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On the canonical metric representation, average distance, and partial Hamming graphs

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Abstract

Average distance of a graph is expressed in terms of its canonical metric representation. The equality can be modified to an inequality in such a way that it characterizes isometric subgraphs of Hamming graphs. This approach simplifies recognition of these graphs and computation of their average distance.

MSC: 05C12; 05C75; 05C85

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1. Introduction

Let $W(G)$ denote the sum of distances between all pairs of vertices of a connected graph G. In chemical graph theory $W(G)$ is known as the *Wiener index* of G. Manifestly, $W(G)/\binom{n}{2}$ is the average distance in G, where $n = |V(G)|$. In this note we show that $W(G)$ can be expressed in terms of the quotient graphs of the canonical metric representation of G. When the metrics of the quotient graphs are omitted, we obtain an inequality between $W(G)$ and a natural, newly introduced graph invariant defined by the

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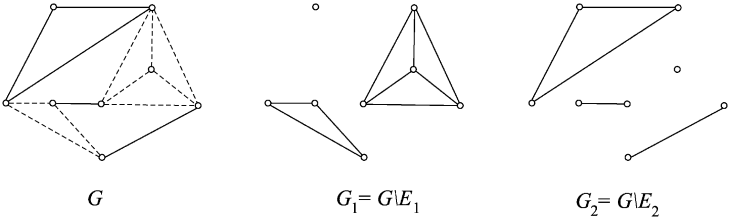

Fig. 1. Θ^*-equivalence classes of G.

canonical representation. The inequality turns into equality if and only if G isometrically embeds into a Hamming graph. This enables us to simplify a recognition algorithm for partial Hamming graphs and to simplify calculation of their Wiener indices.

In the rest of this section we present necessary concepts, while in the next section the main result is proved and its consequences discussed. For any terms and concepts not defined here we refer to the books [8,14].

The *Cartesian product* $G_1 \Box \cdots \Box G_k$ of graphs $G_1, \ldots, G_k$ has the vertex set $V(G_1) \times \cdots \times V(G_k)$, two vertices $(u_1, \ldots, u_k)$ and $(v_1, \ldots, v_k)$ being adjacent if they differ in exactly one position, say in ith, and $u_i v_i$ is an edge of G_i. Let d_G stands for the usual geodesic distance in G. It is well-known that for $G = G_1 \Box \cdots \Box G_k$ and vertices $u, v \in G$ we have $d_G(u, v) = \sum_{i=1}^{k} d_{G_i}(u_i, v_i)$.

A *Hamming graph* is the Cartesian product of complete graphs and a *partial Hamming graph* is a graph that isometrically embeds into a Hamming graph. In the particular case where all the factors are K_2's we speak of *hypercubes* and *partial cubes*, respectively. Partial Hamming graphs have been studied and characterized in [2,5,18].

The canonical metric representation of a connected graph G, due to Graham and Winkler [11], is defined as follows. Edges xy and uv of G are in the Djoković–Winkler [10, 19] relation Θ if $d(x, u) + d(y, v) \neq d(x, v) + d(y, u)$. Let Θ^* be the transitive closure of Θ and let $E_1, \ldots, E_k$ be the Θ^*-equivalence classes, Θ^*-classes for short. For $i = 1, \ldots, k$ let G_i denote the graph $(V(G), E(G) \setminus E_i)$ and $C_1^{(i)}, \ldots, C_{r_i}^{(i)}$ the connected components of G_i. As an example consider the graph G from Fig. 1. It has two Θ^*-equivalence classes E_1 and E_2. The graphs G_1 and G_2 are also shown.

Define the graphs $G_i^*, i = 1, \ldots, k$, with $V(G_i^*) = \{C_1^{(i)}, \ldots, C_{r_i}^{(i)}\}$ where $C_j^{(i)} C_{j'}^{(i)}$ is an edge of G_i^* if some vertex of $C_j^{(i)}$ is adjacent to a vertex of $C_{j'}^{(i)}$. Let the contractions $\alpha_i : V(G) \to V(G_i^*)$ be given by $\alpha_i(v) = C_j^{(i)}$ where $v \in C_j^{(i)}$. Then the mapping

$$\alpha : G \to G_1^* \Box \cdots \Box G_k^*, \tag{1}$$

where $\alpha(v) = (\alpha_1(v), \ldots, \alpha_k(v))$, is the *canonical metric representation* of the graph G. Graham and Winkler proved, among others, that α is an irredundant isometric embedding. Here *irredundant* means that every factor graph G_i^* has at least two vertices and that each vertex of G_i^* appears as a coordinate of some vertex $\alpha(u)$. For more results on the canonical representation we refer to the papers [3,4,12] and the books [8,14].

2. The main result and consequences

Let $X_1, \ldots, X_n$ be graphs and let w be a mapping that to any pair (X_i, X_j) of graphs assigns a real number. Then we introduce the following notation:

$$\Pi_w(X_1, \ldots, X_n) = \sum_{1 \le i < j \le n} w(X_i, X_j) \cdot |X_i| \cdot |X_j|.$$

In the case $w \equiv 1$ we will write $\Pi(X_1, \ldots, X_n)$ for $\Pi_w(X_1, \ldots, X_n)$. With this notation we formulate our main result as follows.

Theorem 2.1. *Let $G = (V, E)$ be a connected graph. Let the notations of its canonical metric representation be as in (1) and let d_i be the distance function of G_i^*. Then*

$$W(G) = \sum_{i=1}^{k} \Pi_{d_i}\left(C_1^{(i)}, \ldots, C_{r_i}^{(i)}\right).$$

Proof. Let $\alpha : G \to G^* = G_1^* \Box \cdots \Box G_K^*$ be the canonical representation of G, where for $u \in V, \alpha(u) = (\alpha_1(u), \ldots, \alpha_k(u))$. Then we can compute as follows:

$$\begin{aligned}
W(G) &= \frac{1}{2} \sum_{u \in V} \sum_{v \in V} d_G(u, v) = \frac{1}{2} \sum_{u \in V} \sum_{v \in V} d_{G^*}(\alpha(u), \alpha(v)) \\
&= \frac{1}{2} \sum_{u \in V} \sum_{v \in V} \sum_{i=1}^{k} d_i(\alpha_i(u), \alpha_i(v)) \\
&= \sum_{i=1}^{k} \left(\frac{1}{2} \sum_{u \in V} \sum_{v \in V} d_i(\alpha(u), \alpha(v)) \right) \\
&= \sum_{i=1}^{k} \sum_{1 \le j < j' \le r_i} d_i\left(C_j^{(i)}, C_{j'}^{(i)}\right) \cdot |C_j^{(i)}| \cdot |C_{j'}^{(i)}| \\
&= \sum_{i=1}^{k} \Pi_{d_i}\left(C_1^{(i)}, \ldots, C_{r_i}^{(i)}\right). \qquad \Box
\end{aligned}$$

Corollary 2.2. *Let $G = (V, E)$ be a connected graph and let the notations of its canonical metric representation be as in (1). Then*

$$W(G) \ge \sum_{i=1}^{k} \Pi\left(C_1^{(i)}, \ldots, C_{r_i}^{(i)}\right).$$

Moreover, equality holds if and only if G is a partial Hamming graph.

Proof. For $u, v \in V$ set $\rho(\alpha_i(u), \alpha_i(v)) = 1$ if $\alpha_i(u) \ne \alpha_i(v)$ and $\rho(\alpha_i(u), \alpha_i(v)) = 0$ otherwise. (Note that rho graphically resembles the Kronecker's delta symbol put upside down.) Then, using the previous proof we have:

$$
\begin{aligned}
W(G) &= \sum_{i=1}^{k} \sum_{1\le j<j'\le r_i} d_i\left(C_j^{(i)}, C_{j'}^{(i)}\right)\cdot |C_j^{(i)}|\cdot|C_{j'}^{(i)}| \\
&\ge \sum_{i=1}^{k} \sum_{1\le j<j'\le r_i} |C_j^{(i)}|\cdot|C_{j'}^{(i)}| \\
&= \sum_{i=1}^{k} \Pi\left(C_1^{(i)},\ldots,C_{r_i}^{(i)}\right).
\end{aligned}
$$

The above inequality turns into equality if and only if for any i, $1 \le i \le k$, and any $C_j^{(i)}$ and $C_{j'}^{(i)}$ we have $d_i(C_j^{(i)}, C_{j'}^{(i)}) = 1$. In other words, equality holds if and only if any G_i^*, $1 \le i \le k$, is a complete graph, which is equivalent to the fact that G is a partial Hamming graph. □

The expression $\sum_{i=1}^{k} \Pi(C_1^{(i)},\ldots,C_{r_i}^{(i)})$ can be considered as a natural (metric) graph invariant of the graph G and might be of some independent interest.

We follow with two applications of the above results. We first discuss the computation of the Wiener index of partial Hamming graphs and continue with the recognition problem for this class of graphs.

2.1. Wiener index of partial Hamming graphs

If G is a partial cube, then, since every factor of the canonical embedding is K_2, Theorem 2.1 implies that

$$W(G) = \sum_{i=1}^{k} |C_1^{(i)}|\cdot|C_2^{(i)}|.$$

This fact has been observed in [16] and later used and elaborated in a series of papers, cf. the survey [15]. Chepoi, Deza, and Grishukhin [6] followed with a far reaching generalization of the above result to ℓ_1-graphs. Before we state their result, some preparation is needed.

By definition, ℓ_1-graphs are the graphs whose geodesic path metric can be isometrically embedded into an ℓ_1-space. Let $\lambda \in \mathbb{N}$ and let G and H be two graphs. Then H is *scale* λ *embeddable* into G if there exists a mapping $\iota : V(H) \to V(G)$ such that for all vertices $u, v \in V(H)$ we have

$$d_G(\iota(u), \iota(v)) = \lambda \cdot d_H(u, v).$$

For $\lambda = 1$ we thus get the usual isometric embedding. By a result of Assouad and Deza [1] a graph G is an ℓ_1-graph if and only if G is scale λ embeddable into a hypercube for some $\lambda \ge 1$. In addition, this is equivalent to the fact that there exists a collection of $\mathcal{C}(G)$ of convex cuts of G such that every edge of G is cut by precisely λ cuts from $\mathcal{C}(G)$ [9]. Chepoi, Deza, and Grishukhin in [6] proved:

Proposition 2.3. *Let G be a scale λ embeddable into a hypercube and let $\mathcal{C}(G)$ be the family of convex cuts defining this embedding. Then*

$$W(G) = \frac{1}{\lambda} \sum_{\{A,B\} \in \mathcal{C}(G)} |A| \cdot |B|.$$

Shpectorov [17] (see [7] for an alternative proof) characterized ℓ_1-graphs as the graphs isometrically embeddable into the Cartesian product of (complete graphs), half-cubes, and cocktail-party graphs. Therefore, partial Hamming graphs are ℓ_1-graphs. However, the computation of $W(G)$ using Corollary 2.2 is simpler than using Proposition 2.3 since using Proposition 2.3 one first has to obtain the family of convex cuts (and the corresponding embedding), while for Corollary 2.2 the computation of Θ^* suffices.

Partial Hamming graphs are scale 2 embeddable into hypercubes. Indeed, complete graphs are scale 2 embeddable, and so are then Hamming graphs and their isometric subgraphs. Hence combining Proposition 2.3 with Corollary 2.2 we get:

Corollary 2.4. *Let G be a partial Hamming graph scale* 2 *embedded into a hypercube and let $\mathcal{C}(G)$ be the family of convex cuts defining this embedding. Then with the notations of Corollary* 2.2,

$$\sum_{i=1}^{k} \Pi\left(C_1^{(i)}, \ldots, C_{r_i}^{(i)}\right) = \frac{1}{2} \sum_{\{A,B\} \in \mathcal{C}(G)} |A| \cdot |B|.$$

2.2. *Recognizing partial Hamming graphs*

Corollary 2.2 in particular characterizes partial Hamming graphs and this characterization can be used to simplify the recognition of partial Hamming graphs. Namely, the present simplest recognition algorithm, cf. [13] or the books [8,14], uses the fact, that any isometric irredundant embedding of a graph into a Hamming graph is the canonical embedding. Therefore the algorithm computes the canonical representation and verifies whether all factors of the representation are complete. Corollary 2.2 further simplifies this approach since it suffices to compute the Θ^*-classes $E_1, \ldots, E_k$, graphs $G \setminus E_i$, and then to check the condition of the theorem. Using this approach the number of vertices in the connected components of $G \setminus E_i$ can be obtained along the way of determining the components. Thus we need not to construct the quotient graphs G_i^* and to check whether they are complete. The recognition complexity remains the same: $O(nm)$, where $n = |V(G)|$ and $m = |E(G)|$.

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