Wiener index in weighted graphs via unification of Θ^*-classes

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Abstract

It is proved that the Wiener index of a weighted graph (G, w) can be expressed as the sum of the Wiener indices of weighted quotient graphs with respect to an arbitrary combination of Θ^*-classes. Here Θ^* denotes the transitive closure of the Djoković-Winkler's relation Θ. A related result for edge-weighted graphs is also given and a class of graphs studied in [25] is characterized as partial cubes.

Key words: Wiener index; weighted graph; Djoković-Winkler's relation; partial cube

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1 Introduction

The cut method (see the survey [17]) turned out to be extremely handy when dealing with distance-based graph invariants which are in turn among the central concepts of chemical graph theory. The method was initiated in [19] where it was shown how cuts can be used to compute the Wiener index (see the surveys [8, 9]) of graphs which admit isometric embeddings into hypercubes. These graphs are know as

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partial cubes. About ten years later, the result was extended in [16] to general graphs by establishing a connection between the Wiener index of a graph and its canonical metric representation. (The result of [19] is then obtained by specializing to bipartite graphs.) The latter representation is due to Graham and Winkler [12], while in [1] a recent application of the main result from [16] can be found.

Our primary motivation for this paper was the recent paper [25] in which it is demonstrated that the cut method is applicable also to the edge-Wiener index [6, 15] and the edge-Szeged index [13]. (For some recent invetigations on the relation between the Wiener index and the Szeged index see [10, 20, 21, 22].) The results in [25] are stated for graphs that admit certain edge partitions. In Section 2 we show that this class of graphs is the class of partial cubes, a class of graphs extensively studied by now, cf. [2, 11, 23].

The main result of this paper, stated and proved in Section 3, is a generalization of the above mentioned theorem from [16]. The generalization is two-fold. First, the variety of factor graphs is extended by allowing arbitrary combinations of the edge classes from the canonical metric representation. Second, the result is extended to weighted graphs. We add here that very recently, Dankelmann [5] studied the Wiener index on trees, cycles, and graphs with minimum degree at least 2.

A special case of our main result should be mentioned here. In [4] it was demonstrated that the Wiener index of benzenoid graphs can be computed in linear time. The main idea is to merge all parallel cuts into a single set and to deduce the Wiener index from the three corresponding quotient graphs (that turned out to be trees [3]), cf. [4, Proposition 2]. This can be seen as another motivation for our investigation.

2 Preliminaries

We consider the usual shortest path distance and write $d_G(u,v)$ for the distance in a graph G between u and v and simplify the notation to $d(u,v)$ when the graph will be clear from the context. The *Wiener index* of G is the sum of distances between all pairs of vertices of G.

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. A subgraph of a graph is called *convex* if for any two vertices of the subgraph all shortest path (of the entire graph) between then belong to the subgraph. For a connected graph G and an edge ab of G we set $W_{ab} = \{x \in V(G) \mid d(x,a) < d(x,b)\}$. Note that if G is bipartite then $V(G) = W_{ab} \cup W_{ba}$ for any edge ab. By abuse of language we consider (when appropriate) W_{ab} also as the subgraph induced by W_{ab}.

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 a graph G, the Djoković-Winkler's relation Θ [7, 24] 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 an equivalence relation. The partition of $E(G)$ induced by Θ^* will be called the *Θ^*-partition.*

A *weighted graph* (G, w) is a graph $G = (V(G), E(G))$ together with the weight function $w : V(G) \to \mathbb{R}^+$. The Wiener index $W(G, w)$ of (G, w) is then defined as [18]:

$$W(G,w) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} w(u)\ w(v)\ d_G(u,v)\,.$$

Clearly, if $w \equiv 1$ then $W(G, w) = W(G)$.

As already mentioned in the introduction, the cut method was developed in [25] for the edge-Wiener/Szeged index. More precisely, the method was developed for graph G that admit a partition $\{F_i\}$ of the edge set such that $G \setminus F_i$ is a two component graph with convex components. We close this section by pointing out that these graphs are precisely the partial cubes.

Proposition 2.1 *Let G be a connected graph. Then G admits a partition $\{F_i\}$ of $E(G)$ such that $G \setminus F_i$ is a two component graphs with convex components if and only if G is a partial cube.*

Proof. It is well-known that if G is a partial cube, then the Θ^*-partition has the required property.

Suppose now that G is an arbitrary connected graph that admits a partition as stated. Then G is bipartite, cf. [25, Theorem 2]. Indeed, consider a shortest odd cycle C of G. Since $G \setminus F_i$ has two (convex) components, either $|C \cap F_i| = 0$ or $|C \cap F_i| \geq 2$ holds for any i. As C is odd, there exists an index j such that $|C \cap F_j| \geq 3$. But this contradicts the minimality of C.

We now claim that if $e = ab \in F_i$, then the two connected components C' and C'' of $G \setminus F_i$ are induced by the sets W_{ab} and W_{ba}. Clearly, a and b are in different components, hence assume without loss of generality that $a \in C'$ and $b \in C''$. Suppose that $x \in V(G)$, $x \neq a, b$. Since G is bipartite, $d(x, a) \neq d(x, b)$. We may assume without loss of generality that $d(x, a) < d(x, b)$. If $x \in C''$ then a shortest x, a-path together with the edge ab is a shortest x, b-path. But then C'' is not convex. Therefore, $x \in C'$ which in turn implies that $C' = W_{ab}$ and similarly $C'' = W_{ba}$. The proof is complete by recalling Djoković's classical theorem from [7] asserting that a connected graph is a partial cube if and only if it is bipartite and all the subgraphs W_{ab} are convex. $\square$

3 The main result

In this section we prove that the Wiener index of a connected weighted graph can be expressed as the sum of the Wiener indices of weighted quotient graphs with respect to an arbitrary combination of Θ^*-classes.

Let G be a connected graph. In the rest of the paper let

$$\mathcal{F} = \{F_1, \ldots, F_k\}$$

denote the Θ^*-partition of $E(G)$. A partition $\mathcal{E} = \{E_1, \ldots, E_r\}$ of $E(G)$ is *coarser than* $\mathcal{F}$ if each set E_i is the union of one or more Θ^*-classes of G.

Lemma 3.1 *Let G be a connected graph and let $\mathcal{E} = \{E_1, \ldots, E_r\}$ be a partition of $E(G)$ coarser than $\mathcal{F}$. Then every connected component of $G \setminus E_j$, $1 \le j \le r$, induces a convex subgraph of G.*

Proof. Let C be a connected component of $G \setminus E_j$ and suppose it is not convex in G. Then there exists vertices $x, y \in C$ and a shortest x, y-path P, not all of its edges belonging to C. Let e be an edge from $(P \setminus C) \cap E_j$ and assume that e is from the Θ^*-class F_i. Let Q be a x, y-path in C. Since P is a shortest path, e is in relation Θ with no edge on P, hence by [14, Lemma 11.4], e is in relation Θ with an edge f on Q. But this is not possible because then f does not belong to C. $\square$

Lemma 3.2 *Let G be a connected graph and let $\mathcal{E} = \{E_1, \ldots, E_r\}$ be a partition of $E(G)$ coarser than $\mathcal{F}$. Let C and C' be connected components of $G \setminus E_j$ and let $x, y \in V(C)$ and $x', y' \in V(C')$. If P_1 and P_2 are shortest x, x'- and y, y'-paths in G, respectively, then $|E(P_1) \cap E_j| = |E(P_2) \cap E_j|$.*

Proof. From the key lemma of [12] (see [14, Lemma 13.1]) we know that if R is a shortest u, v-path in G and Q is an arbitrary u, v-path in G, then $|E(R) \cap F| \le |E(Q) \cap F|$ holds for any Θ^*-class F. Because E_j is a union of one or more Θ^*-classes it follows that $|E(R) \cap E_j| \le |E(Q) \cap E_j|, 1 \le j \le r$.

Consider now the shortest paths P_1 and P_2. Let in addition Q_1 be an x, x'-path that is a concatenation of a shortest x, y-path in C, the path P_2, and a shortest y', x'-path in C'. Similarly, let Q_2 be a y, y'-path that is a concatenation of a shortest y, x-path in C, the path P_1, and a shortest x', y'-path in C'. By the above, $|E(P_1) \cap E_j| \le |E(Q_1) \cap E_j|$ and $|E(P_2) \cap E_j| \le |E(Q_2) \cap E_j|$. On the other hand, $|E(P_2) \cap E_j| = |E(Q_1) \cap E_j|$ and $|E(P_1) \cap E_j| = |E(Q_2) \cap E_j|$. Therefore, $|E(P_1) \cap E_j| \le |E(Q_1) \cap E_j| = |E(P_2) \cap E_j| \le |E(Q_2) \cap E_j| = |E(P_1) \cap E_j|$ so that the equality holds everywhere. $\square$

Let G be a connected graph and let $F_1, \ldots, F_k$ be a partition of $E(G)$. Then the *quotient graph* G/F_i, $1 \le i \le k$, is defined follows: its vertices are the connected components of $G \setminus F_i$, two vertices C and C' being adjacent if there exist vertices $x \in C$ and $y \in C'$ such that $xy \in F_i$.

We are now ready for the main result of this paper.

Theorem 3.3 *Let (G, w) be a connected, weighted graph, and let $\mathcal{E} = \{E_1, \ldots, E_r\}$ be a partition of $E(G)$ coarser than $\mathcal{F}$. Then*

$$W(G, w) = \sum_{j=1}^{r} W(G/E_j, w_j)\,,$$

where $w_j : V(G/E_j) \to \mathbb{R}^+$ is defined by $w_j(C) = \sum_{x\in C} w(x)$, for all connected components C of $G \setminus E_j$.

Proof. Let C and C' be two vertices of $(G/E_i, w_i)$, that is, connected components of $G \setminus E_j$. Then, by Lemma 3.2, $d_{(G/E_j,w_j)}(C, C') = |E(P) \cap E_j|$, where P is a shortest x, x'-path in G and $x \in C$, $x' \in C'$.

Select shortest paths $Y = \{P_1, P_2, \ldots, P_{\binom{n}{2}}\}$ in G such that for every pair of vertices $u, v \in V(G)$, $u \neq v$, there exists a unique shortest u, v-path in the list. Let $M = [m_{ij}]$ be the $\binom{n}{2} \times r$ matrix with entries $m_{ij} = w(u)w(v)|E(P_i) \cap E_j|$, where u and v are the endvertices of the path P_i.

Since $\sum_{j=1}^{r} |E(P_i) \cap E_j|$ is equal to the distance between the endpoints of P_i, the sum of the entries of the i^{th} row of M equals $w(u)w(v)|E(P_i)|$. Therefore, the sum of all entries of M is equal to $W(G, w)$.

Let $C_{j,1}, \ldots, C_{j,i_j}$ be the connected components of $G \setminus E_j$ and let $|C_{j,t}| = n_{j,t}$. The number of non-zero elements in the j^{th} column of M is equal to the number of shortest path from Y that pass through the edges of E_j. By Lemma 3.1 every component $C_{j,t}$ is convex, hence this number is equal to $\sum_{p=1}^{i_j} \sum_{q=p+1}^{i_j} n_{j,p} n_{j,q}$. Moreover, for any vertex $u \in C_{j,p}$ and any vertex $v \in C_{j,q}$ we have $d_{(G/E_j,w_j)}(C_{j,p}, C_{j,q}) = |E(P_i) \cap E_j|$, where u and v are the endvertices of P_i. Thus the summation of the j^{th} column of M yields

$$\sum_{p,q} w(C_{j,p})w(C_{j,q})d_{(G/E_j,w_j)}(C_{j,p}, C_{j,q})\,.$$

Summing over all columns we thus get:

$$W(G, w) = \sum_{j=1}^{r} \sum_{p,q} w(C_{j,p})w(C_{j,q})d_{(G/E_j,w_j)}(C_{j,p}, C_{j,q}) = \sum_{j=1}^{r} W(G/E_j, w_j)\,,$$

which completes the argument. $\square$

For an example illustrating Theorem 3.3 consider the family of graphs G_n, $n \geq 3$, depicted in Fig. 1. Here n denotes the number of inner faces in one layer, so that the total number of the inner faces of G_n is $2n$.

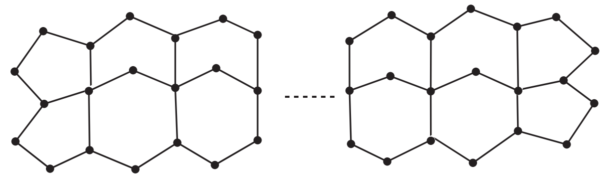

Figure 1: Graphs G_n

G_n has $2(n-2)+1 = 2n-3$ Θ^*-classes. We merge them into classes E_1, E_1', E_2, where E_1 is shown in Fig. 2, E_1' is constructed symmetrically (that is, containing the other horizontal edges of the hexagons), and E_2 is formed by the remaining edges. In other words, E_2 is the Θ^*-class that contains the edges of the pentagons and the vertical edges of the hexagons, see Fig. 3.

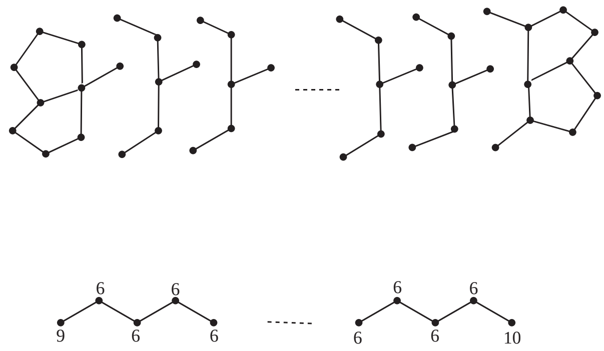

Figure 2: Graphs $G_n \setminus E_1$ and $(G_n/E_1, w)$

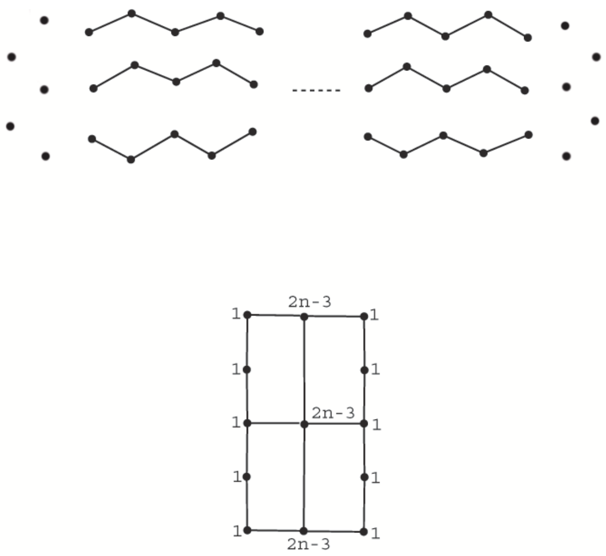

Figure 3: Graphs $G_n \setminus E_2$ and $(G_n/E_2, w)$

Now we have

$$\begin{aligned} W(G_n/E_1, w) &= W(G_n/E_1', w) = 3(n-2)(2n^2+5n-3)\,, \\ W(G_n/E_2, w) &= 16n^2 + 76n - 28\,, \end{aligned}$$

so that

$$W(G_n) = W(G/E_1, w) + W(G/E_1', w) + W(G/E_2, w) = 12n^3 + 22n^2 - 2n + 8\,.$$

4 Concluding remarks

It is also natural to consider *edge-weighted graphs*, that is, pairs (G, w_E), where G is a graph and $w_E : E(G) \to \mathbb{R}^+$. The Wiener index $W(G, w_E)$ of an edge-weighted graph (G, w_E) is defined just as the usual Wiener index, that is, $W(G, w_E) = \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} d(u, v)$, where the distance function is of course computed in (G, w_E). Again, if all the edges have weight 1, then $W(G, w_E) = W(G)$.

With methods analogous to those from Section 3 the following result can be proved:

Theorem 4.1 *Let (G, w_E) be a connected, edge-weighted graph. If $\mathcal{E} = \{E_1, \ldots, E_r\}$ is a partition of $E(G)$ coarser than $\mathcal{F}$ such that for any $j = 1, \ldots, r$, the edges from E_j have the same weight, $w(E_j)$, then*

$$W(G, w_E) = \sum_{j=1}^{r} w(E_j)W(G/E_j, w_j)\,.$$

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