Computing distance moments on graphs with transitive Djoković-Winkler's relation

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Abstract

The cut method proved to be utmost useful to obtain fast algorithms and closed formulas for classical distance based invariants of graphs isometrically embeddable into hypercubes. These graphs are known as partial cubes and in particular contain numerous chemically important graphs such as trees, benzenoid graphs, and phenylenes. It is proved that the cut method can be used to compute an arbitrary distance moment of all the graphs that are isometrically embeddable into Cartesian products of triangles, a class much larger than partial cubes. The method in particular covers the Wiener index, the hyper-Wiener index, and the Tratch-Stankevich-Zefirov index.

Key words: Isometric embedding; distance moment; Wiener index; partial cube; Cartesian product of graphs

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1 Introduction

Several central graph invariants in mathematical chemistry (and elsewhere) are defined using the distance function of a graph. The most famous is certainly the *Wiener index* $W(G)$ of a graph G defined as $W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v)$. It was introduced (for the case of trees) back in 1947 by Wiener in [29], hence the name of this graph invariant. It is, however, still extensively investigated, cf. [5, 21, 23]. The Wiener index can be naturally and widely generalized by setting

$$W_\lambda(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v)^\lambda\,,$$

where λ is some real number [8, 14]. When λ is a positive integer, $W_\lambda(G)$ is called the *k-th distance moment of* G [19]. The distance moment is clearly a fundamental metric graph concept and was in particular (very recently) applied in an appealing way in [27]. More precisely, closed formulas using distance moments were obtained for the n-th order Wiener index [7] and for a recently related invariant from [1].

Of course, $W_1(G) = W(G)$, other special cases from the literature include W_{-2}, W_{-1}, $\frac{1}{2}W_2 + \frac{1}{2}W_1$, and $\frac{1}{6}W_3 + \frac{1}{2}W_2 + \frac{1}{3}W_1$, invariants known as the Harary index [24], the reciprocal Wiener index [3], the hyper-Wiener index [20, 23, 26], and the Tratch-Stankevich-Zefirov index [19, 28], respectively. Therefore, a good method for computing the distance moments graph yields a good method for computing all these classical indices and more.

A partial cube is a graph isometrically embeddable into a hypercube [4, 6, 22, 25]. This class of graphs includes trees, median graphs, as well as several chemically important families of graphs such as hexagonal (benzenoid) systems. Numerous distance-based invariants can be computed on partial cubes with the so-called cut method initiated in [16], see the survey [13]. The paper [16] developed the cut method for the Wiener index, later the method was designed in particular for the hyper-Wiener index [12] (see also [18]). Recently the cut method was used in [31] for the edge-Wiener index and the edge-Szeged index (in [17] it has been shown that the graphs studied in [31] are precisely partial cubes), and very recently the method was proved to be applicable also for the generalized terminal Wiener index [11]. The latter index is a generalization of the terminal Wiener index introduced in [9], see also [2]. A recursive approach for computing $W_\lambda(G)$ for a partial cube G and any λ was developed in [15].

Partial cubes can be characterized as the bipartite graphs in which the so-called Djoković-Winkler's relation is transitive. A more general class of graphs is obtained by omitting the requirement for a graph to be bipartite. As proved by Winkler [30], these graphs are precisely the graphs that admit isometric embeddings into the Cartesian product of triangles.

In this note we prove that the cut method can be extended to obtain an arbitrary distance moment of these graphs. Roughly speaking, the method reduces to the computation of intersections of parts generated by the Djoković-Winkler's relation. The method is formulated and proved in the next section, while in the rest of this section the concepts needed are formally introduced.

The *distance* $d_G(u, v)$ between the vertices u and v of a graph G is the usual shortest path distance. The notation will be simplified to $d(u, v)$ when the graph will be clear from the context. A subgraph of a graph is called *isometric* if the distance between any two vertices of the subgraph is independent of whether it is computed in the subgraph or in the entire graph. For a graph G, the Djoković-Winkler's relation Θ [4, 30] is defined on $E(G)$ as follows. If $e = xy \in E(G)$ and $f = uv \in E(G)$, then $e\Theta f$ if $d(x, u) + d(y, v) \neq d(x, v) + d(y, u)$. Relation Θ is reflexive and symmetric, its transitive closure Θ^* is hence an equivalence relation, its parts are called Θ^*-classes or also Θ-classes when $\Theta = \Theta^*$.

The *Cartesian product* $G \,\square\, H$ of graphs G and H is the graph with vertex set

$V(G) \times V(H)$ where the vertex (g, h) is adjacent to the vertex (g', h') whenever $gg' \in E(G)$ and $h = h'$, or $g = g'$ and $hh' \in E(H)$. For more information on this fundamental graph operation see [10]. Winkler [30] proved that if G is a connected graph G, then $\Theta = \Theta^*$ if and only if G admits an isometric embedding into the Cartesian product whose factors are K_3.

Finally, $[k]$ denotes the set $\{1, 2, \ldots, k\}$.

2 The main result

In order to state the main result of this paper some technical preparation is needed. Let G be a graph with transitive Θ and let $L_1, \ldots, L_k$ be the Θ-classes of G. Then for any $1 \leq i \leq k$, the graph $G - L_i$ consists of two or three connected components denoted $C_1^{(i)}$, $C_2^{(i)}$ and $C_3^{(i)}$. If there are only two such components we assume that $C_3^{(i)}$ is the empty graph. For any $p \geq 1$, for any pairwise different $i_1, i_2, \ldots, i_p \in [k]$ and for any $j_1, j_2, \ldots, j_p \in [3]$ let

$$n_{j_1,j_2,\ldots,j_p}^{i_1,i_2,\ldots,i_p} = \left| V(C_{j_1}^{(i_1)}) \cap V(C_{j_2}^{(i_2)}) \cap \cdots \cap V(C_{j_p}^{(i_p)}) \right| .$$

This notation is illustrated in Fig. 1. The graph in question has 5 Θ-classes and the components of the corresponding graphs $G - L_i$ are indicated. The order of the intersection of the gray parts is then $n_{3,2,3,1}^{1,2,3,5}$.

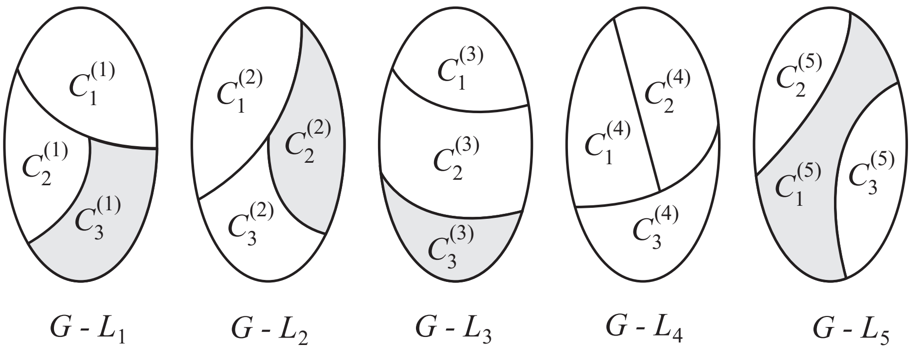

Figure 1: Intersection of parts from $G - L_i$

We now set

$$N_{i_1,i_2,\ldots,i_p} = \sum_{\forall r: j_r \neq j'_r} n_{j_1,j_2,\ldots,j_p}^{i_1,i_2,\ldots,i_p} \cdot n_{j'_1,j'_2,\ldots,j'_p}^{i_1,i_2,\ldots,i_p} ,$$

where the summation is made over all admissible indices $j_1, j_2, \ldots, j_p$ and $j'_1, j'_2, \ldots, j'_p$, and where, as indicated, $j_r \neq j'_r$ for $r = 1, 2, \ldots, k$.

With this preparation in hand we can formulate the main result of this paper as follows.

Theorem 2.1 *Let G be a graph with transitive Θ and let s be a positive integer. Then with the above notation,*

$$W_s(G) = \sum_{\substack{t_{i_1}, t_{i_2}, \dots, t_{i_p} > 0 \\ t_{i_1} + t_{i_2} + \cdots + t_{i_p} = s}} \binom{s}{t_{i_1}, t_{i_2}, \dots, t_{i_p}} N_{i_1, i_2, \dots, i_p} \,.$$

Proof. Let $|V(G)| = n$ and let $Y = \{P_1, \dots, P_{\binom{n}{2}}\}$ be a set of shortest paths of G such that each pair of vertices of G is connected with exactly one path from Y. Let $A = [A_{ij}]$ be the $\binom{n}{2} \times k$ matrix with entries $A_{ij} = 1$ if $P_i \cap L_j \neq \emptyset$ and $A_{ij} = 0$ otherwise. Since Θ is transitive, and no two edges on a shortest path are in relation Θ, we infer that $\sum_{j=1}^{k} A_{ij}$ is the length of the path P_i. Using the multinomial theorem we get:

$$\begin{aligned}
W_s(G) &= \sum_{i=1}^{\binom{n}{2}} |E(P_i)|^s = \sum_{i=1}^{\binom{n}{2}} (A_{i1} + A_{i2} + \cdots + A_{ik})^s \\
&= \sum_{i=1}^{\binom{n}{2}} \left(\sum_{\substack{t_1, t_2, \dots, t_k \geq 0 \\ t_1 + t_2 + \cdots + t_k = s}} \binom{s}{t_1, t_2, \dots, t_k} A_{i1}^{t_1} A_{i2}^{t_2} \cdots A_{ik}^{t_k} \right) \\
&= \sum_{\substack{1 \leq r_1 \leq k \\ t_{r_1} = s}} \binom{s}{t_{r_1}} \sum_{i=1}^{\binom{n}{2}} A_{ir_1} + \sum_{\substack{1 \leq r_1 \neq r_2 \leq k \\ t_{r_1}, t_{r_2} > 0 \\ t_{r_1} + t r_2 = s}} \binom{s}{t_{r_1}, t_{r_2}} \sum_{i=1}^{\binom{n}{2}} A_{ir_1} A_{ir_2} \\
&\quad + \cdots + \sum_{\substack{t_1, t_2, \dots, t_k > 0 \\ t_1 + t_2 + \cdots + t_k = s}} \binom{s}{t_1, t_2, \dots, t_k} \sum_{i=1}^{\binom{n}{2}} A_{i1} A_{i2} \cdots A_{ik} \,.
\end{aligned}$$

The term $A_{ir_1} A_{ir_2} \cdots A_{ir_t}$ is nonzero if and only if $A_{ir_j} = 1$, for $1 \leq j \leq t$. In other words, $A_{ir_1} A_{ir_2} \cdots A_{ir_t}$ is nonzero if and only if P_i contains edges from each of the Θ-classes $L_{r_1}, \dots, L_{r_t}$. It follows that $\sum_{i=1}^{\binom{n}{2}} A_{ir_1} A_{ir_2} \cdots A_{ir_t}$ is equal to the number of shortest paths from Y that contain edges from each of the classes $L_{r_1}, \dots, L_{r_t}$. On the other hand, if P is one of the shortest path between vertices a and b which contains an edge from L_r, then $a \in C_j^{(r)}$ and $b \in C_{j'}^{(r)}$ for some $j \neq j'$. We conclude that the number of shortest paths of Y that contain the edges of $L_{r_1}, \dots, L_{r_t}$ is $N_{r_1, \dots, r_t}$. Hence we can continue the above computation as follows:

$$
\begin{aligned}
W_s(G) &= \sum_{\substack{1\le r_1\le k\\ t_{r_1}=s}} \binom{s}{t_{r_1}} \sum_{j_1\ne j_1'} n^{r_1}_{j_1}\cdot n^{r_1}_{j_1'} + \sum_{\substack{1\le r_1\ne r_2\le k\\ t_{r_1},t_{r_2}>0\\ t_{r_1}+t_{r_2}=s}} \binom{s}{t_{r_1},t_{r_2}} \sum_{\substack{j_1\ne j_1'\\ j_2\ne j_2'}} n^{r_1,r_2}_{j_1,j_2}\cdot n^{r_1,r_2}_{j_1',j_2'} \\
&\quad + \cdots + \sum_{\substack{t_1,t_2,\ldots,t_k>0\\ t_1+t_2+\cdots+t_k=s}} \binom{s}{t_1,t_2,\ldots,t_k} \sum_{\substack{1\le i\le k\\ j_i\ne j_i'}} n^{i_1,i_2,\ldots,i_k}_{j_1,j_2,\ldots,j_k}\cdot n^{i_1,i_2,\ldots,i_k}_{j_1',j_2',\ldots,j_k'} \\
&= \sum_{\substack{t_{i_1},t_{i_2},\ldots,t_{i_p}>0\\ t_{i_1}+t_{i_2}+\cdots+t_{i_p}=s}} \binom{s}{t_{i_1},t_{i_2},\ldots,t_{i_p}} N_{i_1,i_2,\cdots,i_p}\,,
\end{aligned}
$$

and the proof is complete. $\square$

We conclude the note with an example illustrating Theorem 2.1. Let G be the graph from Fig. 2. Then it is straightforward to verify that $\Theta = \Theta^*$ partitions $E(G)$ into classes L_1, L_2, L_3, L_4, where the edges of the triangle lie in L_4, while the remaining three classes contain four edges each. Fig. 2 shows $G - L_1$ and $G - L_4$, the graphs $G - L_2$ and $G - L_3$ are not presented as they are symmetric to $G - L_1$.

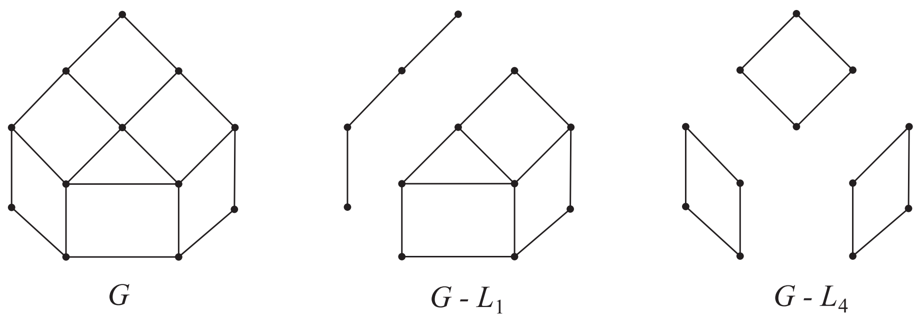

Figure 2: Graphs G, $G - L_1$ and $G - L_4$

Then $W_1(G) = W(G) = 3\cdot(4\cdot 8) + (4\cdot 4 + 4\cdot 4 + 4\cdot 4) = 144$. Moreover, $W_2(G) = W_1(G) + 2\,[3\,(1\cdot 5 + 3\cdot 3) + 3\,(2\cdot 2 + 2\cdot 4 + 2\cdot 2 + 2\cdot 4 + 0\cdot 2 + 0\cdot 2)] = 144 + 228 = 372$. The factor 2 comes from the multinomial coefficient, the first factor 3 is due to symmetry between L_1, L_2, L_3, the second factor 3 comes when intersections with one part in L_i, $1 \le i \le i$, the other part in L_4 are considered. Then the hyper-Wiener index of G is equal to $W_1(G)/2 + W_2(G)/2 = 258$. Similarly, $W_3 = W_1 + \left(\binom{3}{2,1} + \binom{3}{1,2}\right)[3\cdot 24 + 3\cdot 14] + \binom{3}{1,1,1}[3\,(1\cdot 0+1\cdot 2+2\cdot 2+1\cdot 0+2\cdot 0+2\cdot 1+2\cdot 0+0\cdot 1+0\cdot 0+0\cdot 1+2\cdot 1+2\cdot 1)+(2\cdot 1+1\cdot 2+0\cdot 3+2\cdot 1)] = 144+6\cdot 114+6\cdot 42 = 1080$. Hence the Tratch-Stankevich-Zefirov index of G is equal to $\frac{1}{6}\,W_3 + \frac{1}{2}\,W_2 + \frac{1}{3}\,W_1 = 414$.

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