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CALCULATING THE DEGREE DISTANCE OF PARTIAL HAMMING GRAPHS

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Abstract

If G is a connected graph with vertex set $V(G)$, then the degree distance of G is defined as $DD(G) = \sum_{\{u,v\}\in V(G)}(\deg u + \deg v)d(u,v)$, where $\deg u$ is the degree of vertex u, and $d(u,v)$ denotes the distance between u and v. In the chemical literature, $DD(G)$ is better known under

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the name *Schultz index*, introduced by Gutman. In the class of partial Hamming graphs, which include trees, benzenoid and phenylene systems among others, we express the degree distance in terms of the canonical metric representation, thus simplifying its computation.

1 Introduction

Let G be a connected graph of order n and $V(G)$ its vertex set. We denote the degree of a vertex $u \in V(G)$ by $\deg u$ and the distance between vertices u and $v \in V(G)$ by $d(u, v)$. The *degree distance* of G is defined as

$$DD(G) = \sum_{\{u,v\} \in V(G)} (\deg u + \deg v)\, d(u, v).$$

The degree distance seems to have been considered first in connection with certain chemical applications by Dobrynin and Kochetova [1] and at the same time by Gutman [2], who named it the *Schultz index*. This name was eventually accepted by most other authors (see, e.g., [3, 4, 5]). In fact, there are several names (degree distance, MTI index, Schultz index, Zagreb index) associated to this index or closely related indices, we refer to [6] for a clarification of these notions.

The degree distance may be considered as a weighted version of the Wiener index [7, 8]. Recall that the Wiener index of G is defined as

$$W(G) = \sum_{\{u,v\} \in V} d(u, v).$$

The relations between the degree distance and the Wiener index were studied in [2, 3, 9, 10, 11, 12]. An example of such relation,

$$DD(T) = 4W(T) - n(n-1),$$

which holds whenever T is a tree of order n may be found in [2, 11].

In the mathematical literature, extremal properties of $DD(G)$ were investigated in [6, 13, 14, 15, 16]. For the recent results on the Schultz molecular topological index see [17, 18, 19].

Here we show that $DD(G)$ can be expressed in terms of the quotient graphs of the canonical metric representation of G. The metrics of the quotient graphs can be ommited when G is isometrically embeddable into a Hamming graph, which significantly simplifies calculation of

the degree distance for partial Hamming graphs. A similar approach has been recently used to calculate the Wiener index of a graph via its canonical metric representation [20].

In the rest of this section we present necessary concepts, while in the next section the main result is proved. In Section 3 we give few examples on chemically important partial cubes – benzenoid and phenylene systems. In Section 4 we propose a linear algorithm for calculating the degree distance of benzenoid systems.

The *Cartesian product* $G_1 \Box \cdots \Box G_k$ of graphs $G_1, \cdots, G_k$ 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 $d_G(u, v) = \sum_{i=1}^{k} d_{G_i}(u_i, v_i)$, see [21].

A *Hamming graph* is the Cartesian product of complete graphs and a *partial Hamming graph* is a graph that isometrically (that is, distance preserving) embeds into a Hamming graph. In the particular case where all the factors are K_2's we speak of *hypercubes* Q_n and *partial cubes*, respectively, whose important examples include trees, median graphs, benzenoids, phenylenes, grids, bipartite torus graphs, etc. Partial Hamming graphs have been studied and characterized in [22, 23, 24].

The canonical metric representation of a connected graph G, due to Graham and Winkler [25], is defined as follows. Edges xy and uv of G are in the Djoković–Winkler [26, 27] 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^*-classes E_1 and E_2.

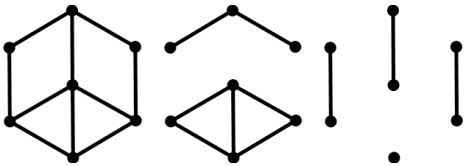

Figure 1: Θ^*-equivalence classes of G.

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 in G to a vertex of $C_{j'}^{(i)}$. Let the contractions $\alpha_i \colon V(G) \to V(G_i^*)$ be given by $\alpha_i(v) = C_j^{(i)}$ where $v \in C_j^{(i)}$. Then the mapping

$$\alpha \colon G \to G_1^* \,\square\, \cdots \,\square\, G_k^*, \tag{1}$$

where $\alpha(v) = (\alpha_1(v), \ldots, \alpha_k(v))$, is the *canonical metric representation* of the graph G. Graham and Winkler proved 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 [28, 29, 30] and the books [21, 31].

2 The main result

Theorem 2.1 *Let $G = (V, E)$ be a partial Hamming graph. Let the notations of its canonical metric representation be as in (1) and let d_i be the distance function of G_i^*. For $i = 1, \ldots, k$ and $j = 1, \ldots, r_i$, let $\deg C_j^{(i)}$ be the sum of degrees in G of vertices that are mapped to $C_j^{(i)}$ by α_i. Then*

$$DD(G) = \sum_{i=1}^{k} \sum_{j=1}^{r_i} \deg C_j^{(i)} \, (n - |C_j^{(i)}|).$$

Proof. Let $\alpha \colon G \to G^* = G_1^* \,\square\, \cdots \,\square\, G_k^*$ 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:

$$\begin{aligned} DD(G) &= \sum_{\{u,v\} \in V} (\deg u + \deg v) d_G(u, v) = \sum_{\{u,v\} \in V} (\deg u + \deg v) d_{G^*}(\alpha(u), \alpha(v)) \\ &= \sum_{\{u,v\} \in V} (\deg u + \deg v) \sum_{i=1}^{k} d_i(\alpha_i(u), \alpha_i(v)) \\ &= \sum_{i=1}^{k} \sum_{\{u,v\} \in V} (\deg u + \deg v) d_i(\alpha_i(u), \alpha_i(v)). \end{aligned}$$

Since G is a partial Hamming graph, each G_i^* is a complete graph, so that $d_i(\alpha_i(u), \alpha_i(v)) = 1$

whenever $\alpha_i(u) \neq \alpha_i(v)$. Thus,

$$\begin{aligned} DD(G) &= \sum_{i=1}^{k} \sum_{\{u,v\}\in V,\ \alpha_i(u)\neq\alpha_i(v)} \deg u + \deg v \\ &= \sum_{i=1}^{k} \sum_{u\in V} \deg u\,(n - |\alpha_i(u)|) \\ &= \sum_{i=1}^{k} \sum_{j=1}^{r_i} \sum_{u\in\alpha_i^{-1}(C_j^{(i)})} \deg u\,(n - |C_j^{(i)}|) \\ &= \sum_{i=1}^{k} \sum_{j=1}^{r_i} \deg C_j^{(i)}\,(n - |C_j^{(i)}|). \end{aligned}$$

□

In the case of partial cubes, Theorem 2.1 specializes to an even more applicable form. For this sake some preparation is needed. It is not difficult to observe that G is a partial cube if and only if every G_i^* of its canonical metric representation is isomorphic to K_2. Hence every corresponding graph G_i consists of two connected components, they are denoted $W_{i,0}$ and $W_{i,1}$ and called *halfspaces* of G. In other words, $W_{i,\chi}$ consists of those vertices u of G for which $\alpha_i(u) = \chi$, $\chi \in \{0,1\}$.

Let G be a partial cube with halfspaces $W_{i,\chi}$, $1 \leq i \leq k$, $\chi \in \{0,1\}$. For any $1 \leq i \leq k$ and any $\chi \in \{0,1\}$ we set

$$D_{(i,\chi)} = \sum_{u\in W_{(i,\chi)}} \deg(u)\,.$$

Since $r_i = 2$ for any i and $|W_{(i,\chi)}| + |W_{(i,\chi)}| = n$, Theorem 2.1 reduces to:

Corollary 2.2 *Let G be a partial cube with halfspaces $W_{i,\chi}$, $1 \leq i \leq k$, $\chi \in \{0,1\}$. Then*

$$DD(G) = \sum_{i=1}^{k} \left(|W_{(i,0)}|D_{(i,1)} + |W_{(i,1)}|D_{(i,0)}\right)\,.$$

An advantage of Corollary 2.2 comparing to computing $DD(G)$ by the definition is that we need not to compute distance but only count vertices and sum up the degrees. This result can be considered as another instance of the so-called cut method. For its general description and an overview of its applications in chemical graph theory see [32]. The method got its name because of benzenoid graph in which the Θ^*-classes are precisely the orthogonal cuts. We also mention

a related result on the Wiener index of weighted graphs from [33]. In that case, however, the weighted Wiener index was defined as $\sum_{u,v} w(u)w(v)d(u,v)$, where w is an arbitrary weight function.

3 Applications to chemical graphs

In this section, we will apply Corollary 2.2 to a particular, but chemically very important class of partial cubes – benzenoid graphs. The term *benzenoid graph* is used for graphs constructed in the following manner. Consider the hexagonal lattice $\mathcal{H}$. Let Z be a circuit on this lattice. Then benzenoid graphs are formed by the vertices and edges of $\mathcal{H}$ lying on some circuit Z or in its interior. The vertices and edges belonging to Z form the perimeter of the respective benzenoid graph, while the vertices (if any) not belonging to the perimeter are said to be the internal vertices.

The third example is a linear phenylene PH_h, chain consisting of hexagons and squares.

3.1 Linear benzenoid chains

Consider the linear benzenoid chain L_h, see Fig. 2 for its description.

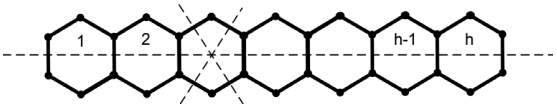

Figure 2: The linear benzenoid chain L_h

The number of vertices equals $n_h = 4h + 2$, while the sum of all degrees equals $d_h = 2m_h = 10h + 2$ since there are $2(h-1)$ vertices of degree three and $(2h+4)$ vertices of degree two. For the horizontal orthogonal cut we have the contribution $2(2h+1)(5h+1)$. For the hexagon C_i, there are two symmetrical orthogonal cuts with contributions

$$(n_{i-1}+1)\cdot(d_{n-i}+4) + (n_{h-i}+1)\cdot(d_i+4).$$

Using again the symmetry, it follows

$$\begin{aligned} DD(L_h) &= 2(2h+1)(5h+1) + 4\sum_{i=1}^{h}(4(i-1)+3)(10(h-i)+6) \\ &= 2\left(10h^2+7h+1+2\sum_{i=1}^{h}\left(40ih-10h-40i^2+34i-6\right)\right) \\ &= \frac{2}{3}\left(40h^3+72h^2+47h+3\right). \end{aligned}$$

3.2 Coronene/circumcoronene series

We next obtain a closed expression for the degree distance of the coronene/circumcoronene homologous series H_k, $k \geq 1$. The first terms of this series are H_1 = benzene, H_2 = coronene, H_3 = circumcoronene, H_4 = circumcircumcoronene, see Fig. 3 where H_3 is shown.

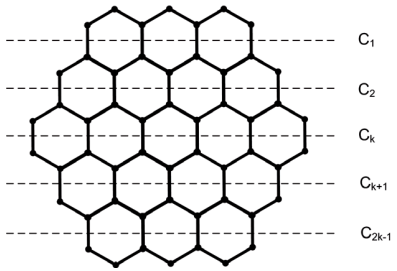

Figure 3: The Coronene / Circumcoronene H_3.

In Fig. 3, $2k-1$ horizontal elementary cuts of H_k are indicated. There exist two additional groups of $2k-1$ equivalent cuts, obtained by rotating the former group by $+60°$ and $-60°$. The number of vertices of H_k equals $n_k = 6k^2$, while there are exactly $6k$ vertices of degree two. Therefore, the sum of all degrees equals

$$d_k = 2m_k = 2 \cdot 6k + 3 \cdot (6k^2 - 6k) = 6k(3k-1).$$

It should be observed that because of symmetry, the contribution of the elementary cut C_i is equal to the contribution of C_{2k-i}, $i = 1, 2, \ldots, k-1$. It can be shown by induction that for $i = 1, 2, \ldots, k$ the number of vertices above cut C_i equals $i(2k+i)$, while the sum of degrees of

the vertices is $(6k-1)i-2i+3i^2$. Therefore,

$$\begin{aligned}\frac{1}{3}DD(H_k) &= 2\cdot(3k^2)(9k^2-3k)\\ &+ 2\sum_{i=1}^{k-1} i(2k+i)\cdot(18k^2-6k-((6i-1)k-2i+3i^2))\\ &+ 2\sum_{i=1}^{k-1}(6k^2-i(2k+i))\cdot((6i-1)k-2i+3i^2)\\ &= \frac{2h}{15}\cdot(3+25h-45h^2-205h^3+492h^4).\end{aligned}$$

Finally, we derive the fifth-order polynomial formula for the degree distance of H_k.

$$DD(H_k)=\frac{2}{5}\cdot h\left(3+25h-45h^2-205h^3+492h^4\right).$$

3.3 Linear phenylenes

Consider the linear phenylene PH_h, consisting of $h-1$ four-membered (cyclobutadiene) and h six-membered (benzene) rings, in which each cyclobutadiene unit is adjacent to two benzene rings, whereas benzene rings are not adjacent to each other, see Fig. 4.

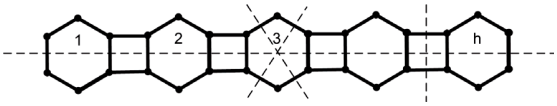

Figure 4: The linear phenylene PH_h

The number of vertices equals $n_h=6h$, while the sum of all degrees equals $d_h=2m_h=2(8h-2)$. The horizontal cut of PH_h contains $2h$ edges, while any of the remaining $(h-1)+2h$ cuts contains two edges. For the horizontal orthogonal cut we have the contribution $2\cdot 3h(8h-2)$. For vertical cut at cyclobutadiene i, we have contribution $6i(16(h-i)-2)+6(h-i)(16i-2)$, and for the hexagon C_i, there are two symmetrical orthogonal cuts with contributions $(6i-3)(16(h-i)+6)+(6(h-i)+3)(16i-10)$. Therefore,

$$\begin{aligned}DD(PH_h) &= 2\cdot 3h(8h-2)\\ &+ \sum_{i=1}^{h-1}(6i(16(h-i)-2)+6(h-i)(16i-2))\\ &+ 2\sum_{i=1}^{h}((6i-3)(16(h-i)+6)+(6(h-i)+3)(16i-10))\\ &= 12h^2(8h+1).\end{aligned}$$

4 Linear algorithm for benzenoid systems

Let B be a benzenoid graph. The edge set of B can be partitioned into three cuts as follows: each cut consists of all parallel edges. Then, making quotient graphs just as it is done in the canonical metric representation, we obtain three trees T_1, T_2, T_3. The key observation of Chepoi [34] is that B embeds isometrically into $T_1 \Box T_2 \Box T_3$ (see [35, 36, 37, 38] for algorithms for calculating the Wiener index, the Szeged index and the hyper-Wiener index in benzenoid systems and trees).

Let

$$W(T, a, b) = \sum_{v \in T} \sum_{u \in T} (a(u)b(v) + a(v)b(u))d(u, v)$$

be the modified weighted Wiener index of tree T, such that every vertex $v \in T$ has two weight values $a(v)$ and $b(v)$.

For $i = 1, 2, 3$, define the weight a_i to be the number of vertices and b_i to be the sum of degrees in the corresponding connected component.

Theorem 4.1 *Let G be a benzenoid system and let α be the canonical embedding of G into $H = T_1 \Box T_2 \Box T_3$. Then*

$$DD(G) = W(T_1, a_1, b_1) + W(T_2, a_2, b_2) + W(T_3, a_3, b_3).$$

Proof. For $u \in V$, let $\alpha(v) = (v_1, v_2, v_3)$.

$$\begin{aligned}
DD(G) &= \sum_{v \in V} \sum_{u \in V} (deg(v) + deg(u)) \cdot d(u, v) \\
&= \sum_{v \in V} \sum_{u \in V} (deg(v) + deg(u)) \cdot d_H(\alpha(u), \alpha(v)) \\
&= \sum_{v \in V} \sum_{u \in V} (deg(v) + deg(u)) \cdot \sum_{i=1}^{3} d_{T_i}(u_i, v_i) \\
&= \sum_{i=1}^{3} \left(\sum_{v \in V} \sum_{u \in V} (deg(v) + deg(u)) \cdot d_{T_i}(u_i, v_i) \right) \\
&= \sum_{i=1}^{3} \left(\sum_{v_i \in V(T_i)} \sum_{u \in V(T_i)} (b_i(v)a_i(u) + b_i(u)a_i(v)) \cdot d_{T_i}(u_i, v_i) \right) \\
&= W(T_1, a_1, b_1) + W(T_2, a_2, b_2) + W(T_3, a_3, b_3).
\end{aligned}$$

Let us take a closer look at the identity

$$\sum_{v\in V}\sum_{u\in V}(deg(v)+deg(u))\cdot d_{T_i}(u_i,v_i)=\sum_{v_i\in V(T_i)}\sum_{u\in V(T_i)}(b_i(v)a_i(u)+b_i(u)a_i(v))\cdot d_{T_i}(u_i,v_i).$$

Consider two vertices v_k and u_k from T_k, $k=1,2,3$, and assume that they represent components consisting of vertices $v'_1,v'_2,\ldots,v'_p$ and $u'_1,u'_2,\ldots,u'_q$ from T, respectively.

$$\begin{aligned} S &= \sum_{i=1}^{p}\sum_{j=1}^{q}(deg(v'_i)+deg(u'_j))\cdot d_{T_k}(v_k,u_k) \\ &= d_{T_k}(v_k,u_k)\cdot\left(p\sum_{j=1}^{q}deg(u'_j)+q\sum_{i=1}^{p}deg(v'_j)\right) \\ &= d_{T_k}(v_k,u_k)\cdot(a_k(v)b_k(u)+a_k(u)b_k(v))\,. \end{aligned}$$

□

We will present the linear algorithm for calculating the following generalization of weighted Wiener index, and consequently for calculating DD in benzenoid systems using Theorem 4.1.

Lemma 4.2 *Let (T,a,b) be a double vertex-weighted tree. For an edge e of T, denote with T_1 and T_2 the connected components of $T\setminus e$, and for $i=1,2$ set*

$$A_i(e)=\sum_{u\in T_i}a(u)\qquad\text{and}\qquad B_i(e)=\sum_{u\in T_i}b(u).$$

Then,

$$W(T,a,b)=\sum_{e\in T}(A_1(e)B_2(e)+A_2(e)B_1(e))\,.$$

The proof relies on the cut method for calculating the weighted Wiener index.

Notice that $A_1(e)+A_2(e)=\sum_{v\in T}a(v)=A$ and $B_1(e)+B_2(e)=\sum_{v\in T}b(v)=B$. One can easily design a dynamic programming algorithm for calculating the sums $A_1(e)$ and $B_1(e)$ in tree T. Choose an arbitrary vertex v as the root and perform a depth-first search from v. Denote with $p(v)$ the parent of vertex v in the DFS tree. Let $A(v)$ be the sum of vertex weights a in the subtree rooted at v (including $a(v)$), while let $B(v)$ be the sum of vertex weights b in the subtree rooted at v (including $b(v)$). Using the formulas

$$A(v)=a(v)+\sum_{(u,v)\in E(T)}A(u)\qquad\text{and}\qquad B(v)=b(v)+\sum_{(u,v)\in E(T)}B(u),$$

we can calculate the arrays A and B, while traversing vertices in the recursive call of a depth-first search. Finally notice that $A_1((v, p(v))) = A(v)$ and $B_1((v, p(v))) = B(v)$ from Lemma 4.2.

The time complexity of the algorithm for calculating the modified weighted Wiener index is $O(n)$, and the memory used is $O(n)$, since we need three additional arrays of length n.

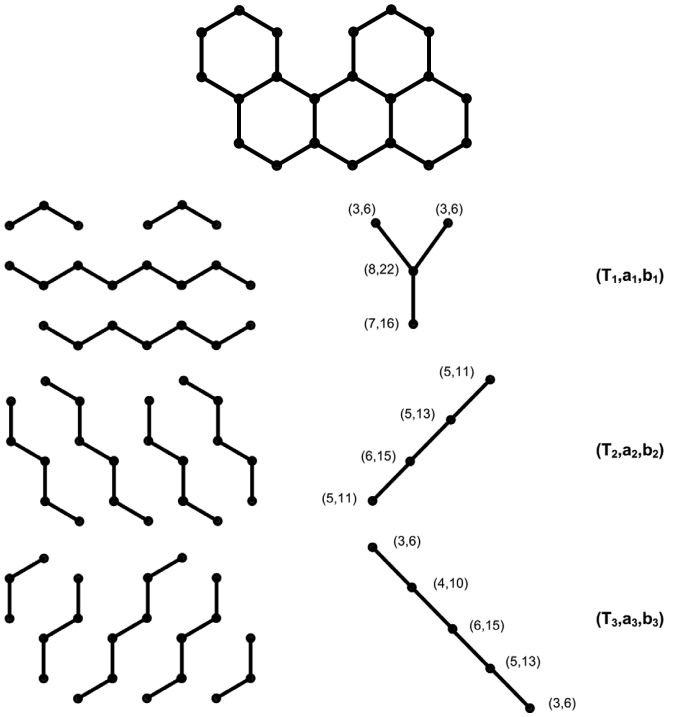

Figure 5: Steps in computing DD of the benzenoid system G

The graph G on Fig. 5 has 5 hexagons, 21 vertices and 25 edges.

$$DD(T_1, a_1, b_1) = (3 \cdot 44 + 18 \cdot 6) + (3 \cdot 44 + 18 \cdot 6) + (7 \cdot 34 + 14 \cdot 16) = 942$$

$$DD(T_2, a_2, b_2) = (5 \cdot 39 + 16 \cdot 11) + (10 \cdot 26 + 11 \cdot 24) + (16 \cdot 11 + 5 \cdot 39) = 1266$$

$$DD(T_3, a_3, b_3) = (3 \cdot 44 + 18 \cdot 6) + (7 \cdot 34 + 14 \cdot 16) + (13 \cdot 19 + 8 \cdot 31) + (18 \cdot 6 + 3 \cdot 44) = 1437$$

By Theorem 4.1, we have $DD(G) = 942 + 1266 + 1437 = 3645$.

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