6
Isometric Embeddings of Graphs

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1. Introduction

With any connected graph $G = (V, E)$ one can associate a metric $d_G: V \times V \to \mathbf{N}$ (the set of non-negative integers) by defining $d_G(v, w)$, for $v, w \in V$, to be the minimum number of edges in any path between v and w. This is the most common definition of *distance* in a graph and has been investigated by many researchers over the years.

In this chapter we combine the basic concepts of distance and subgraph. More precisely, we say that G' is an **isometric** (or **distance-preserving**) **subgraph** of G if, for all vertices v and w, $d_{G'}(v, w) = d_G(v, w)$. Note that this is a natural strengthening of the concept of induced subgraph, since G' is an induced subgraph of G if, for all vertices v and w in V, $d_{G'}(v, w) = 1$ if and only if $d_G(v, w) = 1$.

We shall see that the requirements for a subgraph to be isometric are rather restrictive, and, consequently, a number of surprisingly strong conclusions can be deduced in this case.

2. A General Formulation

Suppose that (M, d) is a metric space—that is, M is a set and d is a mapping from $M \times M$ into $\mathbf{R}$ (the set of real numbers) satisfying, for all $x, y, z \in M$:

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(*i*) $d(x, y) = d(y, x) \geq 0$, with equality if and only if $x = y$;

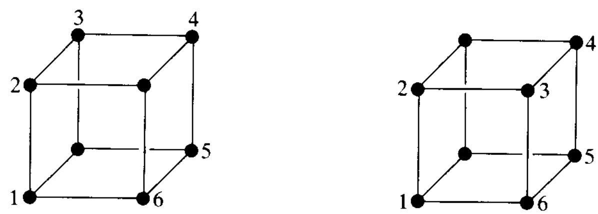
(*ii*) $d(x, y) + d(y, z) \geq d(x, z)$ (the triangle inequality).

A mapping $\lambda: V \to M$ is said to be an **isometric embedding** of $G = (V, E)$ into M if

$$d(\lambda(v), \lambda(w)) = d_G(v, w),$$

for all $v, w \in V$. We will often abbreviate this by writing $\lambda: G \xrightarrow{I} V$, or even $G \xrightarrow{I} M$ if we mean that a suitable λ exists.

In Fig. 1(a) we show an example of an isometric embedding of C_6 into the cube Q_3, and in Fig. 1(b) we show an embedding of C_6 into Q_3 in which C_6 is an induced subgraph of Q_3 but the embedding is not isometric.



(a) (b)

Fig. 1

Many of the spaces (M, d) we shall be concerned with are *product spaces*—that is, spaces formed as Cartesian products of smaller spaces with a much simpler distance structure. Specifically, if (M_k, d_k) $(1 \leq k \leq r)$ are metric spaces, then the product space (M^*, d^*) is defined by

$$M^* = \prod_{k=1}^{r} M_k = \{(m_1, \ldots, m_r): m_k \in M_k, \quad 1 \leq k \leq r\},$$

and

$$d^*((m_1, \ldots, m_r), (m_1', \ldots, m_r')) = \sum_{k=1}^{r} d_k(m_k, m_k').$$

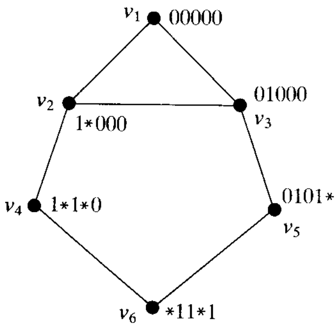
For example, if each M_k consists of the 2-point space $\{0, 1\}$ in which the distance between the two points 0 and 1 is 1, then (M^*, d^*) is just (Q_r, d_H), the r-cube Q_r equipped with the *Hamming metric* for which the distance between two binary r-triples is equal to the number of coordinate positions in which they differ.

3. Extended Binary Labelings

Our first set of results deals with one of the earliest developments of isometric embeddings of graphs. In this case, we wish to find efficient embeddings of graphs into B_*^r, where B_* consists of the set $\{0, 1, *\}$ with the distance d_* defined by

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

In other words, we wish to label each vertex v with an appropriate r-tuple $\lambda(v)$ so that the distances between vertices in V are exactly given by the distances between their corresponding labels. (This problem arose in connection with early work on routing algorithms for packet switching in data networks; see **[29]**, **[22]** and **[11]**.) In Fig. 2(a) we show a graph G and an appropriate labeling; in Fig. 2(b) we give its distance matrix $\mathbf{D}(G) = (d_{ij})$, where $d_{ij} = d_G(v_i, v_j)$.



(a)

	v_1	v_2	v_3	v_4	v_5	v_6
v_1	0	1	1	2	2	3
v_2	1	0	1	1	2	2
v_3	1	1	0	2	1	2
v_4	2	1	2	0	2	1
v_5	2	2	1	2	0	1
v_6	3	2	2	1	1	0

$\mathbf{D}(G)$

(b)

Fig. 2

To begin with, it is not clear that such isometric embeddings always exist. For example, if we are not allowed to use the symbol $*$, then we are asking for isometric embeddings of G into $\{0, 1\}^r$ (that is, Q_r), and this is certainly *not* possible for most graphs (such as non-bipartite graphs). However, this is taken care of by the following result:

Lemma 3.1. *For each connected graph G there exists a least integer $r = r(G)$ such that $G \xrightarrow{I} B_*^r$.*

Proof. Let R denote the integer $\sum_{i<j} d_G(v_i, v_j) = \sum_{i<j} d_{ij}$. We claim that $G \xrightarrow{I} B_*^R$. To see this, for each i and j with $i < j$, select d_{ij} fixed (and mutually disjoint) coordinate positions $D_{ij} \subseteq \{1, 2, \ldots, R\}$ and define

$$\lambda(v)_k = \begin{cases} 0, & \text{if } v = v_i,\ k \in D_{ij}, \\ 1, & \text{if } v = v_j,\ k \in D_{ij}, \\ *, & \text{otherwise.} \end{cases}$$

Since $\{1, 2, \ldots, R\} = \bigcup_{i<j} D_{ij}$, an easy computation shows that $\lambda\colon G \xrightarrow{I} B_*^R$, and we are done. ||

An important question, open for many years, was *how large* $r(G)$ can ever be. This was finally settled by the following elegant result of Winkler [**36**]:

Theorem 3.2. $r(G) \le |V(G)| - 1$. ||

This inequality improves earlier estimates of Yao [**37**] and others (see [**11**], [**22**]), and is best possible for many infinite classes of graphs, as we shall see shortly.

In the other direction, the following lower bound for $r(G)$ was found by Witsenhausen (see [**22**]):

Theorem 3.3. $r(G) \ge \max\{n_+(G), n_-(G)\}$, *where* $n_+(G)$ *and* $n_-(G)$ *denote the number of positive and negative eigenvalues of the distance matrix of* G.

Proof. Suppose that $\lambda\colon G \xrightarrow{I} B_*^r$ is given. For $1 \le k \le r$, define subsets X_k and Y_k of $I = \{1, 2, \ldots, |V(G)|\}$ by $X_k = \{i \in I\colon \lambda(v_i)_k = 0\}$ and $Y_k = \{i \in I\colon \lambda(v_i)_k = 1\}$. From the hypothesis that λ is an isometry and the definition of d_*, we have

$$d_{ij} = d_G(v_i, v_j) = \sum_{k=1}^{r} d_*(\lambda(v_i)_k, \lambda(v_j)_k),$$

for all i and j. We can summarize this information in the following way:

$$\sum_{i<j} d_{ij} x_i x_j = \sum_{k=1}^{r} \Big(\sum_{i \in X_k} x_i\Big)\Big(\sum_{j \in Y_k} x_j\Big),$$

where the x_i are indeterminates. Thus, the existence of an isometric embedding of G into B_*^r implies the existence of a decomposition of the associated quadratic form $\sum_{i<j} d_{ij} x_i x_j$ into a sum of certain products. We

can go one step further and rewrite this equation as

$$\sum_{i<j} d_{ij}x_i x_j = \tfrac{1}{4}\sum_{k=1}^{r}\left\{\left(\sum_{i\in X_k} x_i + \sum_{j\in Y_k} x_j\right)^2 - \left(\sum_{i\in X_k} x_i - \sum_{j\in Y_k} x_j\right)^2\right\},$$

where we have simply used the algebraic identity

$$xy = \tfrac{1}{4}\left((x+y)^2 - (x-y)^2\right).$$

However, this is a decomposition of $\sum_{i<j} d_{ij}x_i x_j$ into a sum and difference of squares, to which we can apply Sylvester's classical law of inertia (see [**25**, p. 352]). This implies that the number of positive squares must be at least $n_+(G)$, and the number of negative squares must be at least $n_-(G)$. Since each of the numbers of positive and negative squares in the above decomposition is at most r, we have $r \geq n_+(G)$, $r \geq n_-(G)$, and the result follows. ||

Theorems 3.2 and 3.3 can be used to determine $r(G)$ exactly, for many graphs G. For example, if G is the complete graph K_p, then an easy computation shows that $n_-(K_p) = p - 1$, and consequently $r(K_p) = p - 1$. Similarly, for the odd circuit C_{2k+1}, we have

$$n_-(C_{2k+1}) = 2k = |V(C_{2k+1})| - 1,$$

and so $r(C_{2k+1}) = 2k$. In the case that G is a tree, much more can actually be said. This we do in the next section.

Before closing this section, we point out that the assertion $r(K_p) = p-1$ has the following equivalent combinatorial interpretation (see [**22**]):

Theorem 3.4. *It is not possible to decompose the edge-set of K_p into fewer than $p - 1$ edge-disjoint complete bipartite subgraphs.*

Remark. At present, no purely combinatorial proof of this is known. However, Tverberg [**32**] has given the following nice algebraic argument:

Proof. Suppose that $E(K_p) = \bigcup_{k=1}^{t} K(A_k, B_k)$ is a decomposition of the edge-set of K_p into t edge-disjoint complete bipartite subgraphs $K(A_k, B_k)$ $(1 \leq k \leq t)$. Then

$$\sum_{1\leq i<j\leq p} x_i x_j = \sum_{k=1}^{t}\left(\sum_{a\in A_k} x_a\right)\left(\sum_{b\in B_k} x_b\right).$$

Consider the following system of $t + 1$ homogeneous linear equations in the p variables x_i:

$$\sum_{a \in A_k} x_a = 0 \ (1 \le k \le t), \text{ and } \sum_{i=1}^{p} x_i = 0.$$

If $(y_1, \ldots, y_p)$ is any solution to this system, then we must have

$$\begin{aligned} 0 &= \left(\sum_{i=1}^{p} y_i\right)^2 = \sum_{i=1}^{p} y_i^2 + 2 \sum_{i<j} y_i y_j \\ &= \sum_{i=1}^{p} y_i^2 + 2 \sum_{k=1}^{t} \left(\sum_{a \in A_k} y_a\right)\left(\sum_{b \in B_k} y_b\right) \\ &= \sum_{i=1}^{p} y_i^2; \end{aligned}$$

that is, $y_i = 0$ for all i. Hence, the number of equations in the system must be as least as large as the number of variables, giving $t + 1 \ge n$. ||

4. Distance Matrices of Trees

Suppose that T_p is a tree with p vertices. An unexpected fact concerning the distance matrix $\mathbf{D}(T_p)$, first noted in **[22]**, is given by the following theorem. The main point of this result is that the value of the determinant is independent of the *structure* of T_p, and depends only on its order.

Theorem 4.1. $\det \mathbf{D}(T_p) = (-1)^{p-1}(p-1)2^{p-2}$.

Sketch of proof. We simply designate an arbitrary fixed vertex of T_p as a root, and sequentially perform row and column operations on $\mathbf{D}(T_p)$ by subtracting from the row and column of each vertex v the row and column of its immediate predecessor v' (so that v' is adjacent to v and lies on the path in T_p from v to the root), always processing the vertices furthest from the root first. When this is done, the resulting matrix $\mathbf{M} = (m_{ij})$ has the form

$$m_{ij} = \begin{cases} 1, & \text{if } i = 1 \text{ or } j = 1, \text{ but } (i, j) \ne (1, 1), \\ -2, & \text{if } i = j = 1, \\ 0, & \text{otherwise,} \end{cases}$$

and the result follows at once. ||

However, one suspects from the form of Theorem 4.1 that much more is going on here. This has led to a number of extensions which help shed light on its particularly simple form.

To state the first of these extensions, let cof $\mathbf{D}(H)$ denote the sum of the cofactors of the distance matrix $\mathbf{D}(H)$ of a graph H. The following result is given in **[20]**:

Theorem 4.2. *If a connected graph G has blocks $G_1, \ldots, G_r$, then*

$$(i)\ \operatorname{cof} \mathbf{D}(G) = \prod_{k=1}^{r} \operatorname{cof} \mathbf{D}(G_k);$$

$$(ii)\ \det \mathbf{D}(G) = \sum_{k=1}^{r} \det \mathbf{D}(G_k) \prod_{i \neq k} \operatorname{cof} \mathbf{D}(G_i).\ \|$$

Since any tree T_p with p vertices has exactly $p - 1$ blocks, each of which is a single edge K_2 with $\det \mathbf{D}(K_2) = -1$, $\operatorname{cof} \mathbf{D}(K_2) = 2$, Theorem 4.1 follows at once.

Note that, when $\operatorname{cof} \mathbf{D}(G) \neq 0$, then part (*ii*) of Theorem 4.2 can be written in the suggestive form

$$\frac{\det \mathbf{D}(G)}{\operatorname{cof} \mathbf{D}(G)} = \sum_{k=1}^{r} \frac{\det \mathbf{D}(G)}{\operatorname{cof} \mathbf{D}(G_k)}.$$

It is not difficult to see that, in fact, there always exist mappings $T_p \xrightarrow{I} B_*^{p-1}$ in which the symbol $*$ is never used. In other words, $T_p \xrightarrow{I} \{0, 1\}^{p-1}$.

The next generalization of Theorem 4.1 is the following:

Theorem 4.3. *Let* $\{\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_p\} \subseteq \{0, 1\}^{p-1}$. *Then*

$$\det(d_H(\mathbf{a}_i, \mathbf{a}_j)) = (-1)^{p-1}(p - 1)2^{p-2}V^2,$$

where V denotes the p-dimensional volume of the parallelepiped spanned by the vectors $\mathbf{a}_k - \mathbf{a}_0$ $(1 \leq k \leq p)$. ||

The proof of this relies on the use of special determinants of the form $\det(\mathbf{x}_i \cdot \mathbf{x}_j)$, called *Gramians* (see [**18**, p. 250]), where $\mathbf{x}_i \cdot \mathbf{x}_j$ denotes the inner product of the vectors $\mathbf{x}_i$ and $\mathbf{x}_j$. The values of these determinants turn out to represent volumes of parallelepipeds in Euclidean space, and the factor 2^{p-1} arises directly from this interpretation.

The final remark we make concerning Theorem 4.1 is the following. Rather than just looking at the determinant of $\mathbf{D}(T_p)$, we could investigate the characteristic polynomial

$$\Delta_{T_p}(x) = \det(\mathbf{D}(T_p) - x\mathbf{I}) = \sum_{k=0}^{p} d_k(T_p)x^k.$$

It turns out (see [**21**], [**16**]) that each coefficient $d_k(T_p)$ represents a fixed *linear combination* (independent of T_p) of the number of occurrences of various subforests in T_p (multiplied by a factor of 2^{p-k-2}). For the case $k = 0$, the coefficient

$$d_0(T_p) = \det \mathbf{D}(T_p)$$

depends only on the number of edges in T_p. The coefficients of these linear combinations themselves satisfy some rather mysterious relations which are not yet completely understood. However, a fuller description of this intriguing subject is beyond the scope of the present discussion. We point out that a curious lemma needed in **[21]** is the following:

Lemma 4.5. *For a tree T_p on p vertices, let ρ_i denote the degree of vertex v_i in T_p, and let $a_{ij} = 1$ if $\{v_i, v_j\} \in E(T_p)$, and 0, otherwise. Then the inverse $\mathbf{D}^{-1}(T_p) = (d_{ij}^*)$ of $\mathbf{D}(T_p)$ is given by*:

$$d_{ij}^* = \frac{(2-\rho_i)(2-\rho_j)}{2(p-1)} + \begin{cases} \frac{1}{2}a_{ij}, & \text{if } i \neq j, \\ -\frac{1}{2}\rho_i, & \text{if } i = j. \end{cases} \quad \|$$

5. Cartesian Products of Graphs

In this section we consider isometric embeddings of graphs into metric spaces formed from the Cartesian product of graphs. To begin with, suppose that $G = (V, E)$ is a given connected graph. Define a relation θ on E as follows:

if $e = \{v, w\} \in E$ and $e' = \{v', w'\} \in E$, then $e\ \theta\ e'$ if and only if
$$d_G(v, v') + d_G(w, w') \neq d_G(v, w') + d_G(v', w).$$

This relation was first introduced in an alternative form by Djoković **[15]**. It is easily seen to be well defined, reflexive and symmetric. Let $\hat{\theta}$ denote the transitive closure of θ, and let E_i $(1 \leq i \leq r)$ be the equivalence classes of $\hat{\theta}$.

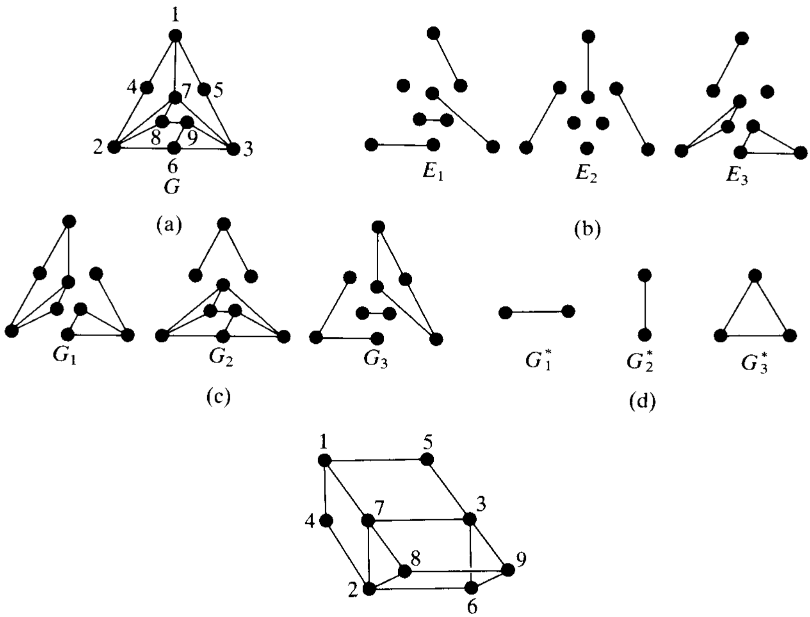
For each i $(1 \leq i \leq r)$, let G_i denote the graph $(V, E \backslash E_i)$, and let $C_i(1)$, $C_i(2)$, $\ldots$, $C_i(m_i)$ denote the connected components of G_i. Form the graphs $G_i^* = (V_i^*, E_i^*)$ $(1 \leq i \leq r)$ by letting $V_i^* = \{C_i(1), \ldots, C_i(m_i)\}$ and taking $\{C_i(j), C_i(j')\}$ to be an edge of G_i^* if and only if some edge in E_i joins a vertex in $C_i(j)$ to a vertex in $C_i(j')$. For $v \in C_i(j)$, denote by α_i: $V \to V_i^*$ the natural contraction sending $v \in C_i(j)$ into V_i^*. Define an embedding α: $G \to \prod_{i=1}^{r} G_i^*$, called the **canonical embedding** of G, by

$$\alpha(v) = (\alpha_1(v), \alpha_2(v), \ldots, \alpha_r(v)).$$

In Fig. 3 we illustrate these concepts for a particular graph G.

We call r, the number of factors G_i^* in the canonical embedding of G, the **isometric dimension** of G (for reasons soon to be made clear) and denote it by $\dim_I(G)$.

An isometric embedding $G \xrightarrow{I} \prod_{i=1}^{m} H_i$ is said to be **irredundant** if $|H_i| > 1$



$$\alpha : G \to \prod_{i=1}^{r} G_i^* = K_2 \times K_2 \times K_3$$

(e)

Fig. 3

for all i $(1 \leq i \leq m)$, and for all $h \in H_i$, h occurs as a coordinate value of the image of some $g \in G$. It is not difficult to see that any β: $G \xrightarrow{I} \prod_{i=1}^{m} H_i$ can be made irredundant by discarding unused vertices and factors.

Finally, let us call G **irreducible** if $G \xrightarrow{I} \prod_{i=1}^{m} H_i$ always implies that $G \xrightarrow{I} H_i$ for some i. The following result of **[24]** summarizes the main properties of the preceding concepts:

Theorem 5.1. *If* α: $G \xrightarrow{I} \prod_{i=1}^{r} G_i^*$ *is the canonical embedding, then*

(*i*) α *is isometric*;

(*ii*) α *is irredundant*;

(*iii*) *each factor* G_i^* *is irreducible*;

(*iv*) α *has the largest possible number* $\dim_I(G)$ *of factors among all irredundant isometric embeddings of* G;

(*v*) *the* only *irredundant isometric embedding of* G *into a product of*

$\dim_I(G)$ *factors is the canonical embedding;*

(vi) *each factor H_j of an irredundant isometric embedding $G \xrightarrow{I} \prod_{j=1}^{m} H_j$ embeds canonically into a product of G_i^*s.* ||

A key fact on which the proof in **[24]** of Theorem 5.1 rests is the following:

Lemma 5.2. *For $v, w \in V$, let P be a minimal path connecting v and w, and let Q be any path connecting v and w. Then for any E_i $(1 \le i \le r)$,*

$$|P \cap E_i| \le |Q \cap E_i|. \quad \|$$

As an immediate corollary of Theorem 5.1 we have the following result:

Corollary 5.3. *G is irreducible if and only if G has a single $\hat{\theta}$-equivalence class.* ||

6. Almost All Graphs are Irreducible

In the usual random graph model, a random graph $G = (V, E)$ has $V = \{1, 2, \ldots, n\}$ and each pair $\{i, j\}$ is chosen to be an edge with (independent) probability $\frac{1}{2}$. With this model, it is not difficult to show that almost all graphs with n vertices are irreducible as $n \to \infty$. What this means precisely is that the number of graphs with n vertices which are not irreducible, divided by the total number of graphs of this order, tends to zero as n increases. An easy way to see this is to consider the graph G shown in Fig. 4. The dotted lines indicate that an edge may or may not be present. In any case, it is immediate to verify that:

$$d_G(\alpha, x) + d_G(\beta, y) = 2 < 4 = d_G(\alpha, y) + d_G(\beta, x),$$

and $$d_G(\alpha', x) + d_G(\beta', y) = 2 < 4 = d_G(\alpha', y) + d_G(\beta', x),$$

so that if $\{\alpha, \beta\} = e \in E$, $\{\alpha', \beta'\} = e' \in E$, then $e\ \theta\ \{x, y\}$, $e'\,\theta\{x, y\}$, and consequently, $e\ \hat{\theta}\ e'$.

Lemma 6.1. *In almost all random graphs H, for any two pairs of vertices $\{\alpha, \beta\}$, $\{\alpha', \beta'\}$ of H there exist vertices x, y of H such that the vertices x and y are connected to α, β, α', β' and each other, as shown in Fig. 4.*

Proof. For two fixed (arbitrary) disjoint pairs of vertices $\{\alpha, \beta\}$, $\{\alpha', \beta'\}$ of a random graph H with n vertices, we call H *bad* if no such vertices x and y exist. Since the edges of H are chosen independently and uniformly, the probability that a *given* pair $\{x, y\}$ fails to induce G is at most $1 - 2^{-9}$. Since we can actually form at least $\lfloor\frac{1}{2}(n - 4)\rfloor \ge \frac{1}{2}n - 3$ disjoint candidate pairs $\{x_i, y_i\}$, the probability that all of them fail to induce G is at most

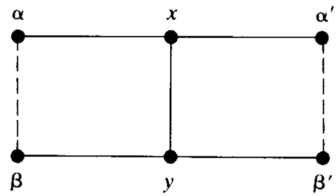


Fig. 4

$(1 - 2^{-9})^{\frac{1}{2}n-3}$. Finally, since there are at most n^4 choices for the initial pairs $\{\alpha, \beta\}$, $\{\alpha', \beta'\}$, the probability that H is bad for *some* choice $\{\alpha, \beta\}$, $\{\alpha', \beta'\}$ is at most $n^4(1 - 2^{-9})^{\frac{1}{2}n-3}$ which certainly tends to 0 as $n \to \infty$. ||

Thus, by Lemma 6.1, in almost all random graphs H any two edges e and e' satisfy $e \ \hat{\theta} \ e'$; that is, H is irreducible. In fact, the preceding argument can be strengthened to show that almost all graphs with n vertices and $cn^{2-\delta}$ edges are irreducible, for an appropriate $\delta > 0$.

It is not difficult to check that, if e and e' are edges belonging to different *blocks* of a connected graph G, then we can never have $e \ \hat{\theta} \ e'$ This implies the following:

Lemma 6.2. *If G is irreducible, then G is 2-connected.* ||

Similar considerations show that if any two edges e and e' of G can be connected by a sequence of triangles in G (that is, there exist triples

$$\{a_1, a_2, a_3\}, \{a_2, a_3, a_4\}, \ldots, \{a_{m-2}, a_{m-1}, a_m\}$$

such that all $\{a_i, a_{i+1}\}$ are edges of G and $e \subseteq \{a_1, a_2, a_3\}$, $e' \subseteq \{a_{m-2}, a_{m-1}, a_m\}$), then G is irreducible. Thus, any triangulated planar graph is irreducible. An analogous result holds for bipartite graphs in which any two edges are connected by a sequence of C_4s.

Irreducible graphs possess many other strong properties which we will not pursue here.

7. Isometric Embeddings into Cubes

In this section we apply some of the preceding theory and investigate graphs G which embed isometrically into Q_r, the r-dimensional cube. Indeed, the early fundamental paper of Djoković **[15]** was devoted to an investigation of such graphs.

Suppose $G \xrightarrow{I} Q_r$ for some r. Then certainly G must be bipartite. Furthermore, suppose $\{v, w\}$ is an edge of G, and assume (without loss of generality) that $v \to (0, 0, \ldots, 0)$ and $w \to (1, 0, \ldots, 0)$. Then any

u with $d_G(u, v) < d_G(u, w)$ must be mapped by the embedding into $(0, u_2, \ldots, u_r)$. In fact, it is not difficult to see that, if

$$d_G(u, v) < d_G(u, w) \text{ and } d_G(v, v) < d_G(v, w),$$

then all points z on any shortest path between u and v must be mapped $z \to (0, z_2, \ldots, z_r)$ by the isometry—that is, z must satisfy $d_G(z, v) < d_G(z, w)$.

The following result of Djoković [15], which can be obtained as a corollary of the previous results on embeddings into Cartesian products, shows that these two necessary conditions are in fact sufficient:

Theorem 7.1. *$G \xrightarrow{I} Q_r$ for some r if and only if*

(*i*) *G is bipartite*;

(*ii*) *for any edge $\{v, w\}$ of G, the set of vertices of G which are closer to v than w is closed under taking shortest paths.* ||

It turns out that when $G \xrightarrow{I} Q_r$, then $\theta = \hat{\theta}$; in fact, this can be used as an alternative characterization, as shown in [24]:

Theorem 7.2. *$G \xrightarrow{I} Q_r$ for some r if and only if*

(*i*) *G is bipartite*;

(*ii*) *the relation θ is transitive.* ||

Another characterization of these graphs was found by Roth and Winkler [30]:

Theorem 7.3. *$G \xrightarrow{I} Q_r$ for some r if and only if*

(*i*) *G is bipartite*;

(*ii*) $n_+(G) = 1$. ||

The proof involves producing a list of forbidden metric subspaces for graphs not isometrically embeddable in Q_r, showing that each of these spaces has at least two positive eigenvalues, and then applying an eigenvalue interlacing theorem.

As noted by Djoković in [15], when $G \xrightarrow{I} Q_r$ then $\dim_I(G)$ is equal to the number of θ-equivalence classes. However, there is also an explicit expression for the value of $\dim_I(G)$, depending only on the signs of the eigenvalues of $\mathbf{D}(G)$ (see [23]):

Theorem 7.4. *If $G \xrightarrow{I} Q_r$, then*

$$\dim_I(G) = n_-(G),$$

the number of negative eigenvalues of the distance matrix $\mathbf{D}(G)$ *of* G.

Proof. First, recall from Theorem 3.3 that $r(G) \geq n_-(G)$. Next, we claim that

$$G \xrightarrow{I} Q_r \Rightarrow n_+(G) = 1.$$

This can be seen by observing (as was done in [**11**]) that no *s are used in the proof of Theorem 3.3, $X_k \cup Y_k$ is always a partition of $V(G)$, and consequently the quadratic form $\sum d_{ij}x_i x_j$ is expressible as a sum of *one* positive square and some negative squares. This implies that $n_+(G) \leq 1$, and since $n_+(G) > 0$ (the trace of $\mathbf{D}(G)$ is zero), we have $n_+(G) = 1$.

We now claim that rank $\mathbf{D}(G) = n + 1$. To see this, observe that, on the one hand,

$$\text{rank } \mathbf{D}(G) = n_-(G) + n_+(G) = n_-(G) + 1 \leq r(G) + 1 \leq r + 1.$$

On the other hand, since G is connected there must exist vertices v_0, $v_1, \ldots, v_r \in V(G)$ such that, if $\lambda\colon G \xrightarrow{I} Q_r$ is an isometry, then the set $\{\lambda(v_0), \lambda(v_1), \ldots, \lambda(v_r)\}$ is full-dimensional in Q_r. Thus the submatrix

$$d_G(v_i, v_j) = (d_H(\lambda(v_i), \lambda(v_j))$$

is non-singular, and so rank $\mathbf{D}(G) \geq r + 1$. Consequently, rank $\mathbf{D}(G) = r + 1$, which proves the claim, and

$$n_-(G) = r = r(G) = \dim_I(G),$$

which proves the theorem. ||

It follows from these considerations, for example, that if $G \xrightarrow{I} Q_r$, then

$$\det \mathbf{D}(G) \neq 0 \text{ if and only if } G \text{ is a tree.}$$

8. General Metric Spaces

The problem of embedding graphs isometrically into other graphs is a special case of the more general topic of embedding (finite) metric spaces isometrically into other metric (or semi-metric) spaces. This subject has an extensive literature, some of which can be found in [**1**]–[**10**], [**12**]–[**14**], [**26**]–[**28**] and [**34**]. Many of these more general results apply directly to our problems. For example, it follows from these considerations that if $G \xrightarrow{I} K_3^r$, then $n_+(G) = 1$. The reason for this is as follows.

Let us say that an $r \times r$ distance matrix $\mathbf{D} = (d_{ij})$ is of **negative type** if

$$x_1 + \ldots + x_r = 0 \quad (x_k \in \mathbf{R}) \Rightarrow \sum_{i,j} d_{ij}x_i x_j \leq 0.$$

Similarly, we call **D hypermetric** if

$$x_1 + \ldots + x_r = 1 \quad (x_k \in \mathbf{Z}) \Rightarrow \sum_{i,j} d_{ij} x_i x_j \leq 0.$$

Although these two conditions are similar, the latter is actually much stronger (see [28]). Not only does it imply the former, but it also implies that the space satisfies the triangle inequality (and many stronger related inequalities), something that a matrix of negative type does not have to. It is not difficult to show that if **D** is of negative type, then $n_+(\mathbf{D}) = 1$.

An even more restrictive condition is the following. The matrix **D** is said to be ***l_1*-embeddable** if **D** can be realized as the distance matrix of a set $X \subseteq \mathbf{R}^m$ for some m, where the distance in $\mathbf{R}^m$ is the usual l_1-metric—that is,

$$d((x_1, \ldots, x_m), (y_1, \ldots, y_m)) = \sum_{k=1}^{m} |x_k - y_k|.$$

It is known (see [28]) that any l_1-embeddable space is hypermetric. Of course, if $G \xrightarrow{I} K_2^m$, then G is l_1-embeddable.

It turns out that the properties of l_1-embeddability, hypermetricity and negative type are preserved under taking products, factors and isometric subsets. Thus, for example, since K_3 is of negative type (actually, the matrix

$$\mathbf{D}(K_3) = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

is of negative type, which is easy to check), then

$$K_3^m \text{ is of negative type} \Rightarrow G \xrightarrow{I} K_3^m \text{ is of negative type} \Rightarrow n_+(G) = 1,$$

as claimed previously.

An interesting observation due to H. J. Landau (personal communication) is the following. Suppose that X is a metric space with distance matrix **D**. Let $\mathbf{D}^{(k)}$ denote the distance matrix corresponding to the product space X^k. As we have just remarked, if X is of negative type then so is X^k and, consequently, $n_+(\mathbf{D}^k) = 1$ for any k. It turns out rather unexpectedly that the converse holds. In fact, it can be shown that if $n_+(\mathbf{D}^{(2)}) = 1$, then this already implies that X must be of negative type. More generally, if X and Y are finite metric spaces, each having more than one point, and if $n_+(\mathbf{D}(X \times Y)) = 1$, then X and Y must both be of negative type.

9. Concluding Remarks

We show in Fig. 5 a map of some of the metric spaces which have been mentioned in the preceding sections. We conclude by describing a variety of results and open problems which deal with various regions of this map.

To begin with, it was suspected at one time (see [**34**]) that hypermetricity might imply l_1-embeddability. However, this was shown not to be the case, both by Assouad [**1**] and by Avis [**9**], who proved that the

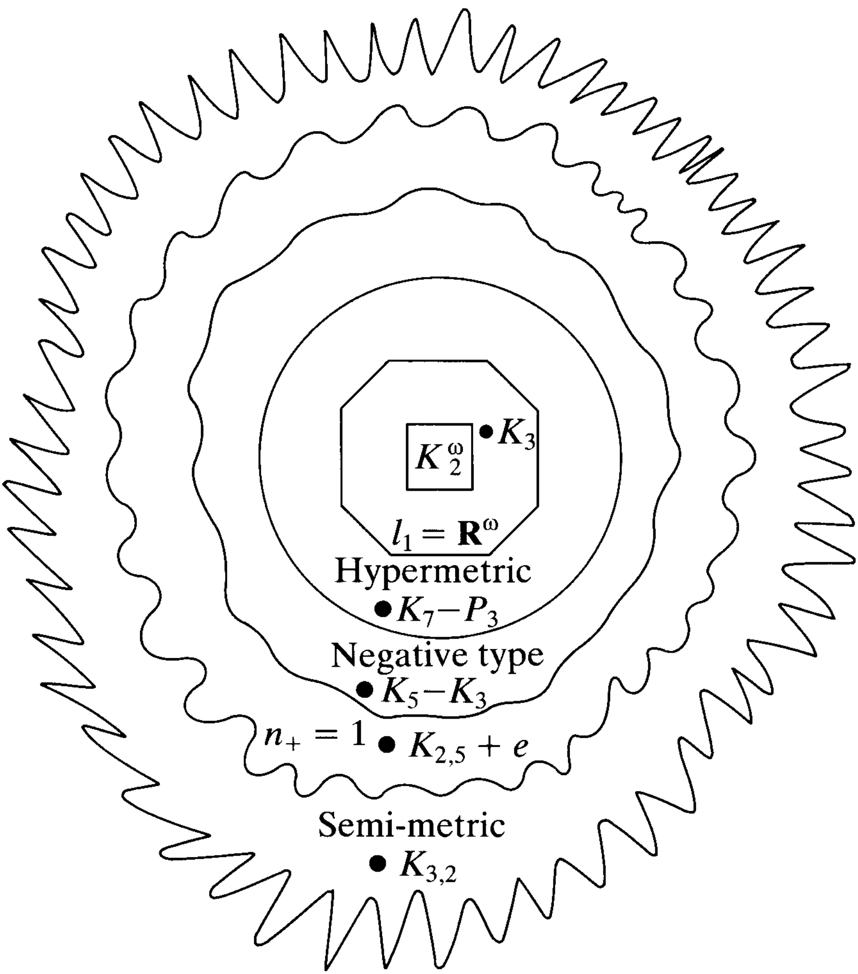


Fig. 5

graph $K_7 - P_3$ is hypermetric but not l_1-embeddable. In the same spirit, it is easy to show that the graph $K_5 - K_3$ is of negative type but not hypermetric (see [7]), and that $K_{2,5} + e$ is an example of a graph *not* of negative type which has $n_+ = 1$ (where the added edge e connects the two vertices in the smaller vertex class of $K_{2,5}$; see [36]).

We point out that the rather simple graph $K_{3,2}$ is exceptional in several respects. Since $n_+(K_{3,2}) = 2$, $K_{3,2}$ is not of negative type, and is therefore not isometrically embeddable into the n-cube Q_n, or even into $\mathbf{R}^n$. In fact, $K_{3,2}$ is not even a *subgraph* of Q_n. It also turns out that

$$r(K_{3,2}) = 4 > \max(n_+(K_{3,2}), n_-(K_{3,2})) = 3,$$

showing that equality need not hold in Theorem 3.3. It is not known how $r(G)$ behaves for random graphs, but it is natural to guess that $r(G) = |G| - 1$ for almost all large graphs G.

It has been shown by L. Babai and C. Godsil (personal communication) that almost all large graphs G have

$$n_+(G) = (\tfrac{1}{2} + o(1))|G|, \text{ and } n_-(G) = (\tfrac{1}{2} + o(1))|G|,$$

so that presumably Theorem 3.3 almost never holds.

At present no necessary and sufficient conditions are known for a graph to be l_1-embeddable, hypermetric, of negative type or have one positive eigenvalue. An old result of Schoenberg [31] shows that a distance matrix $\mathbf{D} = (d_{ij})$ is of negative type if and only if the corresponding distance matrix $\sqrt{\mathbf{D}} = (\sqrt{d_{ij}})$ can be realized by a point set in some Euclidean space. Very recently, Assouad [3] has characterized hypermetric spaces in terms of 'deep holes' in certain lattices in Euclidean space.

An interesting problem which has received some attention in the literature is that of determining the quantity $f(n)$, defined by

$$f(n) = \min\{m\colon |X| = n \text{ and } X \xrightarrow{I} \mathbf{R}^r \text{ for some } r \Rightarrow X \xrightarrow{I} \mathbf{R}^m\},$$

where the l_1-metric is used in $\mathbf{R}^r$ and $\mathbf{R}^m$.

The value of the corresponding function in Euclidean space is clearly $n - 1$, since any set of n points can be embedded isometrically in Euclidean $(n - 1)$-dimensional space. Life is not so simple for the l_1-metric, however. It has been shown by Witsenhausen (personal communication; also see [8]) that

$$f(3) = f(4) = 2, f(5) = 3, f(6) \geq 6, f(7) \geq 10, n - 2 \leq f(n) \leq \binom{n}{2}.$$

Even the correct order of growth of $f(n)$ is rather mysterious at this point.

It would be highly desirable to have analogues of Djoković's theorem for characterizing those $G \xrightarrow{I} H^r$, for general H. For example, Winkler (personal communication) has shown that $G \xrightarrow{I} K_3^r$ for some r if and only if θ is transitive. At present, however, almost nothing is known in this direction. It would seem fruitful to study the characteristic polynomials of the associated distance matrices of various spaces, rather than just the signs of the eigenvalues. This was initiated for trees in **[12]**, **[16]** and **[21]**. It seems quite likely that our understanding of this whole general area would increase substantially if the corresponding results were known for graphs more general than trees. Good candidates for this would appear to be graphs $G \xrightarrow{I} Q_r$.

Note added in proof. Very recently, Terwilliger and Deza **[32]** have characterized certain classes of hypermetric graphs.

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