Partial cubes and other $\ell_1$-graphs

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**$\ell_1$-Graphs**

- By $\ell_1$ we mean the distance space $(X, d)$, where $X = \mathbb{R}^n$ and $d(x, y) = d_1(x, y) = \sum_i |x_i - y_i|$.

- Every (connected) graph $\Gamma$ can also be considered as a distance space by setting $X = V\Gamma$, the vertex set of $\Gamma$, and by taking $d = d_\Gamma$ to be the path distance on $\Gamma$, that is, the number of edges on a shortest path between two vertices.

- We say that a graph $\Gamma$ is $\ell_1$-**embeddable** (or simply, an $\ell_1$-**graph**) if there exists an **isometric** mapping from $(V\Gamma, d_\Gamma)$ to the $\ell_1$ space $(\mathbb{R}^n, d_1)$ for some $n$; that is, a mapping $\phi : V\Gamma \to \mathbb{R}^n$ such that $d_1(\phi(x), \phi(y)) = d_\Gamma(x, y)$ for all $x, y \in V\Gamma$. 
The Hamming cube graph

- Let $Q_n$ be the graph with the vertex set $\{0, 1\}^n$, where two $\{0, 1\}$-tuples are adjacent if and only if they differ at exactly one place.

- $Q_n$ is known as the Hamming cube graph, $d_{Q_n}$ is known as the Hamming distance, that is, $d_{Q_n}(x, y)$ equals the number of places at which the tuples $x$ and $y$ differ.

- $Q_n$ is an $\ell_1$-graph; indeed, $V_{Q_n} \subset \mathbb{R}^n$ and $\phi = id$ is the required isometric embedding.

- The Hamming cube graph has also a different realisation: Take as vertices all subsets of $\Omega = \{1, 2, \ldots, n\}$; two subsets $A$ and $B$ are adjacent if they differ by one elements, that is, if $|A \triangle B| = 1$. In general, for two subsets $A$ and $B$, $d_{Q_n}(A, B) = |A \triangle B|$.
Assouad-Deza Theorem

- We state it just for the case of graphs.

**Theorem** A graph $\Gamma$ is $\ell_1$-embeddable if and only if it is embeddable up to a scale into a Hamming cube $Q_n$.

- Suppose $\Gamma$ and $\Delta$ are graphs. Then a mapping $\phi : V\Gamma \to V\Delta$ is a scale $\lambda$ embedding if $d_\Delta(\phi(x), \phi(y)) = \lambda d_\Gamma(x, y)$ for all $x, y \in V\Gamma$.

- Clearly, $\lambda$ is a positive integer; if $\lambda = 1$ then $\phi$ is an isometric embedding.
Partial cubes

- A subgraph $\Delta$ of $\Gamma$ is isometric if $d_\Delta(x, y) = d_\Gamma(x, y)$ for all $x, y \in V\Delta$. Equivalently, $\Delta$ is an isometric subgraph of $\Gamma$ if the identity mapping from $\Delta$ to $\Gamma$ is an isometric embedding.

- A partial cube is simply any isometric subgraph of the Hamming cube. Note that $Q_n$ is bipartite and so every partial cube is bipartite, too.

- Every partial cube is bipartite; the condition in the Assouad-Deza Theorem is satisfied with $\phi = id$ and $\lambda = 1$. 
The half-cube graph

- The bipartite half of $Q_n$ is known as the *half-cube graph* $\frac{1}{2}Q_n$. Thus, the vertices of $\frac{1}{2}Q_n$ are all even-size subsets of $\Omega = \{1, 2, \ldots, n\}$ and two such subsets $A$ and $B$ are adjacent if $|A \triangle B| = 2$. In general we have for two vertices $A$ and $B$ of $\frac{1}{2}Q_n$ that $d_{\frac{1}{2}Q_n}(A, B) = \frac{1}{2}|A \triangle B|$.

- Although $\frac{1}{2}Q_n$ is not a subgraph of $Q_n$, the identity mapping from $\frac{1}{2}Q_n$ to $Q_n$ is a scale two embedding, and so $\frac{1}{2}Q_n$ is an $\ell_1$-graph.

- Similarly, every isometric subgraph of $\frac{1}{2}Q_n$ is scale two embeddable in $Q_n$, and so it is an $\ell_1$-graph.

- Most $\ell_1$-graphs require scale two; the most well-known examples of $\ell_1$-graphs requiring $\lambda > 2$ are the complete graphs and the cocktail-party graphs (aka hyperoctahedra).
Suppose $\Gamma$ is an $\ell_1$-graph and $\phi : V\Gamma \to VQ_n$ is a scale $\lambda$ embedding. Then we assign to every edge $xy$ of $\Gamma$ a label $\ell(xy) = \phi(x)\triangle\phi(y)$. Every label consists of exactly $\lambda$ elements.

If $x, y \in V\Gamma$ and $x = x_0, x_1, \ldots, x_m = y$ is an arbitrary path from $x$ to $y$ then $\phi(x)\triangle\phi(y) = \ell(x_0x_1)\triangle\ell(x_1x_2)\triangle \ldots \triangle\ell(x_{m-1}x_m)$. Thus, if we know the labels and we know $\phi(x)$ for one vertex $x$ then we know the entire embedding.

Suppose $A \subseteq \Omega$. The shift $\phi_A$ of $\phi$ is defined by $\phi_A(x) = \phi(x)\triangle A$ for all $x \in V\Gamma$. If $\phi$ is a scale $\lambda$ embedding then so is $\phi_A$.

We say that two scale embeddings $\phi$ and $\psi$ are shift-equivalent if $\psi = \phi_A$ for some $A \subseteq \Omega$. Labels define the embedding up to this equivalence.
Key lemma about labels

Here are a few useful facts about some elementary isometric subgraphs of $\Gamma$:

1. Labels along a geodesic path are disjoint.
2. On an isometric cycle of even length, labels of opposite edges are equal; labels on non-opposite edges are disjoint.
3. On an isometric cycle of odd length, labels on opposite edges share exactly half (that is, $\frac{\lambda}{2}$) of their elements; labels on non-opposite edges are disjoint.

Related definitions: A path in $\Gamma$ is called *geodesic* if it is a shortest path between its ends; equivalently, it’s an isometric string subgraph in $\Gamma$. Two edges in a cycle are called *opposite* if they are at maximal distance in that cycle. Clearly, in a cycle of even length every edge has a unique opposite edge; in a cycle of odd length each edge has two opposite edges.
Zones

- We will call the elements of $\Omega$ the *coordinates* of the cube $Q_n$.

- For a coordinate $i$, the set of all edges $xy$ such that $i \in \ell(xy)$ is called the $i$-zone of $\Gamma$.

- Given a partition $\Omega = A \cup B$, the *cut* corresponding to this partition consists of all edges going across the partition. We note that every zone is a cut; indeed, we set $A = \{x \in V\Gamma \mid i \in \phi(x)\}$ and $B = \{x \in V\Gamma \mid i \notin \phi(x)\}$.

- Furthermore, every zone is a *convex cut*, that is, both parts $A$ and $B$ of the partition induce convex subgraphs of $\Gamma$. We call these convex subgraphs the *halves* (or $i$-halves, to be precise) of $\Gamma$. Recall that a subgraph is convex if it contains every shortest path between its vertices. Every convex subgraph is isometric.
Graphs $q_n$

- These are trivalent plane graphs, whose faces are all $q$-gons or hexagons, $q = 3, 4,$ or $5$. The graphs $5_n$ are also known as fullerene graphs.

- It is easy to see that among $3_n$’s only the smallest graph, the tetrahedron $K_4$, is $\ell_1$-embeddable.

- Deza and Dutour did an extensive computer search of $\ell_1$-embeddable $4_n$ and $5_n$ graphs and found five examples in each case. This led them to conjecture that the examples they found were the only $\ell_1$-embeddable $4_n$ and $5_n$ graphs in existence.

- The case of $4_n$ was resolved in affirmative by Deza, Dutour, and Sh. The fullerene case turned out to be much harder; however, it was finally resolved (again, in affirmative) this year by Marcușanu and Sh.
Suppose $\Gamma$ is a fullerene graph. As a first step, we prove the following useful properties of $\Gamma$:

- The only cycles (without returns) in $\Gamma$ of length up to six are the *face cycles*.

- Furthermore, the face cycles are convex and hence isometric.
Zones in fullerenes

Now suppose that the fullerene $\Gamma$ is $\ell_1$-embeddable (in $Q_n$ via $\phi$). Combining the fact that the face cycles are isometric with the result on the labeling of isometric cycles, we obtain a nice description of zones in $\Gamma$, namely:

- Edges in the $i$-zone form a “railroad”-like cyclic structure.

- Switching to the dual graph, we visualize the $i$-zone as a true cycle in the dual graph, or maybe a union of several cycles. The cycles cannot intersect each other, nor can they self-intersect.

- Furthermore, using the convexity of $i$-halves, we can show that in fact every $i$-zone produces a single cycle in the dual graph, which we call the $i$-zone cycle.

- This also gives a nice visualization of the $i$-halves: Cut the sphere through the zone cycle. The resulting two discs contain the two $i$-halves.
The core argument

The fullerene $\Gamma$ contains twelve pentagonal faces and an unknown number of hexagonal faces. The core part of the proof is where we show that $\Gamma$ cannot be too big, that is, the pentagonal faces cannot be too far from each other.

- This step is easy for $4_n$'s, because it can be done locally. Namely, considering a quadrangular face $F$ and assuming that $F$ is surrounded by several (just two!) layers of hexagonal faces, we get a contradiction.

- This “local” type of argument is impossible for fullerenes. Indeed, a single pentagon surrounded by any number of layers of hexagons never yields a contradiction because all such configurations are $\ell_1$-embeddable!!

- Hence the proof must involve two pentagonal faces.
Shaping the seed

Choose two closest pentagonal faces $F$ and $G$ in $\Gamma$. (The distance is measured in the dual graph.) Then $F$ and $G$ can be included in a subgraph called a seed. The idea and terminology go back to the PhD thesis of Puharic.

- Two shortest paths between $F$ and $G$ in the dual graph are called *elementary equivalent* if they differ in just one vertex (i.e., face of $\Gamma$). Extending this by transitivity, we get an equivalence on the shortest paths between $F$ and $G$.

- Pick an equivalence class. The faces of $\Gamma$ involved in the paths from this class form a parallelogram structure as in the hexagonal lattice, but with $F$ and $G$ at the corners with acute angles.

- Say, this has sides of $s$ and $t$ faces, with $s \leq t$. If $s \neq 0$, extend the parallelogram with two additional triangles at the sides of length $s$. The resulting subgraph is the *seed*. All faces involved in the seed, apart from $F$ and $G$, are hexagons.
The contradiction and small cases

- If \( s + t \geq 3 \) then next to the seed we find two straight zone segments. (\textit{Straight} means that only hexagonal faces are involved) The seed together with these two zone segments forms an impossible configuration, thus yielding a contradiction.

- This leaves the small cases: \((s,t) = (0,1), (1,1), \) and \((0,2)\). The case \((s,t) = (1,1)\) is eventually ruled out; the case \((s,t) = (0,2)\) yields the largest example on 80 vertices; while the case \((s,t) = (0,1)\) (adjacent pentagonal faces) branches to yield the remaining four examples: the dodecahedron on 20 vertices and three further fullerenes on 26, 40, and 44 vertices.
$C_{26}(D_{3h})$
$C_{40}(T_d)$
$C_{44}(T)$
$C_{80}(I_h)$
Let $\Gamma$ now be a partial cube.

- Recall that partial cubes are isometric subgraphs of Hamming cubes. In particular, $\lambda = 1$ and partial cubes inherit the bipartite property of $Q_n$.

- Since $\lambda = 1$, the label of each edge of $\Gamma$ consists of a single coordinate, that is, every edge is contained in a single zone. In fact, the zones in partial cubes are usually called the $\Theta$-classes, because they are the equivalence classes of a certain equivalence relation $\Theta$ defined on the edge set $E\Gamma$. Let $i(\Gamma)$ denote the number of $\Theta$-classes of $\Gamma$.

- Since convex subgraphs have played an important role in this talk, let us define the convex excess of $\Gamma$ (denoted $e(\Gamma)$) as $\sum_{C \in \mathcal{C}} \frac{|C| - 4}{2}$, where $\mathcal{C}$ denotes the set of all convex cycles of $\Gamma$. 
An Euler-type inequality

**Theorem** (Klavžar-Sh) *If $\Gamma$ is a partial cube then*

$$2|V_\Gamma| - |E_\Gamma| - i(\Gamma) - e(\Gamma) \leq 2.$$  

- This inequality is a generalization of a similar inequality $2|V_\Gamma| - |E_\Gamma| - i(\Gamma) \leq 2$, which is true for all median graphs. A graph is called a *median graph* if for any three vertices there is a fourth point that belongs to a shortest path between any two of the three original vertices.

- Note that a median graph contains no convex cycles of length more than four, so the convex excess is zero.

- The proof is done by induction on $i(\Gamma)$. 


Contraction and extension

- The induction step is based on the operation of contraction. Namely, given a partial cube $\Gamma$ we can construct a new partial cube $\Gamma'$ by contracting a single zone (say, the $i$-zone) of $\Gamma$. Under this operation edges from the $i$-zone turn into vertices and quadrangles involving edges from the $i$-zone turn into edges.

- The reverse operation is called the expansion. We note that the images of the $i$-halves (which are convex in $\Gamma$) are isometric in $\Gamma'$, and so they form an isometric cover. Every expansion operation starts from an isometric cover.
Exact cases

- It is an interesting problem to see for which partial cubes our inequality is in fact an equality.

- For median graphs the answer is known: If $\Gamma$ is a median graph then $2|V\Gamma| - |E\Gamma| - i(\Gamma) = 2$ if and only if $\Gamma$ is cube-free.

- We don’t have an ultimate answer for the general partial cubes; however, here is an attempt at an answer (and, as a by-product, an interesting related concept).
The zone graph

Suppose $\Gamma$ is a partial cube and $i \in \Omega$.

- The $i$-zone graph is a weighted graph, whose vertex set is the set of edges from the $i$-zone and whose edges are all convex cycles containing edges from the $i$-zone. The edge $C$ carries the weight $\frac{|C|-2}{2}$.

- Every zone graph is connected.

- Every zone graph is $\ell_1$-embeddable (as a naturally defined distance space).

- (?) We have $2|V\Gamma| - |E\Gamma| - i(\Gamma) - e(\Gamma) = 2$ if and only if all zone graphs in $\Gamma$ are weighted trees.