimetric cone MET_3.

4 ℓ_1-graphs

We study in this section ℓ_1-graphs, i.e., the graphs whose path metric can be isometrically embedded into an ℓ_1-space. As was recalled in Section 1, a graph G is an ℓ_1-graph if it is hypercube embeddable, up to scale. A **λ-embedding** of G into the hypercube $H(\Omega)$ is any mapping

$$x \in V \mapsto X \subseteq \Omega$$

such that

$$\lambda d_G(x,y) = |X \triangle Y|$$

for all nodes x, y of G. If G has a λ-embedding into a hypercube, we also say that G is hypercube embeddable with scale λ. A 1-embedding in a hypercube is nothing but an isometric embedding in a hypercube.

Three classes of graphs play a crucial role in the theory of ℓ_1-graphs: complete graphs, cocktail-party graphs, and half-cube graphs. All of them are ℓ_1-graphs, so is any cartesian product of them. Actually, we show below that any ℓ_1-graph arises as an isometric subgraph of such a cartesian product. Complete graphs K_m ($m \geq 3$) and half-cube graphs $\frac{1}{2}H(m,2)$ ($m \geq 3$) have minimum scale 2. Note that $\frac{1}{2}H(2,2) = K_2$, $\frac{1}{2}H(3,2) = K_{4\times 2}$, and K_m is an isometric subgraph of both $K_{m\times 2}$ and $\frac{1}{2}H(m,2)$. The following holds clearly.

Lemma 4.1. *A graph G is hypercube embeddable with scale 2, i.e., $2d_G$ is hypercube embeddable, if and only if G is an isometric subgraph of a half-cube graph.* ∎

On the other hand, determining the minimum scale of cocktail-party graphs is a hard problem. See [DL93b] and the survey [DL94b]. We state a preliminary result that we need here.

Lemma 4.2. *$K_{2^k\times 2}$ has a 2^{k-1}-embedding in a hypercube. Therefore, if $2^{k-1} < m \leq 2^k$, then $K_{m\times 2}$ has a 2^{k-1}-embedding in a hypercube.*

Proof. Consider the vector space $GF(2)^k$. Every hyperplane in $GF(2)^k$ consists of 2^{k-1} points and the symmetric difference of two hyperplanes also contains 2^{k-1} points. We obtain a 2^{k-1}-embedding of $K_{2^k\times 2}$ in the hypercube defined on the set of points of $GF(2)^k$ by labeling the nodes by the 2^k-1 hyperplanes, together with their complements, the full set and $\emptyset$. ∎

We already know from Theorem 2.14 that every connected bipartite ℓ_1-graph is hypercube embeddable. For nonbipartite graphs we have the following observation ([BG73]).

Lemma 4.3. *Let G be an ℓ_1-graph and suppose that G has a λ-embedding in a hypercube. If G is not a bipartite graph, then λ is an even integer. Therefore, the minimum scale of an ℓ_1-graph is equal to 1 or is even.*

Proof. Suppose that G is not bipartite. Let C be an odd cycle in G of minimal length. Then, C is an isometric subgraph of G. Say, $C = (a_1, \ldots, a_{2k+1})$. We can suppose that, in the λ-embedding of G in a hypercube, the nodes a_1, a_{k+1}, a_{k+2} are labeled by $\emptyset$,A,B, respectively. Then, as $d_G(a_1,a_{k+1}) = d_G(a_1,a_{k+2}) = k$ and $d_G(a_{k+1},a_{k+2}) = 1$, we have $\lambda = |A\triangle B|$ and $|A| = |B| = \lambda k$. Hence, $\lambda = 2\lambda k - 2|A\cap B|$. Therefore, λ is an even integer. ∎

The following Theorem 4.4 and Corollaries 4.5-4.10, due to Shpectorov [Shp93], are the main results of this section.

Theorem 4.4. *Let G be an ℓ_1-graph. Then, there is a graph $\widehat{G}$ and an isometric embedding $\widehat{\sigma}$ from G into $\widehat{G}$ such that*
(i) $\widehat{G} = \widehat{G}_1 \times \ldots \times \widehat{G}_k$, where each $\widehat{G}_h$ is isomorphic to a complete graph, a cocktail-party graph $K_{m\times 2}$ ($m \geq 3$), or a half-cube graph, and

(ii) if ψ is a λ-embedding of G into the hypercube, then there is a λ-embedding $\widehat{\psi}$ of $\widehat{G}$ into the same hypercube such that $\psi = \widehat{\psi}\widehat{\sigma}$.

COROLLARY 4.5. *A connected graph G is an ℓ_1-graph if and only if all the factors of its canonical metric representation are ℓ_1-graphs.*

COROLLARY 4.6. *A connected graph G is an ℓ_1-graph if and only if G is an isometric subgraph of a cartesian product of cocktail-party graphs and half-cube graphs.*

COROLLARY 4.7. *Let G be an ℓ_1-graph. Then, G is ℓ_1-rigid if and only if $\widehat{G}$ is ℓ_1-rigid.*

COROLLARY 4.8. *Every ℓ_1-rigid graph is an isometric subgraph of a half-cube graph and, therefore, its minimum scale η is equal to 1 or 2.*

COROLLARY 4.9. *Let G be an ℓ_1-graph on $n \geq 4$ nodes. Then its minimum scale η satisfies $\eta \leq n-2$.*

COROLLARY 4.10. *One can check in polynomial time whether a given graph is an ℓ_1-graph.*

We present in Section 4.1 a concrete construction of the graph $\widehat{G}$ from Theorem 4.4, using a specific λ-embedding of G. We group in Section 4.2 the proofs of Theorem 4.4 and Corollaries 4.5-4.10.

Corollary 4.6 was also obtained in [DG93] as an application of the corespondance existing between Delaunay polytopes in lattices and hypermetrics. However, the proof method from [DG93] does not permit to obtain further results as the characterization of ℓ_1-rigidity and the fact that ℓ_1-graphs can be recognized in polynomial time. In contrast, the proof method presented here uses only elementary notions. It is, in a way, a continuation of the theory of canonical metric representations of graphs. Indeed, the essential step of the proof will be to show that each factor of the canonical metric representation of an ℓ_1-graph can be further embedded into a complete graph, a cocktail-party graph, or a half-cube graph.

We saw in Proposition 2.3 that every hypercube embeddable graph is ℓ_1-rigid. Hence, we have the following chain of implications:

G is an isometric subgraph of a hypercube
$\Longrightarrow$ G is ℓ_1-rigid
$\Longrightarrow$ G is an isometric subgraph of a half-cube graph

Several classes of graphs were shown to be ℓ_1-rigid in [DL94a], including the half-cube graph $\frac{1}{2}H(n,2)$ for $n \neq 3, 4$, the Johnson graph $J(n,d)$ for $d \neq 1$, the Petersen graph, the

Shrikhande graph, the dodecahedron, the icosahedron, any weighted cycle. The method of proof is analogue to that of Proposition 2.3, namely, one shows that the path metric of the graph in question lies on a simplex face of the corresponding cut cone. We refer to [DL94a] for details.

An interesting fact is that, if an ℓ_1-graph G is not ℓ_1-rigid, then this is essentially due to the fact that complete graphs on at least four nodes are not ℓ_1-rigid. Indeed, it follows from Theorem 4.4 that any ℓ_1-embedding of G arises from an ℓ_1-embedding of its extension $\widehat{G}$. As $\widehat{G}$ is a cartesian product of complete graphs, cocktail-party graphs and half-cube graphs, the variety of ℓ_1-embeddings of $\widehat{G}$ follows from the variety of ℓ_1-embeddings of its factors. But the half-cube graph is ℓ_1-rigid unless it coincides with K_4 or $K_{4\times 2}$. Moreover, any ℓ_1-embedding of $K_{n\times 2}$ arises from some ℓ_1-embedding of K_n, since the path metric of $K_{n\times 2}$ can be constructed from the path metric of K_n via the antipodal operation (see [DL94a] for details). Therefore, the variety of ℓ_1-embeddings of $\widehat{G}$, hence of G, arises from the variety of ℓ_1-embeddings of the complete graph. The variety of embeddings of the complete graph is studied in [DL93b].

Unlike the case of isometric subgraphs of hypercubes, no structural characterization is known for the ℓ_1-graphs, or for the isometric subgraphs of half-cube graphs. However, a structural characterization is known for the graphs with a universal node that are ℓ_1-graphs [AD80, AD82]. In particular, it is shown there that, if G is a graph on $n \geq 28$ (resp. $n \geq 37$) nodes, then its suspension ∇G (obtained by adding a new node adjacent to all nodes of G) is an ℓ_1-graph if and only if ∇G is hypermetric (resp. ∇G satisfies the 5-gonal inequalities and is of negative type).

We conclude with a result on the maximum size of the possible ℓ_1-embeddings of an ℓ_1-graph. Let $G = (V, E)$ be a connected ℓ_1-graph. In other words, its path metric can be decomposed as a nonnegative combination of cut semimetrics: $d_G = \sum_{S\in\mathcal{S}} \lambda_S \delta(S)$, where $\mathcal{S}$ is a collection of nonempty proper subsets of V and $\lambda_S > 0$ for $S \in \mathcal{S}$. The quantity $\sum_{S\in\mathcal{S}} \lambda_S$ is called the **size** of the ℓ_1-embedding. We let $S_{\ell_1}(d_G)$ denote the maximum size of an ℓ_1-embedding of d_G. We saw in Proposition 2.3 that every tree has a unique ℓ_1-embedding whose size is equal to $n-1$ (for a tree on n nodes). The next result shows that the maximum ℓ_1-size of an ℓ_1-graph on n nodes is at most $n-1$.

LEMMA 4.11. [Dez] *Let $G = (V, E)$ be a connected ℓ_1-graph and suppose $d_G = \sum_{S\in\mathcal{S}} \lambda_S \delta(S)$ with $\lambda_S > 0$ for all $S \in \mathcal{S}$, where $\mathcal{S}$ is a collection of nonempty proper subsets of V. For each $S \in \mathcal{S}$, $\lambda_S \leq 1$ holds, and the subgraph $G[S]$ of G induced by S is an isometric subgraph of G.*

PROOF. let $S \in \mathcal{S}$. Let ij be an edge of G with $i \in S, j \in V \setminus S$. Hence, $d_G(i,j) = 1 \geq \lambda_S$. Let $i, j \in S$ and let P be a shortest path in G from i to j. Then, any node k of P belongs to S, as the triangle equality $d_G(i,j) = d_G(i,k) + d_G(j,k)$ holds. Hence, P is a shortest path from i to j in $G[S]$. This shows that $G[S]$ is an isometric subgraph of G. ∎

PROPOSITION 4.12. [Dez] *Let G be a connected ℓ_1-graph on n nodes. Then, its maximum ℓ_1-size satisfies: $S_{\ell_1}(d_G) \leq n-1$, with equality if and only if G is a tree.*

PROOF. The proof is by induction on n. Consider a decomposition of d_G as $\sum_{S\in\mathcal{S}}\lambda_S\delta(S)$ with $\lambda_S > 0$ for $S \in \mathcal{S}$. Let $T \in \mathcal{S}$. By Lemma 4.11, $G[T]$ is an isometric subgraph of G. Hence, $d_{G[T]} = \sum_{S\in\mathcal{S},S\cap T\neq\emptyset,T}\lambda_S\delta(S\cap T)$. By the induction assumption, $\sum_{S\in\mathcal{S},S\cap T\neq\emptyset,T}\lambda_S \leq |T|-1$. Similarly, considering the graph $G[V\setminus T]$, we have $\sum_{S\in\mathcal{S},S\cap(V\setminus T)\neq\emptyset,V\setminus T}\lambda_S \leq |V\setminus T|-1$. Hence, $\sum_{S\in\mathcal{S}}\lambda_S \leq \lambda_T + \sum_{S\in\mathcal{S},S\cap T\neq\emptyset,T}\lambda_S + \sum_{S\in\mathcal{S},S\cap(V\setminus T)\neq\emptyset,V\setminus T}\lambda_S \leq 1+(|T|-1)+(|V\setminus T|-1) = n-1$. Moreover, if equality holds, then $G[T], G[V\setminus T]$ are trees and $\lambda_T = 1$. This implies easily that G is a tree. ∎

4.1 Construction of $\widehat{G}$ via the atom graph

In this section, we show how to construct the graph $\widehat{G}$ from Theorem 4.4, using a specific scale embedding of G. It will turn out that, in fact, $\widehat{G}$ does not depend on the choice of the scale embedding and that $\widehat{G}$ is an isometric extension of the canonical metric representataion of G. The main tool for the construction of $\widehat{G}$ is the atom graph of G, as we explain below.

Let $G = (V,E)$ be an ℓ_1-graph. Let

$$\psi : x \in V \mapsto X \subseteq \Omega$$

be a λ-embedding of G into the hypercube $H(\Omega)$. We can suppose without loss of generality that $\Omega = \cup_{x\in V}X$ and that a given node $x_0 \in V$ is assigned to $\emptyset$. Set

$$E_0 = \{e=(x,y)\in E : d_G(x_0,x)\neq d_G(x_0,y)\}. \tag{4.13}$$

For an edge $e=(x,y)\in E_0$, we can suppose that $x_0 \in G(x,y)$. One can easily check the following statements.

$$|X| = \lambda d_G(x_0,x) \quad \text{for all } x\in V. \tag{4.14}$$

$$|X\cap Y| = \frac{\lambda}{2}(d_G(x_0,x)+d_G(x_0,y)-d_G(x,y)) \quad \text{for all } x,y\in V. \tag{4.15}$$

For an edge $e=(x,y)$,

$$\begin{cases} |X\setminus Y| = |Y\setminus X| = \frac{\lambda}{2} & \text{if } e\notin E_0,\\ X\subseteq Y & \text{if } e\in E_0. \end{cases} \tag{4.16}$$

Call **atom** every set of the form $X\triangle Y$ corresponding to an edge $e=(x,y)$ of G, and **proper atom** every set of the form $Y\setminus X$ corresponding to an edge $e=(x,y)\in E_0$ (with $x_0\in G(x,y)$). Atoms have cardinality λ and,

$$\text{if } A,B \text{ are distinct proper atoms, then } |A\cap B| = 0, \frac{\lambda}{2}. \tag{4.17}$$

We define the **atom graph** $\Lambda(G)$ as the graph with node set the set of proper atoms of G and with two proper atoms A,B being adjacent if $|A\cap B| = \frac{\lambda}{2}$. Let $\Lambda_1,\ldots,\Lambda_k$ denote the connected components of $\Lambda(G)$. For $h=1,\ldots,k$, let Ω_h denote the union of the proper atoms that are nodes of Λ_h. Hence, each proper atom is either contained in Ω_h, or disjoint from Ω_h. Actually, the same property holds for all atoms, as we show in the next Claim 4.18.

Claim 4.18. *Let A be an atom of G. Then, for each $h = 1, \ldots, k$, either $A \subseteq \Omega_h$, or $A \cap \Omega_h = \emptyset$.*

Proof. Let (x, y) be an edge of G corresponding to the atom A, i.e., $A = X \triangle Y$. We suppose that the edge (x, y) does not belong to E_0. Hence, the node x_0 is at the same distance s from x and y. Let $(x_0, x_1, \ldots, x_s = x)$ and $(y_0 = x_0, y_1, \ldots, y_s = y)$ be shortest paths from x_0 to x and y in G. Hence,

$$X = \bigcup_{1 \leq i \leq s} B_i, \; Y = \bigcup_{1 \leq i \leq s} C_i,$$

where B_i is the proper atom $X_i \setminus X_{i-1}$, C_i is the proper atom $Y_i \setminus Y_{i-1}$, for $i = 1, \ldots, s$. We claim that

$$X \setminus Y \subseteq B_{i_0}$$

for some $i_0 \in \{1, \ldots, s\}$. Indeed, take $\alpha \in X \setminus Y$ and suppose, for instance, that $\alpha \in B_1$. Then, $B_1 \cap Y \neq B_1$. On the other hand, $B_1 \cap Y \neq \emptyset$, else $B_1 \subseteq X \setminus Y$ implying that $|X \setminus Y| \geq \lambda$, contradicting (4.16). As the cardinality of $B_1 \cap Y$ is a multiple of $\frac{\lambda}{2}$ by (4.17), we obtain that $|B_1 \cap Y| = \frac{\lambda}{2}$, $|B_1 \setminus Y| = \frac{\lambda}{2}$. Therefore, $X \setminus Y = B_1 \setminus Y \subseteq B_1$. Similarly,

$$Y \setminus X \subseteq C_{j_0}$$

for some $j_0 \in \{1, \ldots, s\}$. Furthermore, as the C_j's are pairwise disjoint, each B_i either coincides with some C_j, or meets exactly two of them, unless $B_i = B_{i_0}$ in which case B_i meets exactly one C_j. The symmetric statement holds for each C_i. This means that the subgraph of the atom graph $\Lambda(G)$ induced by the set $\{B_1, \ldots, B_s, C_1, \ldots, C_s\}$ consists of isolated nodes, cycles, and exactly one path whose endpoints are B_{i_0} and C_{j_0}. Let Λ_{h_0} be the connected component of $\Lambda(G)$ that contains this path. Then, $B_{i_0}, C_{j_0} \subseteq \Omega_{h_0}$, which implies that $A = X \triangle Y \subseteq \Omega_{h_0}$. Moreover, for $h \neq h_0$, B_{i_0}, C_{j_0} are disjoint from Ω_h, implying that A is disjoint from Ω_h. ∎

Let $\overline{G}_h$ denote the graph with node set $\{\overline{X} := X \cap \Omega_h \mid x \in V\}$ and with $(\overline{X}, \overline{Y})$ being an edge if $|\overline{X} \triangle \overline{Y}| = \lambda$. Set $\overline{G} = \prod_{1 \leq h \leq k} \overline{G}_h$.

Claim 4.19. *(i) Each $\overline{G}_h$ is λ-embedded into the hypercube $H(\Omega_h)$ and its atom graph $\Lambda(\overline{G}_h)$ coincides with Λ_h.*
(ii) $\overline{G}$ is λ-embedded into the hypercube $H(\Omega)$.
(iii) The mapping $x \in V \mapsto (X \cap \Omega_1, \ldots, X \cap \Omega_k)$ is an isometric embedding of G into $\overline{G}$.

Proof. Let x, y be two nodes of G, giving the two nodes $\overline{X} = X \cap \Omega_h$, $\overline{Y} = Y \cap \Omega_h$ of $\overline{G}_h$. We show

$$|\overline{X} \triangle \overline{Y}| = \lambda d_{\overline{G}_h}(\overline{X}, \overline{Y}).$$

Set $s = d_G(x, y)$ and $t = d_{\overline{G}_h}(\overline{X}, \overline{Y})$. Let $(y_0 = x, y_1, \ldots, y_s = y)$ be a shortest path from x to y in G. Then,

$$X \triangle Y = \sum_{1 \leq i \leq s} Y_i \setminus Y_{i-1}$$

is a disjoint union of atoms. Let t_h denote the number of atoms $Y_i \setminus Y_{i-1}$ that are contained in Ω_h. By Claim 4.18, we obtain

$$|\overline{X} \triangle \overline{Y}| = |(X \triangle Y) \cap \Omega_h| = t_h \lambda.$$

Moreover, we have found a path of length t_h joining $\overline{X}$ to $\overline{Y}$ in $\overline{G}_h$, which implies that $t_h \geq t$. Let $(\overline{Z}_0 = \overline{X}, \overline{Z}_1, \ldots, \overline{Z}_t = \overline{Y})$ be a shortest path joining $\overline{X}$ to $\overline{Y}$ in $\overline{G}_h$. So,

$$|\overline{X} \triangle \overline{Y}| = |(\overline{X} \triangle \overline{Z}_1) \triangle (\overline{Z}_1 \triangle \overline{Z}_2) \triangle \ldots \triangle (\overline{Z}_{t-1} \triangle \overline{Y})| \leq \sum_{1 \leq i \leq t} |\overline{Z}_{i-1} \triangle \overline{Z}_i| = t\lambda.$$

This implies that $t_h \leq t$ and, therefore, $t_h = t$. Hence, the graph $\overline{G}_h$ is λ-embedded into the hypercube $H(\Omega_h)$. One checks easily that its atom graph is Λ_h. Hence, (i) holds. Moreover, $(X \cap \Omega_1, \ldots, X \cap \Omega_k) \mapsto \cup_h (X \cap \Omega_h) = X$ provides a λ-embedding of $\overline{G}_1 \times \ldots \times \overline{G}_k$ into the hypercube $H(\Omega)$, showing (ii). It also follows that

$$d_G(x, y) = \sum_{1 \leq h \leq k} d_{\overline{G}_h}(X \cap \Omega_h, Y \cap \Omega_h)$$

for all nodes $x, y \in V$. This shows (iii). ∎

We now show that each factor $\overline{G}_h$ can be further embedded into some graph $\widehat{G}_h$ which is isomorphic to a complete graph, a cocktail-party graph, or a half-cube graph. We first deal with the case when the atom graph $\Lambda(G)$ is connected, i.e., $k = 1$. Then, the graph $\overline{G}$ is nothing but the graph G embedded into the hypercube $H(\Omega)$.

Claim 4.20. *If $\Lambda(G)$ is connected, then there exists a unique minimal graph $\widehat{G}$ containing G as an isometric subgraph and such that $\widehat{G}$ is isomorphic to a complete graph, a cocktail-party graph $K_{m \times 2}$ $(m \geq 3)$, or a half-cube graph. Moreover, $\widehat{G}$ is λ-embedded into the hypercube $H(\Omega)$.*

Proof. We distinguish three cases.
Case 1: $\Lambda(G)$ is a complete graph. Then, G itself is a complete graph and $\widehat{G} = G$. Indeed, each node x is adjacent to x_0 (else, X would be a disjoint union of the proper atoms corresponding to the edges of a shortest path from x_0 to x). For two nodes $x, y \in V$, X and Y are adjacent proper atoms, implying that $|X \triangle Y| = \lambda$ and, therefore, x and y are adjacent in G. (In fact, $\Lambda(K_n) = K_{n-1}$.)

Case 2: $\Lambda(G)$ is not a complete graph, but is an induced subgraph of a cocktail-party graph. Let A, B be two proper atoms at distance 2 in $\Lambda(G)$. Each other proper atom C is adjacent to both A and B, which implies that $C \subseteq A \cup B$. Hence, for each node $x \in V$, X is contained in the 2λ-element set $A \cup B$. We claim that G is an induced subgraph of a cocktail-party graph. Indeed, any two nonadjacent nodes in G are necessarily at distance 2 since $|X \triangle Y| \leq 2\lambda$ for all $x, y \in V$. Moreover, each node x is adjacent to all other nodes except maybe one, which is then labeled by the complement of X. Then, we take for $\widehat{G}$ the cocktail-party graph $K_{m \times 3}$, obtained by adding an "opposite" node labeled by the complement of X for each node x which is adjacent to all other nodes in G. Hence, $\widehat{G}$ is λ-embedded into the same hypercube $H(\Omega)$. Moreover, $m \geq 3$. Otherwise, G would be a subgraph of $K_{2\times 2}$, which implies that G is P_3 or C_4 in which cases $\Lambda(G)$ consists of two isolated nodes.

Case 3: $\Lambda(G)$ is not an induced subgraph of a cocktail-party graph. We show that G can isometrically embedded into a half-cube graph. First, we claim the existence of distinct proper atoms A, B, C, D satisfying

$$\begin{cases} A \cap C = \emptyset \\ A \cap D = \emptyset \\ C \text{ is adjacent to } D \text{ in } \Lambda(G) \\ B \text{ is adjacent to } A \text{ and } C \text{ in } \Lambda(G). \end{cases}$$

Indeed, let A, C be two proper atoms at distance 2 in $\Lambda(G)$ and let B be a proper atom adjacent to A and B. Suppose for contradiction that, for each proper atom D, D is adjacent to A if and only if D is adjacent to C. If D is adjacent to A and C, then $D \subseteq A \cup C$. If D' is adjacent to A and C and D is adjacent to D', then D meets A or C and, thus, D is adjacent to both A and C, implying $D \subseteq A \cup C$. By connectivity of the atom graph $\Lambda(G)$, we deduce that each proper atom D is contained in $A \cup C$. Therefore, if D, D' are disjoint proper atoms, then D' is the complement of D. This shows that each proper atom is adjacent to all other proper atoms except at most one, contradicting the assumption that $\Lambda(G)$ is not a subgraph of a coktail-party graph.
Let us call a **half** each set of the form $A \cap B$ or $A \setminus B$, where A, B are adjacent proper atoms. Each half has cardinality $\frac{\lambda}{2}$ and each proper atom is the disjoint union of two halves. We claim that

(4.21) distinct halves are disjoint.

If (4.21) holds then, for each node $x \in V$, X can be uniquely expressed as a disjoint union of halves. Indeed, if $(x_0, x_1, \ldots, x_s = x)$ is a shortest path from x_0 to x in G, then $X = \cup_{1\leq i\leq s} X_i \setminus X_{i-1}$ where each proper atom $X_i \setminus X_{i-1}$ is the union of two halves; this set of halves does not depend on the choice of the shortest path. This gives an isometric embedding of G into the half-cube graph $\widehat{G}$ defined on the set of halves. By construction, $\widehat{G}$ is λ-embedded into the hypercube $H(\Omega)$.
As $\Lambda(G)$ is connected, we can order the proper atoms $A_1, A_2, \ldots, A_p$ in such a way that each A_j $(j \geq 2)$ is adjacent to at least one A_s, $s < j$. We suppose that $A_1 = A, A_2 = B, A_3 = C, A_4 = D$. We show by induction on $j \geq 4$ that the distinct halves that are created by the first j proper atoms $A_1, \ldots, A_j$ are pairwise disjoint.
Consider first the case $j = 4$. By construction, the halves $H_1 = A \setminus B$, $H_2 = A \cap B$, $H_3 = B \cap C$, $H_4 = C \setminus B$ are disjoint. Consider the half $C \cap D$. Since $B \cap D = B \cap C \cap D = (C \cap D) \cap H_3$ has cardinality 0 or $\frac{\lambda}{2}$, we obtain that $C \cap D$ is equal to H_3 or H_4. The half $H_5 = D \setminus C$ is disjoint from H_1, H_2, H_3, H_4.
We suppose now that all halves in the set $\mathcal{H}$ of the halves created by the first $j-1$ $(j \geq 5)$ proper atoms are pairwise disjoint. Call two halves $H, H' \in \mathcal{H}$ neighbouring if $H \cup H'$ is a proper atom A_s for some $s < j$. This defines a graph structure on $\mathcal{H}$, for which $\mathcal{H}$ is connected. Suppose that A_j is adjacent to A_s, for $s < j$, and let $A_s = X_1 \cup X_2$ with $X_1, X_2 \in \mathcal{H}$. Suppose that $A_j \cap A_s$ is not equal to X_1, nor to X_2. Set $\alpha = |A_j \cap X_1|$ and $\beta = |A_j \cap X_2$, where $\alpha, \beta > 0$ and $\alpha + \beta = \frac{\lambda}{2}$. If Y_1, Y_2 are two neighbouring halves and $|A_j \cap Y_1| = \alpha$ or β, then $|A_j \cap Y_2| = \beta$ or α, respectively. By connectivity of $\mathcal{H}$, we deduce

that $A_j \cap Y_1| = \alpha$, $|A_j \cap Y_2| = \beta$, or vice versa, for every pair (Y_1, Y_2) of neighbouring halves. Now, $|A_j \cap (H_1 \cup H_2 \cup H_3 \cup H_4 \cup H_5)| = 2(\alpha+\beta)+\alpha$ or $2(\alpha+\beta)+\beta$, which is greater than λ, yielding a contradiction. Therefore, $A_j \cap A_s$ is equal to X_1 or X_2. Hence, $A_j \setminus A_s$ is either a half from $\mathcal{H}$ or a new half disjoint from all halves in $\mathcal{H}$. This concludes the induction, and the proof of Claim 4.20. ∎

Claim 4.22. *If $\Lambda(G)$ has k connected components $\Lambda_1, \ldots, \Lambda_k$, then there exists a unique minimal graph $\widehat{G}$ containing G as an isometric subgraph and such that*

$$\widehat{G} = \prod_{1 \leq h \leq k} \widehat{G}_h,$$

where each factor $\widehat{G}_h$ is isomorphic to a complete graph, a cocktail-party graph $K_{m\times 2}$ $(m \geq 3)$, or a half-cube graph. Moreover, $\widehat{G}$ is λ-embedded into the hypercube $H(\Omega)$.

Proof. As the atom graph $\Lambda(\overline{G}_h) = \Lambda_h$ is connected, we can apply Claim 4.20. Hence, for each $h = 1, \ldots, k$, there exists a unique minimal graph $\widehat{G}_h$ which contains $\overline{G}_h$ as an isometric subgraph and is isometric to a complete graph, a cocktail-party graph $K_{m\times 2}$ $(m \geq 3)$, or a half-cube graph. Therefore,

$$G \hookrightarrow \widehat{G} = \prod_{1 \leq h \leq k} \widehat{G}_h,$$

providing a minimal graph $\widehat{G}$ satisfying Claim 4.22. Moreover, $\widehat{G}$ is λ-embedded into $H(\Omega)$ as each factor $\widehat{G}_h$ is λ-embedded into $H(\Omega_h)$ and the sets Ω_h are disjoint subsets of Ω. ∎

Remark 4.23. Each of the graphs $\overline{G}_h$ is irreducible since it is an isometric subgraph of a complete graph, a cocktail-party graph on at least 6 nodes, or a half-cube graph, which are all irreducible graphs. As the embedding $G \hookrightarrow \overline{G}$ is clearly irredundant, we deduce from Theorem 3.1 that the metric representation

$$G \hookrightarrow \overline{G} = \prod_{1 \leq h \leq k} \overline{G}_h$$

is, in fact, the canonical metric representation of G (which explains why we denoted the number of connected components of the atom graph by k, the letter used in the previous Section 3 for denoting the isometric dimension of G). In particular, the graph $\overline{G}$ whose construction depends, a priori, on the choice of the scale embedding of G into a hypercube, does not, in fact, depend on the specific embedding. Hence, the graph $\widehat{G}$ too does not depend on the specific embedding. ∎

One can also verify directly that the graph $\overline{G}$ does not depend on the specific scale embedding of G. Indeed, the atom graph can be defined in an abstract way, not using the specific embedding.

Given two edges $e = (x, y)$, $e' = (x', y')$ of G, set

$$\langle e, e' \rangle := \frac{1}{2}(d_G(y', x) - d_G(y', y) - d_G(x', x) + d_G(x', y)). \tag{4.24}$$

The quantity $\langle e, e' \rangle$ takes the values $0, \pm 1, \pm\frac{1}{2}$, depending to which sets of the partition $V = G(x, y) \cup G(y, x) \cup G_=(x, y)$ (defined in (1.1)) the nodes x', y' belong. Observe that $\langle e, e' \rangle \neq 0$ if and only if e, e' are in relation by θ (defined in (1.2)). In the case when both e, e' belong to the set E_0 (recall (4.13)), with $x_0 \in G(x, y) \cap G(x', y')$, then

$$\langle e, e' \rangle = \frac{1}{\lambda}|(Y \setminus X) \cap (Y' \setminus X')| \in \{0, \frac{1}{2}, 1\},$$

if $x \mapsto X$ is a λ-embedding of G into a hypercube. In particular, $\langle e, e' \rangle = 1$ if and only if the edges e, e' correspond to the same proper atom $Y \setminus X = Y' \setminus X'$. For $e, e' \in E_0$, set

$$e \sim e' \text{ if } \langle e, e' \rangle = 1.$$

The relation $\sim$ is an equivalence relation on E_0. Clearly, the set of equivalence classes of E_0 under $\sim$ is in bijection with the set of proper atoms. One can define a graph $\mathcal{E}$ on the set of equivalence classes by letting two classes $\overline{e}$, $\overline{e}'$ be adjacent if $\langle e, e' \rangle = \frac{1}{2}$ (the value of $\langle e, e' \rangle$ does not depend on the choice of e in the class $\overline{e}$ and e' in the class $\overline{e}'$). The graph $\mathcal{E}$ clearly coincides with the atom graph $\Lambda(G)$. Let $\mathcal{E}_1, \ldots, \mathcal{E}_k$ denote the connected components of $\mathcal{E}$. Hence, each edge $e \in E_0$ is assigned to a node in one of the $\mathcal{E}_h$'s. We now see how to assign the other edges of G to some component $\mathcal{E}_h$. Let $e = (x, y)$ be an edge that does not belong to E_0, i.e., $d_G(x_0, x) = d_G(x_0, y)$. Let $(x_0, x_1, \ldots, x_s = x)$ and $(y_0 = x_0, y_1, \ldots, y_s = y)$ be shortest paths joining x_0 to x and y in G and set $e_i = (x_{i-1}, x_i), f_i = (y_{i-1}, y_i)$ for $i = 1, \ldots, s$. Consider the subgraph of $\mathcal{E}$ induced by the set $\{\overline{e}_i, \overline{f}_i : i = 1, \ldots, s\}$. An analogue of Claim 4.18 shows that this graph consists of isolated nodes, cycles, and exactly one path. Moreover, the component $\mathcal{E}_h$ containing this path depends only on the edge (x, y) (not on the choice of the shortest paths from x_0 to x and y). This permits us to partition the edge set E of G into $E_1 \cup \ldots \cup E_k$, where E_h consists of the edges that are assigned to $\mathcal{E}_h$ by the above procedure. Then, let $\mathcal{G}_h$ denote the graph obtained by contracting the edges from $E \setminus E_h$. The graph $\mathcal{G}_h$ coincides with the graph G_h (up to renumbering of the factors).
So we have shown how to construct the graph $\overline{G}$ in an abstract way, not depending on the specific scale embedding of G. We refer to [Shp93] for more details.

4.2 Proofs

PROOF OF THEOREM 4.4. The existence of a graph $\widehat{G}$ satisfying Theorem 4.4 (i) follows from Claim 4.22. We prove the second part of Theorem 4.4. Let $\psi : x \mapsto X$ be a λ-embedding of G into a hypercube $H(\Omega)$. Suppose first that ψ assigns the given node x_0 to $\emptyset$. Using ψ, by the construction of Section 4.1, we obtain a graph $\widehat{G_\psi}$ which is λ-embedded into $H(\Omega)$ and is isomorphic to $\widehat{G}$ (by Remark 4.23). This gives the λ-embedding $\widehat{\psi}$ such that $\psi = \widehat{\psi}\widehat{\sigma}$. Suppose now that ψ assigns the set X_0 to the node x_0. Consider the λ-embedding $x \mapsto X \triangle X_0$, denoted by $\psi \triangle X_0$, of G into $H(\Omega)$. As $\psi \triangle X_0$ maps x_0 to $\emptyset$, we obtain $\widehat{\psi \triangle X_0} \triangle X_0$ for the embedding $\widehat{\psi}$. ∎

PROOF OF COROLLARIES 4.5 AND 4.6. If G is an ℓ_1-graph, then the graph $\overline{G}$ is an ℓ_1-graph (by Claim 4.19) and $\overline{G}$ coincides with the canonical metric representation of G (by Remark 4.23). This shows Corollary 4.5. Corollary 4.6 is an immediate consequence of Corollary 4.5. ∎

PROOF OF COROLLARIES 4.7 AND 4.8. The implication: $\widehat{G}$ is ℓ_1-rigid $\Longrightarrow$ G is ℓ_1-rigid follows from Theorem 4.4 (ii). Conversely, suppose that G is ℓ_1-rigid. We show that $\widehat{G}$ is ℓ_1-rigid. Consider a scale embedding $\widehat{\psi}_i$ of $\widehat{G}$ in the hypercube Ω_i, for $i = 1, 2$. We can suppose that Ω_1 and Ω_2 have the same cardinality (if not, add some redundant elements). We can also suppose that $\widehat{\psi}_1$ and $\widehat{\psi}_2$ have the same scale λ. (If, for $i = 1, 2$, $\widehat{\psi}_i$ has scale λ_i, then replace $\widehat{\psi}_i$ by $\widehat{\psi}'_i$, where $\widehat{\psi}'_1$ is the $\lambda_1\lambda_2$-embedding constructed from $\widehat{\psi}_1$ by replacing the elements of Ω_1 by disjoint sets each of cardinality λ_2 and $\widehat{\psi}'_2$ is the $\lambda_1\lambda_2$-embedding constructed from $\widehat{\psi}_2$ in the same way.) Then, $\psi_i := \widehat{\psi}_i\widehat{\sigma} : x \mapsto X_i$ is a λ-embedding of G into the hypercube $H(\Omega_i)$, for $i = 1, 2$. As G is ℓ_1-rigid, any two isometric ℓ_1-embeddings of G are equivalent (recall the definition from Section 1). It is not difficult to see that this implies the existence of a bijection $\alpha : \Omega_1 \longrightarrow \Omega_2$ and of a set $A \subseteq \Omega_2$ such that $X_2 = \varphi(X_1)$ for each node x of G where, for a subset $Z \subseteq \Omega_1$, we set

$$\varphi(Z) = \sigma(Z)\triangle A.$$

Using ψ_i, by the construction of Section 4.1, we obtain the graph $\widehat{G}_{\psi_i}$, which is λ-embedded into the hypercube $H(\Omega_i)$ via $\widehat{\psi}_i$. By the minimality of the graphs $\widehat{G}_{\psi_1}$,$\widehat{G}_{\psi_2}$ (see Claim 4.22), we deduce that φ establishes the equivalence of the embeddings $\widehat{\psi}_1$ and $\widehat{\psi}_2$. Hence, $\widehat{G}$ is ℓ_1-rigid. This shows Corollary 4.7. Corollary 4.8 now follows easily. Indeed, if G is ℓ_1-rigid, then $\widehat{G}$ is ℓ_1-rigid, which implies that each factor $\widehat{G}_h$ is ℓ_1-rigid (as a product of graphs is ℓ_1-rigid if and only if each factor is ℓ_1-rigid). Therefore, each $\widehat{G}_h$ is one of the following graphs: K_2, K_3, $K_{3\times 2}$, or $\frac{1}{2}H(m, 2)$ for $m \geq 5$, which are all hypercube embeddable with scale 2. Therefore, G is hypercube embeddable with scale 2, i.e., G is an isometric subgraph of a half-cube graph.

∎

PROOF OF COROLLARY 4.9. Suppose G has n nodes. If some factor $\widehat{G}_h$ is a cocktail-party graph $K_{m\times 2}$, then $m < n$. Hence, by Lemma 4.2, $\widehat{G}_h$ is hypercube embeddable with scale 2^{k-1}, if $2^{k-1} < n - 1 \leq 2^k$. All other factors are also hypercube embeddable with scale 2^{k-1} since $k \geq 2$ as $n \geq 4$. Hence, G is hypercube embeddable with scale 2^{k-1}, which implies that its minimum scale η satisfies: $\eta \leq 2^{k-1} < n - 1$. ∎

PROOF OF COROLLARY 4.10. Indeed, the graph $\widehat{G}$ can be constructed in polynomial time and one can check whether $G \hookrightarrow \widehat{G}$ also in polynomial time. ∎

5 Additional results

Among the properties contained in the metric hierarchy from Figure 2.12, we have the hypermetric and the negative type condition. Hypermetric graphs are treated in detail in

[DG93] and in the survey [DGL93]. We saw in Figure 2.13 two characterizations for the distance spaces of negative type. Winkler [Win85] proposes another characterization for the graphs of negative type. Let G be a graph. Consider an orientation G' of G which has, for each edge (a,b) of G, exactly one of the arcs (a,b) or (b,a). Given two arcs $e=(a,b)$ and $e'=(a',b')$ of G', we set, as in relation (4.24),

$$\langle e,e'\rangle := \frac{1}{2}(d_G(a,b') - d_G(a,a') - d_G(b,b') + d_G(b,a')).$$

Observe that, if d_G is of negative type and $u_a \in \mathbb{R}^m$, $a \in V$, are vectors satisfying $d_G(a,b) = (\| u_a - u_b \|_2)^2$ for all $a,b \in V$, then $\langle e,e'\rangle$ coincides with the scalar product $(u_b - u_a)^T(u_{b'} - u_{a'})$.

THEOREM 5.1. [Win85] *Let G be a connected graph on $n+1$ nodes and let G' be an arbitrary orientation of G. Let T be a spanning tree in G, with corresponding arcs $e_1,\ldots,e_n$ in G'. The following assertions are equivalent.*
(i) d_G is of negative type.
(ii) The $n \times n$ matrix $(\langle e_i,e_j\rangle)_{i,j=1,\ldots,n}$ is positive semidefinite.

PROOF. Let $V = \{a_0,a_1,\ldots,a_n\}$ denote the set of nodes of G. By definition, d_G is of negative type if and only if

$$\sum_{0\le r<s\le n} d_G(a_r,a_s)x_rx_s \le 0 \text{ for all } x \in U := \{x \in \mathbb{R}^{n+1} : \sum_{0\le r\le n} x_r = 0\}.$$

For each node $a_r \in V$, set

$$A(a_r) := \{i \in \{1,\ldots,n\} : \text{ the arc } e_i \text{ ends in } a_r\},$$

$$B(a_r) := \{i \in \{1,\ldots,n\} : \text{ the arc } e_i \text{ begins in } a_r\}.$$

For $y \in \mathbb{R}^n$, define $x \in \mathbb{R}^{n+1}$ by setting

$$x_r = \sum_{i\in A(v_r)} y_i - \sum_{i\in B(v_r)} y_i$$

for $r = 0,1,\ldots,n$. One can check that $\sum_{0\le r\le n} x_r = 0$, i.e., $x \in U$, and $x = (0,\ldots,0)$ implies that $y = (0,\ldots,0)$. Hence, we have found a 1-1 linear correspondance between the spaces $\mathbb{R}^n$ and U. We check that, under this correspondance,

$$\sum_{1\le i,j\le n} \langle e_i,e_j\rangle y_iy_j = -\sum_{0\le r<s\le n} d_G(a_r,a_s)x_rx_s.$$

Indeed, $d_G(a_r,a_s)$ appears in $\sum_{1\le i,j\le n} \langle e_i,e_j\rangle y_iy_j$ with the coefficient

$$\sum_{(i,j)\in A(v_r)\times B(v_s)} y_iy_j + \sum_{(i,j)\in B(v_r)\times A(v_s)} y_iy_j - \sum_{(i,j)\in A(v_r)\times A(v_s)} y_iy_j - \sum_{(i,j)\in B(v_r)\times B(v_s)} y_iy_j,$$

which is equal to $-x_rx_s$. This shows the equivalence of (i) and (ii). ∎

Example 5.2. Consider the graph G_n with node set $\{a_0, \ldots, a_n\}$ and with edges the pairs (a_0, a_1), (a_0, a_i) and (a_1, a_i) for $i = 2, 3, \ldots, n$. Then, the path metric of G_n is of negative type if and only if $n \leq 5$. (To see it, consider the oriented spanning tree T with arcs $e_1 = (a_0, a_1), \ldots, e_n = (a_0, a_n)$. The matrix $(\langle e_i, e_j \rangle)_{i,j=1,\ldots,n}$ has all its entries equal to 0 except the diagonal entries equal to 1 and the $(1, i)$- and $(i, 1)$-entries equal to $\frac{1}{2}$ for $i = 2, \ldots, n$. Its determinant is equal to $\frac{5-n}{4}$.) Note that, for $n \geq 6$, G_n provides a counterexample to the converse of the last implication from Figure 2.12, since the distance matrix of G_n has exactly one positive eigenvalue, but G_n is not of negative type. (Indeed, the eigenvalues of the distance matrix of G_n are $2n-1, -1, -2$ with respective multiplicities $1, 1, n-1$.) ∎

Many other aspects of the metric structure of graphs have been considered in the literature, leading to rich theories. For instance, distance-regular graphs, or strongly-regular graphs, are defined by some invariance property of their path metric. The study of such graphs leads to a large and rich area of research, connected to algebraic graph theory. The papers [BK91, Koo90, Koo92, KS94, Wei92] deal with the study of graphs with high regularity that have some specified metric properties as hypermetricity, or some special cases of it (e.g., satisfying the pentagonal inequality, or the hexagonal iunequality), etc... For instance, the distance-regular graphs that are hypercube embeddable are completely classified: they are the hypercubes, the even cycles, and the double-odd graphs [Wei92, Koo90]. The distance-regular graphs of negative type (or, equivalently, whose distance matrix has exactly one positive eigenvalue) are classified in [KS94].

We mention below some other topics related to the metric structure of graphs, as interval-regular graphs, geodetic graphs, or the question of embedding a given distance space into a (weighted) graph.

Remark 5.3. **Interval-regular graphs and geodetic graphs.**
Let $G = (V, E)$ be a connected graph. For two nodes $x, y \in V$, let $\gamma(x, y)$ denote the number of shortest paths joining x to y in G, set

$$I(x, y) = \{z \in V \mid d_G(x, y) = d_G(x, z) + d_G(z, y)\}$$

and, for $i = 0, 1, \ldots, d_G(x, y)$, set

$$N_i(x, y) = \{z \in I(x, y) \mid d_G(x, z) = i\}.$$

Set also

$$N_{-1}(x, y) = \{z \in V \mid d_G(x, z) = 1 \text{ and } d_G(z, y) = d_G(x, z) + 1\}.$$

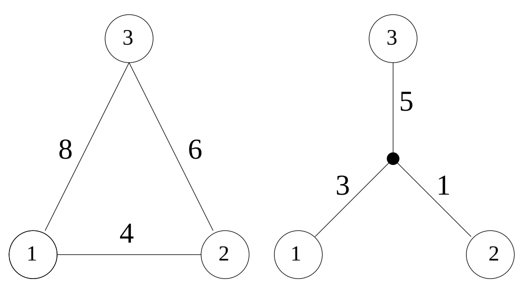
Then, G is **distance-regular** if the numbers $|N_1(x, y)|$ and $|N_{-1}(x, y)|$ depend only on $d_G(x, y)$ (see [BCN89]). The graph G is said to be **interval-regular** if $|N_1(x, y)| = d_G(x, y)$ for all nodes $x, y \in V$ (see [Mul80, Mul82]). G is said to be **uniformely geodetic** [CP83] (or F**-geodetic**, [CS86]) if $\gamma(x, y)$ depends only on $d_G(x, y)$. Every distance-regular graph is uniformely geodetic [CP83], and every Hamming graph is interval-regular (since the subgraph induced by the interval $I(x, y)$ is isomorphic to the $d_G(x, y)$-hypercube). See, e.g., [Sca90, Koo93] for more informations on uniformely geodetic graphs; [Koo93] characterizes the uniformely geodetic bipartite graphs.
Several characterizations of the hypercube are known. Foldes [Fol77] shows that the hypercube

is the only connected bipartite graph for which $\gamma(x,y) = d_G(x,y)!$ holds for any pair of nodes. Ceccherini and Sappa [CS86] show that a connected bipartite graph G is isomorphic to a hypercube if and only if the cartesian product $G \times K_2$ is uniformely geodetic.
Interval-regular graphs are linked to hypercubes in the following way [Mul82]: A connected graph G is interval-regular if and only if, for any two nodes x, y, the subgraph of G consisting of the edges connecting two consecutive levels $N_i(x,y)$ and $N_{i+1}(x,y)$ ($i = 0, 1, \ldots, d_G(x,y) - 1$) is isomorphic to the $d_G(x,y)$-hypercube. Equivalently, G is interval-regular if and only if $\gamma(x,y) = d_G(x,y)!$ for all nodes $x, y \in V$.
Hamming graphs can be characterized in terms of interval-regular graphs in the following way [BM91]: A connected graph G is a Hamming graph if and only if G is an interval-graph, G does not contain $K_{1,1,2}$ as an induced subgraph, and the only isometric odd cycles in G are triangles. More generally, [BM91] characterizes the connected graphs that can be decomposed as a cartesian product where each factor is the suspension of a geodetic graph of diameter at most 2. (A geodetic graph is a graph in which there is exactly one shortest path joining any pair of nodes, and the suspension of a graph H is obtained by adding to H a new node adjacent to all nodes of H.) ▮

REMARK 5.4. **Embedding metrics into graphs.**
We now consider the question of embedding metrics into graphs or, more generally, into weighted graphs. This topic has many applications, in various areas, as psychology [Cun78], or biology [PFH82].
Let $G = (V, E)$ be a graph and let $w_e \in \mathbb{R}_+$, $e \in E$, be nonnegative weights assigned to its edges. The path metric $d_{G,w}$ of the weighted graph (G, w) is defined by letting $d_{G,w}(x,y)$ denote the smallest value of $\sum_{e \in E(P)} w_e$, taken over all paths P joining x and y in G.
Given a finite metric space (X, d), one says that the weighted graph (G, w) **realizes** (X, d) if there exists a mapping $i \in X \mapsto x_i \in V$ such that

$$d(i,j) = d_{G,w}(x_i, x_j)$$

for all $i, j \in X$. The graph G may have more nodes than those corresponding to points of X. Every metric space can clearly be realized by some graph, namely, by the complete graph on $|X|$ nodes with weights $d(i,j)$ on its edges. Consider, for instance, the metric d on $X = \{1,2,3\}$ defined by $d(1,2) = 4,\ d(1,3) = 8,\ d(2,3) = 6$. Then, d can be realized by the following two weighted graphs: K_3 and a tree with one auxiliary node.



The objective is, therefore, to find a graph (G, w) realizing (X, d) whose total weight $\sum_{e \in E} w_e$ is as small as possible. The existence of an optimal realization, i.e., with minimum total weight among all possible realizations, was shown in [ISPZ84]. But finding an optimal realization is an NP-hard problem even if the metric is assumed to be integer valued [Al88, Win88].
On the other hand, the metric spaces that can be realized by weighted trees are well characterized.

Namely, (X, d) is realizable by a weighted tree (then, (X, d) is called a **tree metric**) if and only if d satisfies the following condition, known as the **four-point condition**:

$$d(i,j) + d(r,s) \leq \max(d(i,r) + d(j,s), d(i,s) + d(j,r)),$$

i.e., the two largest of the three sums $d(i,j) + d(r,s), d(i,r) + d(j,s), d(i,s) + d(j,r)$ are equal, for all $i, j, r, s \in X$ [Bun74]. Note that the four point condition implies the metric condition (by taking $r = s$). Moreover, if (X, d) is realizable by a tree, then there is only one such realization; it is optimal among all graph realizations, and it can be found in polynomial time [HY64].
The four point condition is closely related to another metric condition, namely, ultrametricity. Recall that a distance space (X, d) is said to be **ultrametric** if it satisfies

$$d(i,j) \leq \max(d(i,k), d(j,k))$$

for all $i, j, k \in X$. In other words, any three points form an isoceles triangle with the third side shorter or equal to the other two. See [ABBW87] for applications and references on ultrametrics. Clearly, every ultrametric space satisfies the four point condition. Actually, each tree metric can be characterized in terms of an associated ultrametric in the following way [Ban90]. Let (X, d) be a distance space, let $r \in X$, and let c be a constant such that $c \geq \max(d(i,j) : i, j \in X)$. Define the distance $d^{(c)}$ on X by setting

$$d^{(c)}(i,j) = c + \frac{1}{2}(d(i,r) + d(j,r) - d(i,j))$$

for $i \neq j \in X$. Then, d is a tree metric if and only if $d^{(c)}$ is ultrametric. Ultrametrics have also a tree-like representation, which is used in classification theory, in particular, in taxonomy (see [Gor87] and references there for details). Let $T = (V, E)$ be a tree and $w_e \in \mathbb{R}_+$, $e \in E$, be nonnegative weights on its edges. Let $r \in V$ be a specified node (a root) of T and let $X = \{x_1, \ldots, x_k\}$ denote the set of leaves (nodes of degree 1) of T other than r. We assume that $d_{T,w}(r, x) = h$ for all $x \in X$, for some constant h, called the height of T. Then, T is also called a **dendogram**, or **indexed hierarchy**. The height $h(v)$ of a node v of T is defined as the length of a shortest path joining v to some leaf of X. Then, one can define a metric space (X, d_X) on X by letting $d_X(x, y)$ denote the height of the first predecessor of x and y. The metric space (X, d_X) is ultrametric and every ultrametric arises in this way [ABBW87].

∎

Acknowledgements. I thank M. Deza for bringing to my attention some references, in particular, for pointing out the results from [FH93] and [Dez] quoted, respectively, in Theorem 2.17 and Proposition 4.12.

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