Preface

This research monograph is a follow-up to the book Geometry of Cuts and Metrics by M.Deza and M.Laurent, published in 1997 by Springer-Verlag, Berlin (Russian translation was published in 2001 by MCNMO, Moscow). The main object of that book was the ℓ_1-metrics, i.e. those isometrically embeddable, up to a scale, into some hypercube H_m or, if infinite, into some cubic lattice Z_m. During the last six years a lot of work was done on a special case of ℓ_1-metric: the graph distance of the skeleton of (finite or infinite) polytope.

This monograph consists mainly of identifying such polytopes combinatorially ℓ_1-embeddable, within interesting lists of polytopal graphs, i.e. such that corresponding polytopes are either prominent mathematically (regular partitions, root lattices, uniform polytopes and so on), or applicable in Chemistry (fullerenes, polycycles etc.) The embeddability, if any, provides applications to chemical graphs and, in the first case, it gives new combinatorial perspective to ℓ_2-prominent affine polytopal objects.

The lists of polytopal graphs in the book, come from broad areas of Geometry, Crystallography and Graph Theory; so, just to introduce them we need many definitions. The book concentrates on such concise and, as much as possible, independent definitions. The scale-isometric embeddability - the main unifying question, to which those lists will be subjected - will be presented with the minimum of technicalities.

The main families of the considered graphs come from: various generalization of regular polytopes (or tilings), from (point) lattices and from applications in Chemistry.

Some samples of results are:

(i) All embeddable regular tilings and honeycombs of dimension $d > 2$, are, besides the hyper-simplices and hyper-octahedra, exactly those with bipartite skeleton: the hyper-cubes, cubic lattices and 11 special tilings of hyperbolic space.

(ii) If P is an Archimedean polyhedron or a plane partition, other than 3-gonal prism, then exactly one of P and its dual P is embeddable.

(iii) For the regular 4-polytope 24-cell, its usual and golden truncation (Gosset's semi-regular 4-polytope) are embedded into H_{12} and half-H_{12}, respectively.

(iv) The skeletons of Voronoi tiling for the lattice A_n and its dual lattice A_n^* are embedded into Z_{n+1} and $Z_{\binom{n+1}{2}}$, respectively.

The book is organized as follows.

Relatively long introduction (chapter 1) gives main notions, as well as methods of embedding. After reading it, any of the other chapters can be read independently.

Chapters 14 and 15 consider, respectively, specifications and generalizations of the notion of embeddability. Each of chapters 2–13 is centered around embeddability for a particular list of graphs. We tried to give concise and, as much as possible, independent presentation of those lists; so that the readers of different backgrounds will be able to isolate "ready to use" chapters, which are of interest for them.

Chapters 2, 4, 5, 6, 12, 13 treat various lists of 3-polytopes. Chapters 9, 10 and 11 consider infinite graphs coming from the tilings of $\mathbb{R}^2$, $\mathbb{R}^3$ and from lattices. Chapters 3, 7, 11 consider graphs in $\mathbb{R}^n$. Finally, chapters 2, 8 and 11 can be of interest for workers in Mathematical Chemistry and Crystallography.

The authors are grateful to Marie Grindel, Jacques Beigbeder and, especially, to Mathieu Dutour for various help: in drawings, redaction and inspiration.

1991 Mathematics Subject Classification: primary 05C12; secondary 52C99

Contents

Preface v

1. Introduction: Graphs and their Scale-isometric Embedding 1
   - 1.1 Graphs 1
   - 1.2 Embeddings of graphs 3
   - 1.3 Embedding of plane graphs 10
   - 1.4 Types of regularity of polytopes and tilings 14
   - 1.5 Operations on polytopes 17
   - 1.6 Voronoi and Delaunay partitions 18
   - 1.7 Infinite graphs 19
2. An Example: Embedding of Fullerenes 25
   - 2.1 Embeddability of fullerenes and their duals 26
   - 2.2 Infinite families of non-ℓ_1 fullerenes 30
   - 2.3 Katsura model for vesicles cells versus embeddable dual fullerenes 30
3. Regular Tilings and Honeycombs 35
   - 3.1 Regular tilings and honeycombs 35
   - 3.2 The planar case 36
   - 3.3 Star-honeycombs 40
   - 3.4 The case of dimension $d \geq 3$ 40
4. Semi-regular Polyhedra and Relatives of Prisms and Antiprisms 43
   - 4.1 Semi-regular polyhedra 43
   - 4.2 Moscow, Globe and Web graphs 45

4.3 Stellated k-gons, cupolas and antiwebs 48
4.4 Capped antiprisms and columns of antiprisms 50

5. Truncation, Capping and Chamfering 53

5.1 Truncations of regular partitions 53
5.2 Partial truncations and cappings of Platonic solids 54
5.3 Chamfering of Platonic solids 59

6. 92 Regular-faced (not Semi-regular) Polyhedra 63

7. Semi-regular and Regular-faced n-polytopes, $n \geq 4$ 71

7.1 Semi-regular (not regular) n-polytopes 71
7.2 Regular-faced (not semi-regular) n-polytopes 72
7.3 Archimedean 4-polytopes 72
7.4 The embedding of the snub 24-cell 73

8. Polycycles and Other Chemically Relevant Graphs 75

8.1 (r,q)-polycycles 75
8.2 Quasi-$(r,3)$-polycycles 77
8.3 Coordination polyhedra and metallopolyhedra 80

9. Plane Tilings 83

9.1 58 embeddable mosaics 83
9.2 Other special plane tilings 87
9.3 Face-regular bifaced plane tilings 89

10. Uniform Partitions of 3-space and Relatives 99

10.1 28 uniform partitions 100
10.2 Other special partitions 103

11. Lattices, Bi-lattices and Tiles 107

11.1 Irreducible root lattices 107
11.2 The case of dimension 3 108
11.3 Dicings 110
11.4 Polytopal tiles of lattice partitions 111

12. Small Polyhedra 115

12.1 Polyhedra with at most seven faces 115

12.2 Simple polyhedra with at most eight faces 116

13. Bifaced Polyhedra 119

13.1 Goldberg's medial polyhedra 120
13.2 Face-regular bifaced polyhedra 123
13.3 Constructions of bifaced polyhedra 125
13.4 Polyhedra 3_n and 4_n 126
13.5 Polyhedra 5_n (fullerenes) revisited 129
13.6 Polyhedra oc_n (octahedrites) 129

14. Special ℓ_1-graphs 137

14.1 Equicut ℓ_1-graphs 137
14.2 Scale one embedding 145

15. Some Generalization of ℓ_1-embedding 153

15.1 Quasi-embedding 153
15.2 Lipschitz embedding 157
15.3 Polytopal hypermetrics 157
15.4 Simplicial n-manifolds 160

Bibliography 163

Index 171

B are adjacent if and only if $|A \triangle B| = 1$, where $A \triangle B$ is the symmetric difference of the sets A and B. Hence the scale λ embedding $\phi : V \to H_m$ is equivalent to a labeling of each vertex $v \in V(G)$ by a set $\phi(v)$, such that vertices v and u are adjacent if and only if $|\phi(v) \triangle \phi(u)| = \lambda$. On the other hand, this labeling implies a labeling of *edges* (v, u) by the sets $\phi(v) \triangle \phi(u)$. For $i \in \{1, 2, \ldots, m\}$, call the set of edges, labels of which contain i, a *i-zone* or, simply, a *zone*. Both these labeling of vertices and edges of G are used in Figures of the chapter 2, for example.

If G is embedded into a hypercube H_m, then any partition of H_m into two opposite facets induces a partition $S \cup \overline{S} = V$ of the set of vertices of G. Any partition $S \cup \overline{S} = V$ is called the *cut* $\{S, \overline{S}\}$. The edge set $E(S, \overline{S})$ of the cut $\{S, \overline{S}\}$ is the set of edges with one end in S and another one in $\overline{S}$. Evidently, removing $E(S, \overline{S})$ from G we obtain a graph with at least two connected components, i.e. $E(S, \overline{S})$ is a cutset of edges. The edges of the set $E(S, \overline{S})$ *are cut* by the cut $\{S, \overline{S}\}$.

The cut $\{S, \overline{S}\}$ defines the *cut semimetric* $\delta(S)$ on the set V:

$$\delta(S)(i,j) = \delta_{\{S,\overline{S}\}}(i,j) = \begin{cases} 0 \text{ if } i, j \in S \text{ or } i, j \in \overline{S} \\ 1 \text{ otherwise.} \end{cases}$$

Let us project the hypercube H_m with an embedded graph G along the edges connecting two opposite facets. Then we obtain an embedding of G into H_{m-1}, such that some distances of G are diminished by one. In other words, we embed G endowed with the new semimetric $d_G - \delta(S)$.

In such a way we obtain a decomposition of the path-metric d_G of an ℓ_1-embeddable graph G (actually, of any ℓ_1-metric) into a non-negative linear combination of cut semimetrics.

All ℓ_1-semimetrics on n vertices (that is, all ℓ_1-semimetric spaces (V_n, d) with $|V_n| = n$), considered as points of an $\binom{n}{2}$-dimensional space, form a $\binom{n}{2}$-dimensional pointed cone called the *cut cone*. This cone is generated by the $2^{n-1} - 1$ extreme rays. Each extreme ray is a non-zero cut semimetric $\delta(S)$ for some proper subset S of $V_n = \{1, 2, \ldots, n\}$.

In other words, a graph G (or any metric) is ℓ_1-embeddable graph if and only if the path-metric d_G is a linear combination, with non-negative coefficients, of cut semimetrics:

$$d_G = \sum_{S \subset V_n} a_S \delta(S) \text{ with } a_S \geq 0 \text{ for all } S.$$

If G is embeddable into H_m with a scale λ, then the above decomposition can be rewritten as follows

$$\lambda d_G = \sum_{S \subset V_n} a_S \delta(S) \text{ with integer } a_S \geq 0 \text{ for all } S. \tag{1.1}$$

An advantage of using (1.1) is that it allows to classify ℓ_1-embedding of G up to equivalence: different solutions to (1.1) with non-negative integers a_S such that $g.c.d.(\lambda, a_S) = 1$ correspond to different embeddings. If such a solution is unique, the graph G is called ℓ_1*-rigid graph* (see [DeLa94]).

Rigidity of any ℓ_1-metric is defined similarly. Restated in terms of the cut cone, a metric is ℓ_1-rigid if and only if it belongs to a face of the cut cone, which is a simplex subcone.

If G is an ℓ_1-graph, then for every cut $\{S, \overline{S}\}$ occurring in the ℓ_1-decomposition of d_G (i.e. with $a_S > 0$), both sets S and $\overline{S}$ are convex; we call such a cut *convex cut*. The following fact was established in [DeTu96].

Proposition 1.1 *[DeTu96] A graph G is scale λ embeddable into a hypercube if and only if there exists a* complete *collection $\mathcal{C}(G)$ of (not necessary distinct) convex cuts of G, such that every edge of G is cut by exactly λ cuts from $\mathcal{C}(G)$.*

For $\lambda = 1$ this is the well-known Djokovic characterization ([Djok73]) of graphs, which are isometrically embeddable into hypercubes.

Lemma 1.1 *[CDG97] Any ℓ_1-graph, which does not contain K_4, is ℓ_1-rigid.*

We say that a polyhedron P is ℓ_1-embeddable if its *skeleton* $G(P)$ (that is, the graph formed by its vertices and edges) is an ℓ_1-graph. A graph G is called *polytopal graph* if there is a polytope P (possibly, infinite) with $G(P) = G$.

For an embedding of a metric d into m-cube with scale λ, the ratio $s(d) = \frac{m}{\lambda}$ is called *size* of the embedding. For a graph G on n vertices there are the following lower and upper bounds on size $s(d_G)$ (see [DeLa97], page 45):

$$\frac{W(G))}{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil} \leq s(d_G) \leq \frac{W(G)}{n-1}, \tag{1.2}$$

where, recall,

$$W(G) = \sum_{i,j \in V} d_G(i,j).$$

When the equality holds in the left-hand side of the inequality (1.2), we say that G is an *equicut graph*. This means that for such a graph, every S in the formula (1.1) satisfies $a_S \neq 0$ if and only if S partitions V into parts of size $\lceil \frac{n}{2} \rceil$ and $\lfloor \frac{n}{2} \rfloor$, where $n = |V|$.

On the other hand, the equality on the other side of (1.2) only happens in a very special case.

Lemma 1.2 *$s(d_G) = \frac{W(G)}{n-1}$ if and only if G is the star $K_{1,n-1}$.*

As an example, consider embedding of an n-simplex α_n having $G(\alpha_n) = K_{n+1}$. Any $\alpha_n, n \geq 3$, is not ℓ_1-rigid, i.e. it admits at least two different embeddings. We give now three embeddings of α_n into m-cubes H_m with scale λ, realizing, respectively, maximum, minimum and a middle (for $n > 4$) of size $\frac{m}{\lambda}$. For the simplex α_n the bounds (1.2) take the form

$$s_n := \frac{n(n+1)}{2\lfloor \frac{n+1}{2} \rfloor \lceil \frac{n+1}{2} \rceil} \leq s(\alpha_n) \leq \frac{n+1}{2} < \frac{n(n+1)}{2(n-1)} = \frac{W(K_{n+1})}{n-1}.$$

For the left hand side, we have $s_n = 2 - \frac{1}{\lceil \frac{n+1}{2} \rceil}$, i.e. $s_n = \frac{2n}{n+1}$ for odd n, and $s_n = \frac{2(n+1)}{n+2}$ for even n.

The upper bound is realized by the embedding $\alpha_n \to \frac{1}{2}H_{n+1}$, where the vertices of α_n are mapped into vertices x of $\frac{1}{2}H_{n+1}$ with $\sum_{i=1}^{n+1} x_i = 1$ (in odd representation of $\frac{1}{2}H_{n+1}$).

A middle (for $n > 4$) size is realized as follows. Take the set of all $\frac{n(n+1)}{2}$ edges (ij), $1 \leq i < j \leq n+1$, of K_{n+1} as the set of indices V of H_m, i.e. $m = \frac{n(n+1)}{2}$. Map the vertex i of α_n (i.e. of K_{n+1}) into the subset $V_i = \{ij : 1 \leq j \leq n+1, j \neq i\} \subset V$. Then $|V_i \Delta V_j| = 2(n-1)$ is the scale λ. In this case $s(\alpha_n) = \frac{n(n+1)}{4(n-1)}$. For $n = 4$, this gives $s(\alpha_4) = s_4 = \frac{5}{3}$, i.e. the lower bound for $n = 4$.

Define λ_n be the minimal even positive number t such that ts_n is an integer. Then there is an embedding of α_n into $\lambda_n s_n$-cube with scale λ_n realizing the lower bound s_n. This is an equicut embedding (cf. the item (i) of Theorem 1.1 below).

Any $\beta_n, n \geq 4$, is also not ℓ_1-rigid. All embedding of β_n are into 2λ-cube with a such even scale λ that α_{n-1} is embeddable into m-cube, $m \leq 2\lambda$, with scale λ. For minimal such scale, denote it μ_n, the following is known: $n > \mu_n \geq 2\lceil \frac{n}{4} \rceil$ with equality in the lower bound for any $n \leq 80$ and, in the case of n divisible by four, if and only if there exists an Hadamard matrix of order n. In particular, β_3 and β_4 are embeddable into $\frac{1}{2}H_4$ (in fact, $G(\beta_4) = \frac{1}{2}H_4$, but there are two embeddings of β_4 into $\frac{1}{2}H_4$), β_5 is embeddable only with scale four (into H_8).

The size $s(d_G)$ has the following properties formulated in terms of $n = |V|$.

Theorem 1.1 *[DePa01] Let G be an ℓ_1-graph.*

(i) $s(d_G) = s_{n-1} = 2 - \frac{1}{\lceil \frac{n}{2} \rceil}$ if and only if $G = K_n$;

(ii) $s(d_G) = 2$ if and only if G is a non-complete subgraph of a cocktail-party graph $K_{n\times 2}$;

(iii) $s(d_G) = n - 1$ if and only if G is a tree;

(iv) $2 < s(d_G) < n - 1$, otherwise.

Clearly, the scale λ embeddability into H_m implies the scale 2λ embeddability into $\frac{1}{2}H_{2m}$. Moreover, for any graph G, which is scale λ embeddable into a hypercube, we have:

(i) $\lambda = 1 \Leftrightarrow G$ is an isometric subgraph of a hypercube; we write: $G \to H_m$.
(ii) $\lambda = 1$ or $2 \Leftrightarrow G$ is an isometric subgraph of a half-m-cube; we write: $G \to \frac{1}{2}H_m$.

Similarly, for an infinite graph G we have:

(i) $\lambda = 1 \Leftrightarrow G$ is an isometric subgraph of a cubic lattice; we write: $G \to Z_m$.
(ii) $\lambda = 1$ or $2 \Leftrightarrow G$ is an isometric subgraph of a half-cubic lattice graph; we write: $G \to \frac{1}{2}Z_m$.

Lemma 1.3 *[CDG97] The scale λ of a planar ℓ_1-graph is either one or two.*

Finally, we recall that a graph G is called *hypermetric graph* (see [DeGr93] for details) if its path-metric d_G satisfies any *hypermetric inequality* defined by:

$$\sum_{1\le i<j\le n} b_i b_j \, d_G(v_i, v_j) \le 0, \tag{1.3}$$

where $b = \{b_1, b_2, \ldots, b_n\} \in Z^n$, $\sum_{i=1}^{n} b_i = 1$ and v_i, $1 \le i \le n$, are arbitrary distinct vertices of G.

Note that the above definition of a hypermetric is *local*, since it uses only finite sets of vertices. Hence an *infinite* graph is called *hypermetric* graph if each its finite subgraph is a hypermetric graph.

If $\sum_{i=1}^{n} |b_i| = 2k+1$, this inequality is called a $(2k+1)$-*gonal inequality* ([Deza60]) and a graph satisfying all $(2q+1)$-gonal inequalities for $q \leq k$ is called $(2k+1)$-*gonal*.

Clearly, the case $k = 1$ corresponds to the usual triangle inequality. Below we present the case $k = 2$, i.e. the 5-gonal inequality, which is an important necessary and in many cases sufficient (see below) condition for embedding of graphs. Namely, for $b_a = b_b = b_c = 1$, $b_x = b_y = -1$, (1.3) takes the form :

$$d(x,y) + (d(a,b) + d(a,c) + d(b,c)) \leq$$
$$(d(x,a) + d(x,b) + d(x,c)) + (d(y,a) + d(y,b) + d(y,c)) \qquad (1.4)$$

for distances between any five vertices a, b, c, x, y.

Using the given above definition of the cut semimetric $\delta(S)$, it is not difficult to verify that

$$\sum_{1 \leq i < j \leq n} b_i b_j \delta(S)(i,j) = \sum_{i \in S, j \in \overline{S}} b_i b_j = (\sum_{i \in S} b_i)(1 - \sum_{i \in S} b_i) \leq 0,$$

since $\sum_{i \in S} b_i$ is an integer. According to the decomposition (1.1), this implies that every ℓ_1-semimetric is a hypermetric.

For the path-metric of a graph G, the links between those metric properties are given by the following inclusions:

G is an isometric subgraph of a hypercube $\Rightarrow$ d_G is ℓ_1-rigid
$\Rightarrow$ G is an isometric subgraph of a half-cube $\Rightarrow$ G is an ℓ_1-graph
$\Rightarrow$ d_G is hypermetric $\Rightarrow$ d_G is $(2k+1)$-gonal $\Rightarrow$ d_G is $(2k-1)$-gonal
$\Rightarrow$ d_G is 3-gonal (= metric).

We also recall that the Djoković' characterization of ℓ_1-graphs with scale $\lambda = 1$ can be reformulated (see Avis [Avis80]) in the following way: a graph is an isometric subgraph of a hypercube if and only if it is bipartite and 5-gonal.

In general, a graph G is an ℓ_1-graph if and only if G is an isometric subgraph of a Cartesian product of cocktail-party graphs (i.e. the skeletons of the polytopes dual to hypercubes) and half-cube graphs, see [Shpe93] (or [DeGr93] for another proof).

As for complexity results: while recognizing of a metric as ℓ_1-embeddable (that is isometrically embeddable into an ℓ_1^m) is NP-complete (see [Karz85]), recognizing of a graph as ℓ_1-embeddable is polynomial (see [DeSh96]). See also [DeLa97] for a general study of ℓ_1-metrics.

1.3 Embedding of plane graphs

In spite of the fact that recognizing if a graph is ℓ_1-embeddable, is polynomial, a more simple algorithm is suggested in [CDG97] for any planar graphs. This algorithm is very useful, since polytopal graphs of 3-dimensional polytopes and 2-dimensional tilings are planar. A proof of all assertions of chapter 1.3 can be find in [CDG97].

Recall that, according to Lemma 1.3, a planar ℓ_1-graph G has scale λ equal to 1 or 2, and it is 1 if and only if G is bipartite. According to Proposition 1.1, in order to find an ℓ_1-embedding of a planar non-bipartite graph, it is sufficient to find a collection of convex cuts, such that every edge of G is cutted by exactly 2 cuts of this collection. The algorithm, which is mentioned above, finds explicitly this collection.

Let G be a planar *locally* finite graph (i.e. all vertices have finite degree) and assume a plane drawing of G is given, i.e. G is a plane graph. An *interior face* of G is a cycle of G, which bounds a simply connected region. Denote by G^* the plane graph dual to G; suppose that a plane drawing of G^* is given, such that the vertices and the edges of G^* belong to the corresponding faces of G.

Let $Z(S,\overline{S})$ be the family of interior faces of G, which are crossed by the cut $\{S,\overline{S}\}$; we say that $Z(S,\overline{S})$ is the *belt* of the cut $\{S,\overline{S}\}$. Let $C(S,\overline{S})$ be a partial subgraph of G^* defined in the following way: the vertices of $C(S,\overline{S})$ are the faces of $Z(S,\overline{S})$ and two such faces are adjacent in $C(S,\overline{S})$ if and only if they share a common edge from $E(S,\overline{S})$.

Lemma 1.4 *If $\{S,\overline{S}\}$ is a convex cut and F is a face of a plane graph G, then $|E(S,\overline{S})\cap E(F)| = 0$ or 2. In particular, $C(S,\overline{S})$ is either a path, or a cycle.*

Geometrically, Lemma 1.4 asserts that if we cut the plane along $C(S,\overline{S})$, then, once entering a face of $Z(S,\overline{S})$, we must exit this face through some other edge and we will never visit this face again. In particular, the line, along which we cut, has no self-intersections. Furthermore, the sets $S\cap Z(S,\overline{S})$ and $\overline{S}\cap Z(S,\overline{S})$ are either paths, or cycles. Let us denote them by $bd(S)$ and $bd(\overline{S})$, and call them the *border lines* of the cut $\{S,\overline{S}\}$.

Now, we assume that a planar graph G embedded in the Euclidean plane with the following property:

(a) *Any interior face is an isometric cycle of G.*

(Although this property is natural, one can construct planar ℓ_1-graphs, which do not admit a planar embedding obeying the condition (a): for example, take a *book*, i.e. a collection of at least three 4-cycles sharing a common edge.)

Two edges $e = (u, v)$ and $e' = (u', v')$ on a common interior face F are called *opposite* if $d_G(u, u') = d_G(v, v')$ and these distances are equal to the diameter of the cycle F. If F is an *even* face (i.e. if it is bounded by a circuit of even length), then any of its edges has a unique opposite. Otherwise, if F has an odd length, then every edge $e \in E(F)$ has two opposite edges e^+ and e^-. In the latter case, if F is clockwise oriented, we distinguish (for e) the *left opposite edge* e^+ and the *right opposite edge* e^-. If every face of $Z(S, \overline{S})$ is crossed by the cut $\{S, \overline{S}\}$ in two opposite edges, then we say that $\{S, \overline{S}\}$ is an *opposite cut* of G.

If a convex cut $\{S, \overline{S}\}$ of G enters an interior face F through an edge e, then convexity of S and $\overline{S}$, and isometricity of F yield that $\{S, \overline{S}\}$ exits F through an edge opposite to e. We say that $\{S, \overline{S}\}$ is *straight* on an even face F and this cut *makes a turn* on an odd face F. The turn is *left* or *right*, depending on which of the opposite edges e^+ or e^- we cross.

Lemma 1.5 *In a plane graph with isometric faces all convex cuts are opposite.*

If G is a plane graph with isometric faces of even length only (i.e. if G is bipartite), then G is an ℓ_1-graph if and only if every opposite cut is convex. This presents a useful way to verify if G is ℓ_1-embeddable or not.

An opposite cut of a plane graph G is *alternating cut* if the turns on it alternate. For many important plane ℓ_1-graphs the convex cuts, participating in an ℓ_1-decomposition, turn out to be alternating. Consequently, if G is bipartite, then the alternating cuts are exactly the opposite cuts of G. By Lemma 1.5 every convex cut of a bipartite graph G is alternating.

Another class of plane graphs with this property is given in the next lemma (we say that two interior faces are *adjacent* if they share an edge).

Lemma 1.6 *Let G be a plane graph, in which all interior faces are isometric cycles of odd length. If the union of each pair of adjacent faces is an isometric subgraph of G, then any convex cut of G is alternating.*

The most known class of plane graphs verifying the conditions of Lemma 1.6 is that of *triangulations* (i.e. plane graphs, in which all interior faces are triangles) without 4-cliques. It has been established in [BaCh00] that any finite triangulation with the property that all vertices, which do not belong to the exterior face, have degree larger than five is

ℓ_1-embeddable. Moreover, all such graphs are ℓ_1-rigid.

For a triangulation, Lemma 1.6 implies the following property:

If a triangulation G does not contain K_4 as an induced subgraph (i.e. if all interior vertices have degree at least 4*), then any convex cut of G is alternating.*

A circuit C of a plane graph G is said to be *alternating* (or *left-right circuit*, or *Petri walk*, or *zigzag*) if every face of G is either disjoint with C, or shares with it exactly two consecutive edges. Clearly, any edge of G is covered by exactly two circuits from the family of alternating circuits of G; in other words, G has a double cover by its alternating circuits.

The graph G^*, which is the dual to a cubic plane graph G, is a plane triangulation. Every alternating *simple* circuit of G corresponds to an alternating cut of G^* and, conversely, any convex alternating cut of G^* defines a simple alternating circuit of G. Therefore, we obtain the following necessary condition of embedding of G^*:

If the dual of a finite plane cubic graph G is ℓ_1-embeddable, then all its alternating circuits are simple.

Above condition is not sufficient; for example, fullerenes $C_{20a^2}(I_h)$ (see chapter 2) have exactly $6a$ alternating circuits, all of which have length $10a$ and simple, but their dual polyhedra embed only for $a = 1$ (the icosahedron).

A circuit C of a plane *Eulerian* (i.e. with every vertex having even valence) graph G is said to be *central* (or *straight-ahead*) circuit if entering in each its vertex, it leave it by opposite edge. Clearly, any edge of G is covered by exactly one circuit from the family of central circuits of G; in other words, the edge-set of G is partitioned by its central circuits, i.e. G has a cover by its central circuits.

The graph G^*, which is dual to an Eulerian plane graph G, is a plane bipartite one. Every central simple circuit of G corresponds to an opposite cut of G^* and, conversely, any convex opposite cut of G^* defines a simple central circuit of G. Therefore, we obtain the following necessary condition of embedding of G^*:

If the dual of a finite plane Eulerian graph G is ℓ_1-embeddable, then all its central circuits are simple.

Now we present an algorithmic procedure to find the alternating cuts (if they exist) crossing given edge $e = (u, v)$ of a plane graph G. In order to do this we extend the cuts from the edge e, crossing face after face. We go away from e straight through even faces until we arrive to an odd face, say, F. Then in one cut we make a left turn on F and in the other cut we make a right turn on F. After that we have only to alternate the directions when passing through odd faces of G. Namely, if, say, our last turn in a cut was to left, then coming to the next odd face this cut turns to right and conversely. Let $E(e)$ and $E'(e)$ be two subsets of edges, which we cross in this movement. Then any alternating cut $\{S, \overline{S}\}$, which cuts the edge e, satisfies either to $E(S, \overline{S}) = E(e)$, or to $E(S, \overline{S}) = E'(e)$. Indeed, $\{S, \overline{S}\}$ cuts the edges from the common part of $E(e)$ and $E'(e)$ until the face F. At this moment, we have only two possibilities to continue the movement along $E(S, \overline{S})$; namely, $\{S, \overline{S}\}$ cuts the face F in the same fashion as $E(e)$ or $E'(e)$, say as $E(e)$. In this case necessarily $E(S, \overline{S})$ and $E(e)$ coincide everywhere.

We call a set of edges of the form $E(e)$ or $E'(e)$, for some e, an *alternating zone* (of edges). If we label each alternating zone by a number, then each edge obtains a label consisting of two numbers. If G is an ℓ_1-graph, then the alternating zone with a label i is the i-zone defined above.

So, we have the following result.

Lemma 1.7 *Every edge e of a plane l_1-graph G is crossed by at most two alternating cuts, each of them being defined by the alternating zones $E(e)$ or $E'(e)$.*

Denote by $\mathcal{A}(G)$ the collection of all alternating cuts of G, where every cut, which never has to turn is counted twice. In general, there are plane graphs without alternating cuts. This is due to the fact that $E(e)$ and $E'(e)$ do not necessarily define cutsets of G. However, if $E(e)$ and $E'(e)$ are cutsets for all $e \in E(G)$, then Lemma 1.7 infers that the family of alternating cuts $\mathcal{A}(G)$ is rather complete: every edge of G is crossed by exactly two cuts from $\mathcal{A}(G)$.

Unfortunately, only this property together with the property (a) do not imply ℓ_1-embeddability of a plane graph G, because alternating cuts can be non-convex. Neither it can exclude ℓ_1-embeddability: there exist plane ℓ_1-graphs with non-convex alternating cuts and so, such that the complete family of convex cuts (which, by Proposition 1.1, gives the embedding) contains non-alternating convex cuts. Let us call such embeddings *non-standard*. Examples of 3-polytopes having non-standard embedding are: α_3, $(Prism_3)^* \to \frac{1}{2}H_4$, dual $RhDo$-$v_3 \to \frac{1}{2}H_6$ (three amongst six convex cuts are non-alternating), Dürer's octahedron $\to \frac{1}{2}H_8$ (five amongst eight convex cuts are not alternating; see Figure 1.3), $F_{26} \to \frac{1}{2}H_{12}$ (see Figure 2.2 below) and (considered in chapter 5) B-extensions, realizing $P + Prism_3$, and elongations along circuit of graphs with non-standard embedding.

To ensure the ℓ_1-embeddability of G we have to impose the following metric condition on the border lines of alternating cuts constructed by our procedure (fortunately, these natural requirements are easily verified in many important particular cases):

(b) *Any border line* $bd(S)$ *and* $bd(\overline{S})$ *of any alternating cut* $\{S, \overline{S}\}$ *is an isometric cycle or a geodesic.*

Evidently, (b) implies the condition (a).

Proposition 1.2 *If* G *is a plane graph, satisfying condition (b), then a cut* $\{S, \overline{S}\}$ *of* G *is alternating if and only if it is convex. Hence* G *is a rigid* ℓ_1*-graph.*

In fact, from Lemma 1.6 and condition (b) we obtain that every edge of G is crossed by exactly two alternating cuts. By Proposition 1.2 we conclude that G is scale two embeddable into a hypercube. Since every convex cut of G is alternating, we deduce that this ℓ_1-embedding of G is unique.

Recall that a finite planar graph G is *outerplanar graph* if there is an embedding of G in the Euclidean plane, such that all vertices of G belong to the exterior face. Applying the above facts to outerplanar graphs, we obtain

Proposition 1.3 *Any outerplanar graph is a rigid* ℓ_1*-graph.*

Easy to see, that any embeddable finite plane graph embeds into $H_{\frac{p}{2}+z}$, if it is bipartite, and into $\frac{1}{2}H_{p+z}$, otherwise; here p is the length of the perimeter and z is the number of *closed* (i.e. having only non-boundary edges) alternating zones.

1.4 Types of regularity of polytopes and tilings

In this book, we shall consider ℓ_1-embedding of graphs $G(P)$ of 1-skeletons (i.e. edge-skeletons) of (convex) n-polytopes P. We consider also such generalizations of n-polytopes as non-convex n-polytopes, tilings, honeycombs

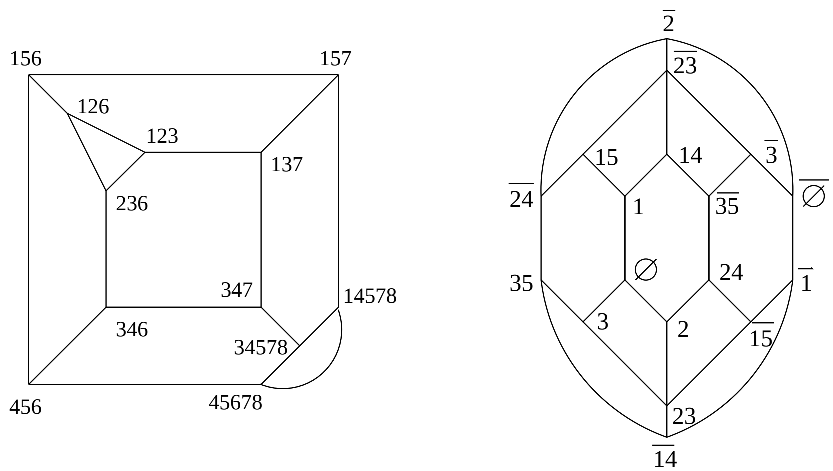


Fig. 1.1 **Examples of embedding: a) Dürer's octahedron** $\rightarrow \frac{1}{2}H_8$**, b) elongated dodecahedron ElDo** $\rightarrow H_5$

etc. We call such P ℓ_1-*embeddable* if its graph $G(P)$ is ℓ_1-embeddable.

A *convex* n*-polytope* is an n-dimensional compact convex subset of Euclidean n-space formed by intersections of finitely many half-spaces, see [Grün67]. The k-dimensional intersection, $0 \leq k \leq n-1$, of n-polytope with supporting hyperplanes are called their k*-faces*. In particular, for $k = 0, 1$ and $n-1$, we have *vertices*, *edges* and *facets*, respectively. An n-polytope is called *simple* n*-polytope* if each its vertex has exactly n neighboring vertices.

For $n = 3$, we sometimes call a 3-polytope by a *polyhedron*. The graph of the edge-skeleton of a polyhedron is planar. We call a polyhedron a k*-hedron* if it has k facets. For example, the tetrahedron is a 4-hedron, the cube is a 6-hedron, the octahedron is an 8-hedron, the dodecahedron is a 12-hedron and the icosahedron is a 20-hedron.

A polyhedron, such that all of its facets are *regular* triangles, is called *deltahedron*. There are exactly eight (convex) deltahedra with regular ones tetrahedron, octahedron and icosahedron amongst them.

A *dual polytope* of a convex n-polytope P is an n-polytope P^* such that the k-faces of P^*, $0 \leq k \leq n-1$, are in one-to-one correspondence with the $(n-k-1)$-faces of P and corresponding faces are orthogonal. The planar graphs of the skeletons of dual polyhedra are also dual.

We shall also consider *non-convex* n*-polytopes*, which are compact sets with interior points and piecewise linear boundary structure. They are homothetic to the n-ball.

An *n-dimensional honeycomb* is an infinite set of n-polytopes fitting together to fill all n-space, such that every facet of each polytope belongs to exactly one other polytope; it is called *tiling* if all above polytopes are convex.

For a definition of regularity a notion of a vertex figure is important. A *vertex figure* of an n-polytope or, more generally, of a tiling or of a honeycomb, is the convex hull of the midpoints of all edges incident to a given vertex. A vertex figure of an n-polytope is a convex $(n-1)$-polytope. But a vertex figure of an n-tiling or of an n-honeycomb can be infinite and/or non-convex.

The regularity of an n-polytope is defined by induction over its dimension supposing that a point is a convex regular 0-polytope.

A convex n-polytope is *regular n-polytope* if all its facets and vertex figures are regular $(n-1)$-polytopes.

A *regular-faced n-polytope* is one, whose facets are regular $(n-1)$-polytopes. All regular-faced n-polytopes are known.

An *isogonal n-polytope* is one, whose group of symmetries is transitive on vertices.

A *semi-regular n-polytope* is a regular-faced isogonal n-polytope. A semi-regular 3-polytope is the same as uniform polyhedron.

With the semi-regular 3-polytopes as a starting point, for $n \geq 4$, an isogonal n-polytope is called *uniform* if all its facets are uniform (that is, for $n = 4$, the facets are semi-regular polyhedra).

A *quasi-regular n-polytope* is a semi-regular polytope, whose symmetry group is transitive on edges.

Five regular polyhedra (Platonic solids) and semi-regular polyhedra (13 Archimedean solids, prisms, antiprisms) have been known since antiquity. Archimedean polyhedra and their dual (Catalan polyhedra) were rediscovered during the Renaissance, and Kepler ([Kepl1619]) gave them their modern names. We give the usual notations of the five Platonic polyhedra:

- simplex α_3 = tetrahedron; it is self-dual, $G(\alpha_3) = K_4$;
- cube γ_3, $G(\gamma_3) = H_3$ and its dual: octahedron β_3, $G(\beta_3) = K_{3\times 2}$;
- icosahedron Ico and its dual: dodecahedron Do.

We denote by $\frac{1}{2}\gamma_n$ the convex hull of a half of vertices of the n-cube γ_n, such that its skeleton form the graph $\frac{1}{2}H_n$. The *Johnson n-polytope* $P_J(n)$ is the convex hull of vertices of γ_{n+1} lying in the hyperplane $\sum_1^{n+1} x_i = 2$. Its skeleton $G(P_J(n))$ is $J(n+1,2) = T(n+1) = L(K_{n+1})$. Similarly as for graphs, we have

$$\tfrac{1}{2}\gamma_2 = \alpha_1 = \beta_1 = \gamma_1, \quad P_J(2) = \alpha_2,\, P_J(3) = \beta_3,$$
$$\tfrac{1}{2}\gamma_4 = BPyr(P_J(3)) = \beta_4.\ \tfrac{1}{2}\gamma_3 = \alpha_3\ .$$

See below for definition of the *n-bipyramid* $BPyr(P)$.

Apropos, for $m = 3, 4$, $(\frac{1}{2}\gamma_m)^* = \alpha_3, \gamma_4$, respectively; for $m \geq 5$, $(\frac{1}{2}\gamma_m)^*$ contains isometric subgraph $K_5 - K_3$ and so, not 5-gonal.

All regular and regular-faced polytopes are known. For each $n > 4$, all regular n-polytopes are: n-simplex α_n with $G(\alpha_n) = K_{n+1}$, n-cross-polytope β_n with $G(\beta_n) = K_{n\times 2}$ and n-cube γ_n with $G(\gamma_n) = H_n$.

All 92 regular-faced polyhedra were found by the work of many people, especially, of Johnson and Zalgaller (see, for example, [John66], [Zalg69], [Berm71], [KoSu92]). Finally, in [BlBl91], the complete list of regular-faced n-polytopes is given.

Semi-regular n-polytopes were found in 1897 by Gosset. It is proved for $n = 4$ in [Maka88] and for any n in [BlBl91] that the Gosset's list is complete (see [Coxe73] and [Grün67] for an historical account). In what follows, we use frequently the names and numbers of 112 regular, Archimedian and regular-faced polyhedra from the list of [Berm71]. For example, Nr.1–5 are regular polyhedra. In [Berm71] and [Zalg69], the regular-faced polyhedra are given as appropriate joints of 28 *basic* polyhedra $M_1 - M_{28}$.

1.5 Operations on polytopes

We use some operations transforming a polytope into another polytope.

- **Direct product**. The *direct product of n-polytope P and m-polytope P'* is an $(n + m)$-polytope $P \times P'$ with $G(P \times P') = G(P) \times G(P')$. Sometimes, it is called the *Cartesian product*.
- **Prisms**. The *prism with the base* P is the polytope $PrismP := \alpha_1 \times P$. $Prism_n$ denotes the prism with an n-gon as the base, i.e. $Prism_n = Prism(C_n)$.
- **Elongation**. Let C be a simple circuit in a 3-polytope (or, in general, in any plane graph) P. An *elongation of P along C* consists of replacing C by the ring of 4-gons. The elongation of P along the circuit C, bounding a face, means putting the prism on this face.
- **Truncation**. A *truncation (at vertex v)* of a polytope P cuts the vertex v. In other words, the vertex v of P is substituted by a facet, which is the vertex figure of P. A polytope P is called *truncated* and denoted

as tr(P) if all vertices of P are truncated. In most cases, we can do truncation at $\frac{1}{3}$ of edge distances.

- **Capping**. In a sense, this operation is an inverse of truncation. A *capping* of a polytope P at its facet F consists of addition of a new vertex v to P, such that v is adjacent to all vertices of F. A *t-capped* polytope P is obtained by cappings at t distinct facets of P.
- **Pyramids**. The convex hull of an n-polytope P and a vertex v, not lying in the space spanned by P, is called *pyramid* over P (with the apex v) and denoted by $Pyr(P)$. We set $Pyr_n = Pyr(C_n)$. We denote by $Pyr^t(P)$ the result of t consecutive applications of taking pyramid. One has $G(Pyr^t(P)) = \nabla^t G(P)$.
  $BPyr(P)$ denotes an $(n+1)$-*bipyramid* with n-polytope P as the base. It has two apexes, which are opposite with respect to the hyperplane spanned by P. $G(BPyr(P))$ is $\nabla^2 G(P)$-e, where e is the edge connecting two apexes of $\nabla^2 G(P)$. We set $BPyr_n = BPyr(C_n)$.
- **Chamfering**. This operation is applied only to 3-polytopes. The *chamfering* of a polyhedron P is the polyhedron, denoted by Cham(P), which is obtained by putting prisms on all facets of P and deleting original edges. t-iterated chamfering is denoted by $\text{Cham}_t(P)$ (see also the end of chapter 5).
- **Ambo**. The convex hull of the midpoints of all edges of a polytope P is called its *ambo-polytope* and denoted by Ambo(P). We restrict ourself only to the cases when the mid-points of edges, which are incident to any given vertex, lie on the same plane. If P is a polyhedron, then each vertex of the polyhedron Ambo(P) has degree four. This is so, since each edge of P is incident to two faces, and, in each face, an edge is adjacent to two edges. The skeleton of Ambo(P) is called also the *medial graph* of the skeleton of P. The skeleton of Ambo(P) is the line graph of the skeleton of P, if P is a simple polyhedron. We have $\text{Ambo}(\alpha_3) = \beta_3$, $\text{Ambo}(\beta_4)$=24-cell.

1.6 Voronoi and Delaunay partitions

A finite or infinite set X of points of $\mathbb{R}^n$ is called *discrete* if there is a positive number r, such that the ball of radius r with the center in a point of X does not contain another points of X.

A special case of an infinite discrete set in $\mathbb{R}^n$ is an *n-dimensional point lattice*. It is the set of end-points of vectors $\sum_{i=1}^{n} z_i b_i$, where the vectors b_i

are linearly independent, and $z_i \in \mathbb{Z}$ for all i.

Any discrete set of points X defines two partitions (tilings) of $\mathbb{R}^n$ by *Voronoi* and *Delaunay* polytopes. Voronoi, who introduced this theory (for lattices) in his last two papers, call them M- and L-*polytopes*, respectively. Any lattice has exactly one affine type of Voronoi polytope and a finite number of types of Delaunay polytopes.

Each Voronoi polytope $P(x)$ of the *Voronoi partition* relates to a point $x \in X$ such that $P(x)$ is the set of all points of $\mathbb{R}^n$, which are not more far from x, than from any other point of X. Denote by $Vo(X)$ the skeleton graph of the Voronoi partition. In particular, for a lattice L, $Vo(L)$ is the skeleton of the Voronoi partition defined by L.

The *Delaunay partition* is dual of the Voronoi partition (dual, in both, combinatorial and metric sense). It can be obtained by the *empty sphere method* of Delaunay. Take a point $y \notin X$ as center of a sphere S_y not containing points of X. Then increase radius of S_y until a point $x \in X$ touches S_y. After that move the center y such that one can again increase radius of S_y remaining x on S_y until another point $x' \in X$ touches S_y. Continuing, one obtains a (locally maximal) *empty* (i.e. not having points of L in its interior) sphere S_y with $n+1$ affinely independent points from X on S_y. The convex hull of all points of X, lying on S_y is a Delaunay polytope P_D of the Delaunay partition. The case when radius of S_y is infinite is not excluded.

Denote by $De(X)$ the skeleton graph of the Delaunay partition. In particular, for a lattice L, $De(L)$ is the skeleton of the Delaunay partition of L. Edges of $De(L)$ are minimal vectors of the simple cosets of $L/2L$. Recall that if L is the root lattice D_n, then the graphs $De(D_n)$ and $\frac{1}{2}Z_n$ have the same vertex-set, but the graphs themselves are distinct.

1.7 Infinite graphs

First, we give an example of a sequence of polytopal graphs, which are embeddable with increasing scale, but the graph in the limit is not embeddable. Consider i points a_j, $1 \le j \le i$, with the positive integer coordinate j on the axe. Let any neighboring points a_{j-1}, a_j be a pair of antipodal vertices of the cross-polytope β_{m_j} of dimension $m_j := 2^j$, such that β_{m_j} has a common vertex only with $\beta_{m_{j-1}}$ (namely, a_{j-1}) and $\beta_{m_{j+1}}$ (namely, a_j). Denote by W_i the graph obtained by such attaching of i cross-polytopes. Clearly, β_{m_i} and W_i are embeddable into Z_{m_i} with scale $\lambda_i = \frac{m_i}{2} = 2^{i-1}$.

Denote by W_∞ the limit of W_i for $i \to \infty$. We have $\lambda_i \to \infty$ for $i \to \infty$; so, W_∞ cannot be embedded, with finite scale, even into Z_∞.

Now (following [DeSt02a]) we consider cubical complexes and, especially, introduce the *infinite dimensional cube*.

Novikov proposed in [Novi86] to study *cubical* complexes, i.e. those consisting (instead of simplexes) of cubes of all dimensions. The simplest example of a cubical complex is an Euclidean cube of an arbitrary dimension (with faces of all dimensions). Another example of a cubical complex is usual cubical lattice giving a partition of Euclidean n-space into n-cubes adjacent by facets. This complex consists of a countable number of cubes of finite dimension. Each point of the complex belongs only to one cube, if it is an inner point, and to a finite number of cubes, if it is a boundary point.

Now, we construct a third example of a cubical complex. Let $\mathcal{E}_\infty = (O, e_1, e_2, \dots, e_k, \dots)$ be limit for $n \to \infty$ of the orthonormal frame $\mathcal{E}_n = (O, e_1, e_2, \dots, e_n)$. We take k arbitrary integers $i_1 < i_2 < \cdots < i_k$ from $\mathbf{N}$, $k \in \mathbf{N}$, and construct on the corresponding k vectors $e_{i_1}, e_{i_2}, \dots, e_{i_k}$ from $\mathcal{E}_\infty$ a closed cube $I^k(O, e_{i_1}, e_{i_2}, \dots, e_{i_k})$ with origin O as a vertex. Take union of all such cubes

$$\cup_{i_1<i_2<\dots,i_k\in\mathbf{N},k\in\mathbf{N}} I^k(O, e_{i_1}, e_{i_2}, \dots, e_{i_k}).$$

The family of cubes of this union, including faces of all dimensions, composes an infinite-dimensional cubical complex. In fact, at first, each cube of the family is either a cube of the form $I^k(O, e_{i_1}, e_{i_2}, \dots, e_{i_k})$, or its face. Hence each face of the cube I^k is a cube of the family. Secondly, any two cubes of the family are obviously faces of a cube of the form $I^k(O, e_{i_1}, e_{i_2}, \dots, e_{i_k})$. Therefore their intersection is again a cube of the family.

Since each cube of the form $I^k(O, e_{i_1}, e_{i_2}, \dots, e_{i_k})$ is a k-dimensional face of the n-dimensional cube $I^n(O, e_1, e_2, \dots, e_n)$, where n is not less than the maximal index i_k, then our family has a more simple description $\cup_{n\in\mathbf{N}} I^n$. Here I^n is a short denotation of $I^n(O, e_1, e_2, \dots, e_n)$. Since $I^1 \subset I^2 \subset \cdots \subset I^n \subset \dots$, our cubical complex can be considered as a family of faces of all dimensions of an infinitely expanding cube I^n when n goes to infinity. Dimensions of the cubes composing the complex are finite, but there is no upper bound for all these dimensions. Hence this complex is not finite-dimensional.

This cubical complex determines a polytope of infinite dimension, let us denote this polytope by W. The body of the polytope W is union of all open cubes of the complex. Hence it is not closed. In fact, the infinite sequence of points $M_i = (\frac{1}{2}, \frac{1}{4}, \dots, \frac{1}{2^i}, \frac{1}{2^{i+1}}, 0, 0, \dots)$, each of which belongs to the polytope W has a limit point $M_\infty = (\frac{1}{2}, \frac{1}{4}, \dots, \frac{1}{2^i}, \frac{1}{2^{i+1}}, \dots)$ if $i \to \infty$. The point M_∞ does not belong to W since it does not belong to any finite dimensional cube I^n of above union. (The polytope W is a proper subset of the *Tikhonov cube* I^τ, i.e. of the topological product of τ copies of the unit interval of the real line, with cardinal number $\tau = \aleph_0$. This special Tikhonov cube is homeomorphic to the *Hilbert cube*, i.e. to the subspace of the Hilbert space ℓ_2 consisting of all the points $x = (x_1, x_2, \dots)$, for which $0 \leq x_n \leq 1$, $n \geq 1$. As a graph, the edge skeleton of the polytope W is a maximal connected component of the edge skeleton of the cube I^∞ of countable dimension.)

We consider a set of points such that their coordinates in the basis $\mathcal{E}_\infty$ are 0 and 1, and the number of ones is finite. These points are not all points with coordinates 0 and 1. The points of this set are just the points, which can be reached from origin O (or from any point of the set) by a finite shortest path, whose edges are unit vectors of the basis $\mathcal{E}_\infty$. These (and only these) points are vertices of the polytope W. The distance between points $y = (y_1, y_2, \dots, y_k, \dots)$ and $z = (z_1, z_2, \dots, z_k, \dots)$ of W (in particular, between vertices of W) is given by the formula $\rho(y, z) = \sum_{k=1}^{\infty} |y_k - z_k|$. For any pair of points (y, z) of W, this sum contains infinitely many members, but only finite number from them are distinct from zero (and are equal to 1 in the case of vertices). Hence, in fact, the distance is computed by a finite formula. We denote by $\mathcal{H}^\infty$ the graph induced by the set of vertices of the polytope W. (The metric space of $\mathcal{H}^\infty$ is a special limit of an infinite sequence of metric spaces $\mathcal{H}^n$ for $n \to \infty$. It contains all $\mathcal{H}^n$, $n \in \mathbf{N}$. It turns out that $\mathcal{H}^\infty$ is a universal carrier of graphic metrics of all graphs embeddable in hypercubes and cubic lattices.)

Since any finite set of vertices of an *infinite dimensional cube* H^∞ has finitely many coordinates equal to 1 (and infinitely many zero coordinates), it belongs to a finite dimensional cube. Hence this finite set of vertices satisfies every hypermetric inequality. Therefore we have

Proposition 1.4 *The metric space H^∞ is hypermetric.*

Now we want to prove that the metric space $\mathcal{Z}^n$ is also hypermetric.

A simple path P_n of length $n-1$ is obviously embedded isometrically into the skeleton of an n-dimensional cube. Any embedding of the path P_n into a cube of dimension less than n, cannot be isometric. In fact, if P_n is embedded into H_k with $k < n$, then there are two parallel edges in the embedded P_n. The sub-path consisting of any two nearest parallel edges and all edges between them composes a path of the form $e_1+e_2+\cdots+e_k-e_1$. Only the border vectors of the sum are colinear. The colinear vectors should be opposite directed, since otherwise the path cannot belong to the cube. The shortest path in the cube between the end-points of above path is $e_2+..+e_k$. It is shorter by 2 of the original path. Hence the embedding is not isometric.

But if an edge path of length n can be embedded isometrically into the finite cube H_n, an edge ray (as an edge path of infinitely many edges) cannot be embedded isometrically in any cube of finite dimension. The edge ray is embedded isometrically into the infinite dimensional cube H_∞.

We use above considerations for a study of an n-dimensional cubic lattice. Let the orthonormal frame $(O, e_1, e_2, \dots, e_n)$ in $\mathbb{R}^n$ be a basis of an n-dimensional cubic lattice. We enlarge the frame up to a countable orthonormal frame $(O, e_1, e_2, \dots, e_n, e_{n+1}, \dots)$, which we consider as a basis of an infinite dimensional cube.

There are $2n$ rays in an n-dimensional lattice such that they goes from O in $2n$ directions along the unit vectors $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n$ and $-\mathbf{e}_1, -\mathbf{e}_2, \dots, -\mathbf{e}_n$. Each of these rays can be mapped into the edge skeleton of the polytope W (which is a proper subset of a cube of countable dimension).

Namely, we map, edge by edge, the rectilinear ray of the skeleton of an n-dimensional lattice, which is directed along $\mathbf{e}_i$, that is, which goes in the positive direction of the i-th axis, $1 \le i \le n$, into the broken path

$$\mathbf{e}_i + \mathbf{e}_{i+1\cdot 2n} + \mathbf{e}_{i+2\cdot 2n} + \cdots + \mathbf{e}_{i+k\cdot 2n} + \dots$$

of the skeleton of the polytope W. Here the first edge begins in the point O, and the edge $\mathbf{e}_{i+j\cdot 2n}$ begins in the end of the edge $\mathbf{e}_{i+(j-1)\cdot 2n}$, $j = 1, 2, 3, \dots$.

In a similar way, we map the rectilinear edge ray in an n-dimensional cubic lattice directed along $-\mathbf{e}_i$, that is, going in the negative direction of the i-th axis, $1 \le i \le n$, into the edge path

$$\mathbf{e}_{i+n} + \mathbf{e}_{i+n+1\cdot 2n} + \mathbf{e}_{i+n+2\cdot 2n} + \cdots + \mathbf{e}_{i+n+k\cdot 2n} + \dots$$

of the edge skeleton of W, where the edge $\mathbf{e}_{i+n}$ begins in the origin O, and the edge $\mathbf{e}_{i+n+j\cdot 2n}$ begins in the end of the edge $\mathbf{e}_{i+n+(j-1)\cdot 2n}$, $j = 1, 2, 3, \dots$.

We take an edge of the skeleton of a standard cubic lattice. We consider the hyperplane, which is orthogonal to this edge and bisects it. This hyperplane gives a *middle cut* of the partition (that is, of the n-dimensional cubic lattice). All edges of the partition, which are intersected by this hyperplane form an *equivalence class*. All edges of the same class are mutually parallel and have the same direction. This equivalence class contains always an edge of the rectilinear ray going from O along the corresponding coordinate axis (into positive or negative direction). This edge is mapped by above map into a vector of the basis $\mathcal{E}_\infty$. Let this vector be a label of all edges of the equivalence class containing this edge. Then edges of distinct equivalence classes obtain distinct labels.

Different equivalence classes correspond to different middle cuts, even if the hyperplanes of middle cuts are parallel. When we label all edges of the one-dimensional skeleton of a standard cubic lattice by vectors of the basis $\mathcal{E}_\infty$, we construct a map of the skeleton of a primitive cubic lattice into the skeleton of the polytope W (and in the skeleton of an infinite-dimensional cube). Above construction shows that this map transforms each shortest edge path (of a finite length) into a shortest path. Hence the constructed map is an embedding, moreover an isometric embedding. (This map can be extended up to a continuous locally isometric cellular map of a normal partition into cubes of n-dimensional Euclidean space into the n-dimensional skeleton of the polytope W.)

Proposition 1.5 *The following embedding $\mathcal{Z}^n \to \mathcal{H}^\infty$ holds.*

Since the embedding $\mathcal{Z}^n \to \mathcal{H}^\infty$ is isometric, and any metric subspace of a hypermetric space is itself hypermetric, the following is true

Corollary 1.1 *The metric space $\mathcal{Z}^n$ is hypermetric.*

It is clear that the metric space $\mathcal{H}^\infty$ is not embedded into the metric space $\mathcal{Z}^n$ for any *finite* n.

In the space with the basis $\mathcal{E}_\infty$, we consider a set of all points, which can be reached from origin O by edge paths, whose links are vectors of the frame $\mathcal{E}_\infty$. The coordinates of any point of this set in the basis $\mathcal{E}_\infty$ are integer, and there are only finitely many non-zero coordinates. Denote this set of points (with the natural ℓ_1-metric) by $\mathcal{Z}^\infty$. Clearly, any finite set of points of $\mathcal{Z}^\infty$ is contained in $\mathcal{Z}^n \subset \mathcal{Z}^\infty$ for some $n \in \mathbf{N}$. Since $\mathcal{Z}^n$ is a hypermetric space, the metric space $\mathcal{Z}^\infty$ is a hypermetric space, too.

Proposition 1.6 *The following embeddings are true*

$$\mathcal{Z}^\infty \to \mathcal{H}^\infty \subset \mathcal{Z}^\infty.$$

The fact that the embedding $\mathcal{Z}^\infty \to \mathcal{H}^\infty$ holds can be proved by the same way as in previous Proposition. The only difference is that now there are countably many rays in both directions. However in this case, we can label edges of each ray by distinct labels. This is true, since a union of countably many countable sets is itself countable.

Chapter 2

An Example: Embedding of Fullerenes

In order to illustrate above notions of ℓ_1-embedding and its applicability, we start with *fullerenes*, a variety of polyhedra important in Chemistry. In this chapter, after introducing fullerenes and giving a general lemma, we report the ℓ_1-status of more than 4000 small fullerenes and their duals. Some infinite families of non-embeddable fullerenes are also considered. The ℓ_1-status was computer-checked by D.Pasechnik and M.Dutour.

A *fullerene* is a carbon molecule, which can be seen as a simple polyhedron. We denote it by F_n. The n vertices - the carbons atoms - are arranged in 12 pentagons and $(\frac{n}{2} - 10)$ hexagons, and the $\frac{3}{2}n$ edges correspond to carbon-carbon bonds. Fullerenes F_n can be constructed for all even $n \geq 20$ except $n = 22$ (see [Grün67], page 271). For a given n, different arrangements of facets are possible; such fullerenes are called *isomers*. For example, there are 1, 1, 1, 2, 3, 40, 271 and 1812 fullerenes F_n for $n = 20$, 24, 26, 28, 30, 40, 50 and 60, respectively.

Any fullerene without pair of pentagons sharing a common edge, is denoted by C_n and called *preferable fullerene* (or also IP-fullerenes, for Isolated Pentagons). For example, the unique preferable fullerene made of 60 carbon atoms C_{60} is the truncated icosahedron, also called *buckminsterfullerene*.

A usual way to somehow distinguish between isomers is to give their symmetry group. For example, $C_{180}(I_h)$ is the unique preferable fullerene with 180 vertices and symmetry group I_h (extended icosahedral group of order 120). While $C_{60}(I_h)$ is a soccer ball, $F_{32}(D_3)$, $C_{70}(D_{5h})$ and $C_{84}(D_{2d})$ resemble to a tennis, rugby and baseball ball, respectively. The general reference for fullerenes is [FoMa95]. In this chapter we focus on the following metric question:

Can we embed into a hypercube the graph formed by the vertices and the *edges of a fullerene while preserving, up to a scale, the path distances?*

2.1 Embeddability of fullerenes and their duals

Lemma 2.1 *A fullerene F_n (and its dual F_n^*)*
(i) is either an ℓ_1-rigid isometric subgraph of a half-cube,
(ii) or violates a $(2k+1)$-gonal inequality for some integer $k \geq 2$.

Proof. In fact, (i) is a direct application of Lemma 1.6. A fullerene F_n being a simple polyhedron and its dual F_n^* having no vertex of valence three, both do not contain K_4 and therefore are ℓ_1-rigid (and are isometric subgraphs of a half-cube by the implications given in chapter 1.2) when ℓ_1-embeddable.

If F_n or F_n^* is not embeddable, then, as remarked in [DeGr93], a hypermetric but not ℓ_1-embeddable graph has diameter two or three. Then, since F_{20}^* is known to be an ℓ_1-polyhedron and since any fullerene (and its dual, except of F_{20}^*) has diameter at least four, it is not hypermetric, and (ii) follows. □

Table 2.1 **Embeddability of small fullerenes: out of all 7916 F_n and F_n^* with $n < 60$, only seven are ℓ_1-embeddable**

Fullerene	ℓ_1-embeddability of F_n	ℓ_1-embeddability of F_n^*
$F_{20}(I_h)$	$\to \frac{1}{2}H_{10}$	$\to \frac{1}{2}H_6$
$F_{26}(D_{3h})$	$\to \frac{1}{2}H_{12}$	not 5-gonal
$F_{28}(T_d)$	not 5-gonal	$\to \frac{1}{2}H_7$
$F_{36}(D_{6h})$	not 5-gonal	$\to \frac{1}{2}H_8$
$F_{40}(T_d)$	$\to \frac{1}{2}H_{15}$	not 5-gonal
$F_{44}(T)$	$\to \frac{1}{2}H_{16}$	not 5-gonal

Amongst fullerenes F_n and their duals with $n < 60$, and all preferable fullerenes C_n and their duals with $n < 86$, only five fullerenes, $F_{20}(I_h)$, $F_{26}(D_{3h})$, $F_{40}(T_d)$, $F_{44}(T)$, and $C_{80}(I_h)$, and only four dual fullerenes,

Table 2.2 **Embeddability of small preferable fullerenes: out of all 102 C_n and C_n^* with $n < 86$, only two are ℓ_1-embeddable**

Fullerene	ℓ_1-embeddability of F_n	ℓ_1-embeddability of F_n^*
$C_{60}(I_h)$	not 5-gonal	$\to \frac{1}{2}H_{10}$
$C_{80}(I_h)$	$\to \frac{1}{2}H_{22}$	not 5-gonal

$F^*_{20}(I_h)$, $F^*_{28}(T_d)$, $F^*_{36}(D_{6h})$ and $C^*_{60}(I_h)$, turn out to be ℓ_1-embeddable (see Tables 2.1 and 2.2). The embedding is given in detail in Figures 2.1, 2.2, 2.3 and 2.5, where a vertex of $\frac{1}{2}H_m$ is labeled by the set $S \subset V_m$ of its non-zero coordinates. The vertices of V are labeled by numbers 0,1,2,...,9 and $0', 1', 2', \dots$ and by letters $a, b, c, \dots$. In Figures 2.3 and 2.4, the edges are labeled by the symmetric difference between sets of nonzero coordinates of corresponding vertices of $\frac{1}{2}H_{16}$ and $\frac{1}{2}H_{22}$, respectively.

While there exist 5-gonal but not 7-gonal polyhedra (for example, the snub square antiprism; see Figure 6.4 c) below), we could not find any such fullerene or its dual. Probably, any non-l_1-embeddable fullerene F_n (or F^*_n) is, moreover, not 5-gonal.

On the other hand, we believe that five F_n and four F^*_n, given in Tables 2.1 and 2.2, are only l_1-embeddable ones.

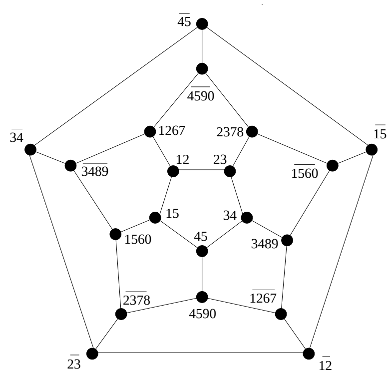


Fig. 2.1 **Embedding of $F_{20}(I_h)$ into $\frac{1}{2}H_{10}$**

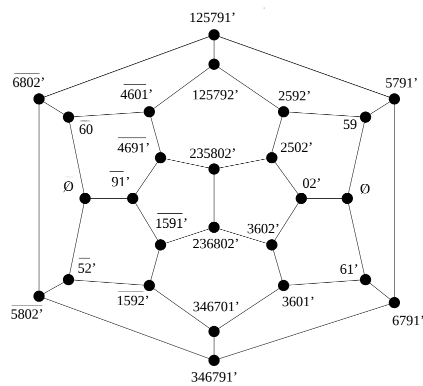


Fig. 2.2 **Embedding of $F_{26}(D_{3h})$ into $\frac{1}{2}H_{12}$**

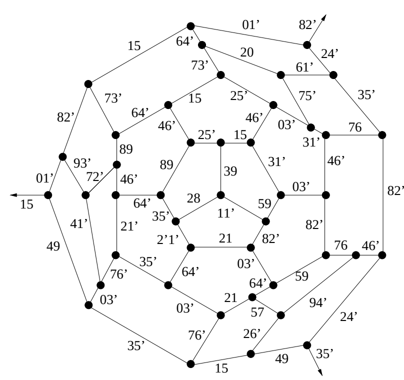


Fig. 2.3 **Embedding of $F_{44}(T)$ into $\frac{1}{2}H_{16}$**

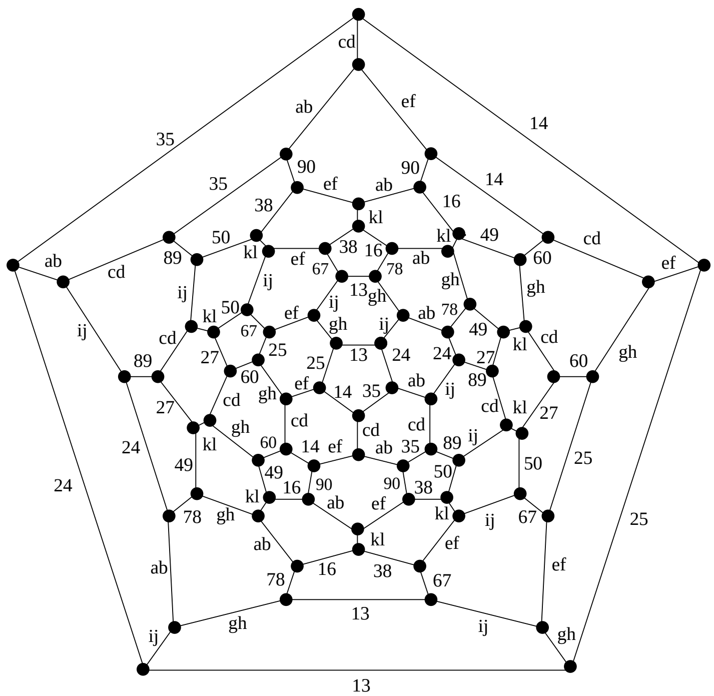


Fig. 2.4 **Embedding of $C_{80}(I_h)$ into $\frac{1}{2}H_{22}$**

2.2 Infinite families of non-ℓ_1 fullerenes

Now we present two families of interesting non-ℓ_1 fullerenes. Starting from a fullerene F_n that we can separate into two hemispheres by cutting five edges (respectively, six), we insert between those hemispheres a layer of five hexagons (respectively, six) as follows. After the cutting of F_n we obtain two hemispheres each with five (or six) *tails*. Similarly, we can represent a ring of k hexagons as a ring of k rectangles with the outer and inner borders having each k tails. Taking $k = 5$ (or $k = 6$) we can glue the outer tails with the tails of one hemisphere and the inner tails with the tails of the other hemisphere for to obtain a fullerene with more hexagons. The obtained fullerene has $n + 10$ vertices (respectively, $n + 12$) and is called a 1-*layered* F_n. By inserting i layers, we get the i-layered F_n. For example, cutting anywhere F_{20} and inserting i layers, we get the i-layered dodecahedron defined as $F_{10(i+2)}(D_{5h})$ for odd i and $F_{10(i+2)}(D_{5d})$ for even i (see Figure 2.6). (It is most *strained, antiaromatic, least stable* fullerene, since, as opposite to preferable fullerenes, it has maximal number of abutting pairs of pentagonal faces.) Starting with $F_{24}(D_{6d})$ and inserting i-layers of 6 hexagons between two hemispheres made of five pentagons surrounding a hexagon, we get the i-layered $F_{24}(D_{6d})$: $F_{12(i+2)}(D_{6h})$ for odd i and $F_{12(i+2)}(D_{6d})$ for even i, see Figure 2.6.

Proposition 2.1 *For any integer $i \geq 1$:*

(i) The i-layered fullerene (and its dual) $F_{10(i+2)}(D_{5h}$ or $D_{5d})$ is not ℓ_1-embeddable, and

(ii) the i-layered fullerene (and its dual except for $i = 1$) $F_{12(i+2)}(D_{6h}$ or $D_{6d})$ is not ℓ_1-embeddable.

Proof. To prove that the above fullerenes are not ℓ_1-embeddable, we simply exhibit a not 5-gonal configuration contained in their skeletons. The coefficients b_i of the violated 5-gonal inequality (see (1.4) in chapter 1.2) are, respectively, 0 for a black vertex, -1 for a square one, and 1 for a white circle. □

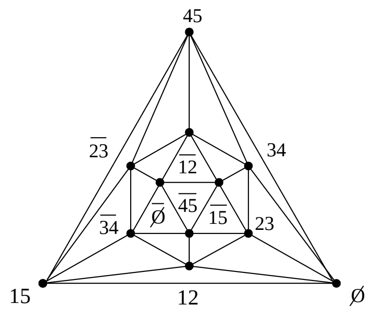
2.3 Katsura model for vesicles cells versus embeddable dual fullerenes

It turns out, that all known fullerenes, for which their duals are ℓ_1-embeddable - including the plane partition by regular hexagons (*the*

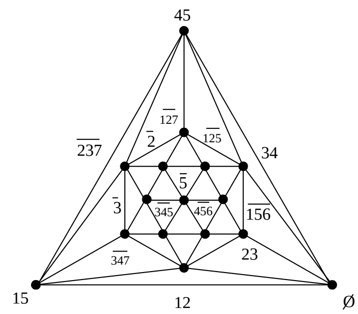
Voronoi partition of *the hexagonal lattice* A_2), which can be seen as an infinite fullerene C_∞ - fit the following Katsura's model for *coated vesicles cells* (see [Kats83]). More precisely, the n vertices of a fullerene F_n are partitioned into four types $T_{a,b}$ according to the number a of pentagons and b of hexagons they are incident to, that is, $T_{3,0}$, $T_{0,3}$, $T_{1,2}$ and $T_{2,1}$. Katsura then considers the average strain energy of its n vertices assuming *Hookean elasticity* and only *short range interactions*. The *stable* fullerenes, that is, with minimal energy under his model (depending on which type of vertices have minimal energy) are the following:

- The dodecahedron (minimal energy on $T_{3,0}$ vertices); its dual $F^*_{20}(I_h) \to \frac{1}{2}H_6$.
- The hexagonal sheet C_∞ (minimal energy on $T_{0,3}$ vertices); its dual (*the Delaunay partition* of A_2) $\to \frac{1}{2}Z_3$.
- The buckminsterfullerene (minimal energy on $T_{1,2}$ vertices); its dual $C^*_{60}(I_h) \to \frac{1}{2}H_{10}$.
- The elongated hexagonal barrel $F_{36}(D_{6h})$ (minimal energy on $T_{2,1}$ vertices); its dual $F^*_{36}(D_{6h}) \to \frac{1}{2}H_8$.
- The $F_{28}(T_d)$ (minimal energy on $T_{2,1}$ vertices); its dual is the hexakis truncated tetrahedron and $F^*_{28}(T_d) \to \frac{1}{2}H_7$.

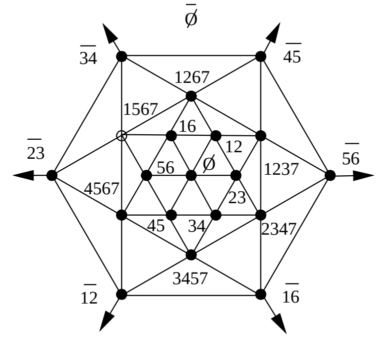
The remaining two stable fullerenes have also minimal energy on $T_{2,1}$ vertices; they are the tennis ball $F_{32}(D_3)$ and $F_{36}(D_{2d})$, whose duals are not embeddable.



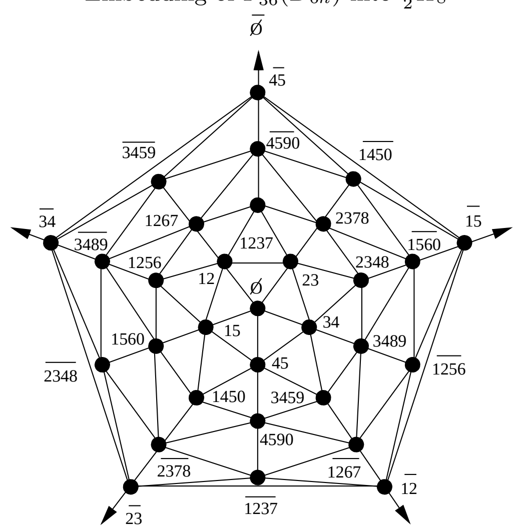
Embedding of $F^*_{20}(I_h)$ into $\frac{1}{2}H_6$



Embedding of $F^*_{28}(T_d)$ into $\frac{1}{2}H_7$



Embedding of $F^*_{36}(D_{6h})$ into $\frac{1}{2}H_8$



Embedding of $C^*_{60}(I_h)$ into $\frac{1}{2}H_{10}$

Fig. 2.5 **Dual Embeddings**