Some Distance-Based Topological Indices of Partial Cubes

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The Wiener index

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The **Wiener index** of a connected graph G is defined as

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

Its history goes back to 1947, when H. Wiener used the distances in the molecular graphs of alkanes to calculate their boiling points.

The Wiener index of a vertex-weighted graph

The Wiener index of (G, w) is defined as

$$W(G,w) = \sum_{\{u,v\} \subseteq V(G)} w(u)w(v)d_G(u,v).$$

The Szeged index

Let G be a connected graph and $e = uv$ an edge of G. We will use the following notation:

$$N_1(e|G) = \{x \in V(G) \mid d_G(x,u) < d_G(x,v)\},$$

$$N_2(e|G) = \{x \in V(G) \mid d_G(x,v) < d_G(x,u)\}.$$

I. Gutman; 1994

The **Szeged index** of a connected graph G is defined as

$$Sz(G) = Sz_v(G) = \sum_{e \in E(G)} |N_1(e|G)| \cdot |N_2(e|G)|.$$

The Szeged index of a weighted graph

The Szeged index of a vertex-edge-weighted graph

$$Sz(G, w, w') = \sum_{e \in E(G)} w'(e) n_1(e|G) n_2(e|G),$$

where for $i = 1, 2$,

$$n_i(e|G) = \sum_{x \in N_i(e|G)} w(x).$$

Hypercubes

Hypercube

The **hypercube** Q_n of dimension n is defined in the following way: all vertices of Q_n are binary strings of length n and two vertices of Q_n are adjacent if the corresponding strings differ in precisely one position.

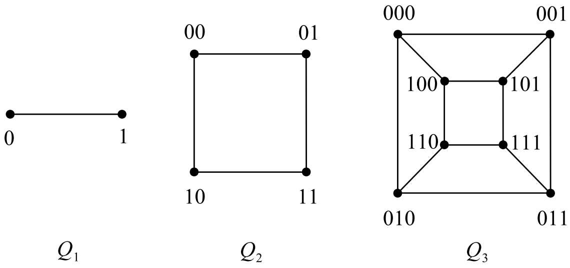

Figure: Hypercubes.

Partial cubes

Definition

A subgraph H of G is called an **isometric subgraph** if for each $u, v \in V(H)$ it holds $d_H(u, v) = d_G(u, v)$. Any isometric subgraph of a hypercube is called a **partial cube**.

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Partial cubes constitute a large class of graphs with a lot of applications and includes, for example, many families of chemical graphs (benzenoid systems, trees, phenylenes, cyclic phenylenes, polyphenyles).

Relation Θ

Definition

Two edges $e_1 = u_1v_1$ and $e_2 = u_2v_2$ of graph G are in relation Θ, $e_1 \Theta e_2$, if

$$d_G(u_1, u_2) + d_G(v_1, v_2) \neq d_G(u_1, v_2) + d_G(v_1, u_2).$$

Note that this relation is also known as Djoković-Winkler relation.

The relation Θ is reflexive and symmetric, but not necessarily transitive. We denote its transitive closure (i.e. the smallest transitive relation containing Θ) by Θ^*.

Relation Θ and partial cubes

Well known facts:

A connected graph G is a partial cube if and only if G is bipartite and $\Theta = \Theta^*$.

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Let E be a Θ-class of a partial cube G. Then $G - E$ has exactly two connected components, i.e. $\langle N_1(e|G) \rangle$ and $\langle N_2(e|G) \rangle$ where $e \in E$.

Example: benzenoid systems

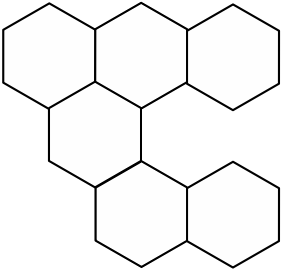

Figure: A benzenoid system.

Example: benzenoid systems

An **elementary cut** of a benzenoid system is a line segment that starts at the center of a boundary edge of a benzenoid system, goes orthogonal to it and ends at the first next boundary edge. Obviously, an elementary cut coincides with a Θ-class.

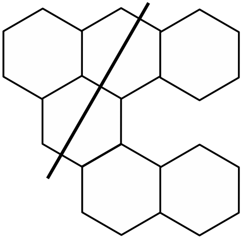

Figure: A benzenoid system with an elementary cut (Θ-class).

Example: C_4C_8 systems

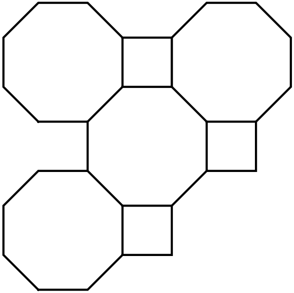

Figure: A C_4C_8 system.

Coarser partition

Let $\mathcal{E} = \{E_1, \ldots, E_r\}$ be the Θ^*-partition of the set $E(G)$. Then we say that a partition $\{F_1, \ldots, F_k\}$ of $E(G)$ is **coarser** than $\mathcal{E}$ if each set F_i is the union of one or more Θ^*-classes of G.

Example

- The edge set of a benzenoid system can be naturally partitioned into sets F_1, F_2, and F_3 of edges of the same direction. Obviously, $\{F_1, F_2, F_3\}$ is a partition coarser than Θ-partition.

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- The edge set of a C_4C_8 system can be naturally partitioned into sets F_1, F_2, F_3, and F_4 of edges of the same direction. Obviously, $\{F_1, F_2, F_3, F_4\}$ is a partition coarser than Θ-partition.

Quotient graphs

Definition

Suppose G is a connected graph and $F \subseteq E(G)$. The **quotient graph** G/F is a graph whose vertices are connected components of the graph $G - F$, such that two components C_1 and C_2 are adjacent in G/F if some vertex in C_1 is adjacent to a vertex of C_2 in G.

Example: benzenoid systems

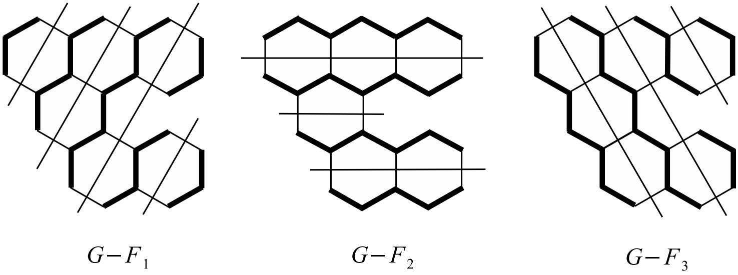
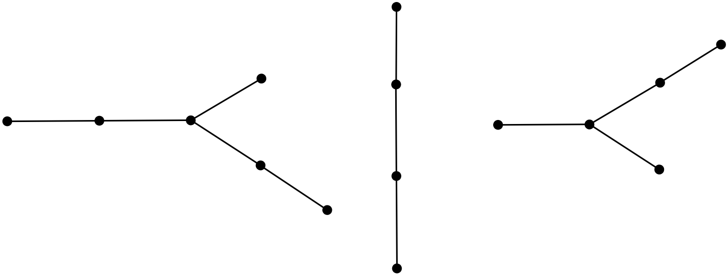


Figure: Graphs $G-F_1$, $G-F_2$, and $G-F_3$.

Example: benzenoid systems

The quotient graphs $G/F_1 = T_1$, $G/F_2 = T_2$, and $G/F_3 = T_3$ are trees.



T_1 T_2 T_3

Figure: Quotient trees T_1, T_2 and T_3.

Example: C_4C_8 systems

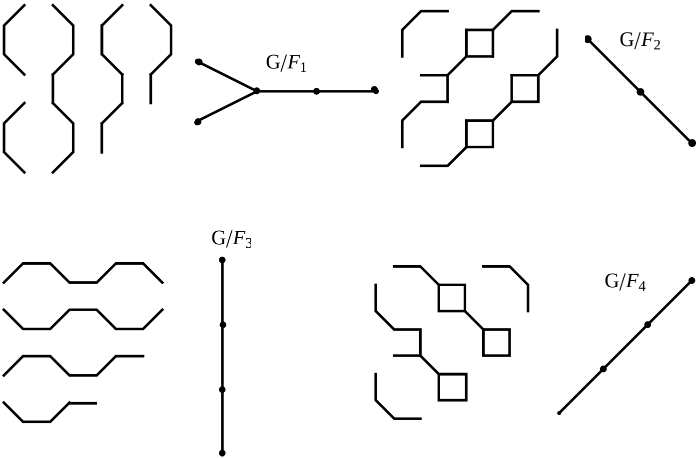


Figure: Quotient trees.

Weighted quotient graphs

Let $\{F_1, \ldots, F_k\}$ be a partition coarser than the Θ^*-partition. We define:

1. for $x \in V(G/F_i)$, let $w_i(x)$ be the number of vertices in the connected component x of $G - F_i$,
2. for $xy \in E(G/F_i)$, let $w_i'(xy)$ be the number of edges in F_i with one end-point in x and another in y.

Example: C_4C_8 systems

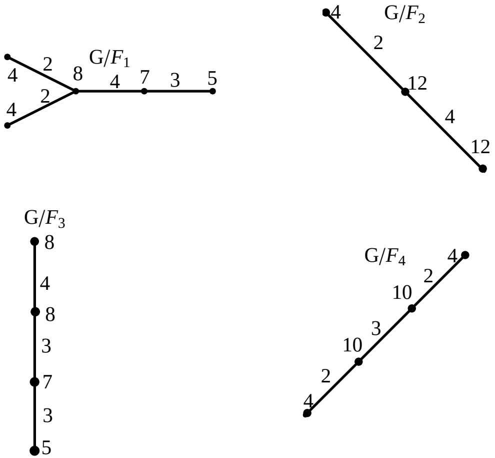


Figure: Weighted quotient trees.

The Wiener index

Theorem (S. Klavžar, M. J. Nadjafi-Arani; 2014)

Let G be a connected graph. If $\{F_1, \ldots, F_k\}$ is a partition coarser than the Θ^*-partition, then

$$W(G) = \sum_{i=1}^{k} W(G/F_i, w_i).$$

The Szeged index of partial cubes

Lemma (M. Črepnjak, N. Tratnik; 2017)

Let G be a partial cube. If $\{F_1, \ldots, F_k\}$ is a partition coarser than the Θ-partition, then G/F_i is a partial cube for each i, $1 \leq i \leq k$.

The Szeged index of partial cubes

Lemma (M. Črepnjak, N. Tratnik; 2017)

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Theorem (M. Črepnjak, N. Tratnik; 2017)

Let G be a partial cube. If $\{F_1, \ldots, F_k\}$ is a partition coarser than the Θ-partition, then

$$Sz(G) = \sum_{i=1}^{k} Sz(G/F_i, w_i, w_i').$$

The cut method on benzenoid systems

Theorem (V. Chepoi, S. Klavžar; 1997)

If G is a benzenoid system, then

$$W(G) = W(T_1, w_1) + W(T_2, w_2) + W(T_3, w_3),$$

$$Sz(G) = Sz(T_1, w_1, w_1') + Sz(T_2, w_2, w_2') + Sz(T_3, w_3, w_3'),$$

The cut method for other indices

Theorem (A. Kelenc, S. Klavžar, N. Tratnik; 2015)

If G is a benzenoid system, then

$$\widehat{W}_e(G) = \sum_{i=1}^{3} \left(\widehat{W}_e(T_i, w_i') + W_v(T_i, w_i) + W_{ve}(T_i, w_i, w_i') \right).$$

Theorem (N. Tratnik; 2017)

If G is a benzenoid system, then

$$\begin{aligned} Sz_e(G) &= \sum_{i=1}^{3} \left(Sz_v(T_i, w_i, w_i') + Sz_e(T_i, w_i') + Sz_{ve}(T_i, w_i, w_i') \right), \\ PI(G) &= \sum_{i=1}^{3} \left(PI_e(T_i, w_i') + PI_v(T_i, w_i, w_i') \right). \end{aligned}$$

The edge-hyper-Wiener index

Definition (M. Randić; 1993 and Iranmanesh et. al.; 2011)

The **hyper-Wiener index** and the **edge-hyper-Wiener index** of G are defined as:

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d_G(u,v) + \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)^2,$$

$$WW_e(G) = \frac{1}{2} \sum_{\{e,f\} \subseteq E(G)} d_G(e,f) + \frac{1}{2} \sum_{\{e,f\} \subseteq E(G)} d_G(e,f)^2.$$

A cut method for the hyper-Wiener index of partial cubes was developed by S. Klavžar in 2000.

Additional notation

If G is a partial cube with Θ-classes $E_1, \ldots, E_d$, we denote by U_k and U_k' the connected components of the graph $G - E_k$. For any $k \neq l$ set

$$\begin{aligned} m_{kl}^{11} &= |E(U_k) \cap E(U_l)|, \\ m_{kl}^{10} &= |E(U_k) \cap E(U_l')|, \\ m_{kl}^{01} &= |E(U_k') \cap E(U_l)|, \\ m_{kl}^{00} &= |E(U_k') \cap E(U_l')|. \end{aligned}$$

The cut method for the edge-hyper-Wiener index

Theorem (N. Tratnik; 2018)

Let G be a partial cube and let d be the number of its Θ-classes. Then

$$WW_e(G) = 2W_e(G) + \sum_{k=1}^{d-1} \sum_{l=k+1}^{d} \left(m_{kl}^{11} m_{kl}^{00} + m_{kl}^{10} m_{kl}^{01} \right) - \binom{|E(G)|}{2}.$$

Benzenoid systems

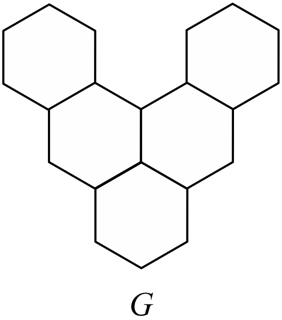

Figure: Benzenoid system G.

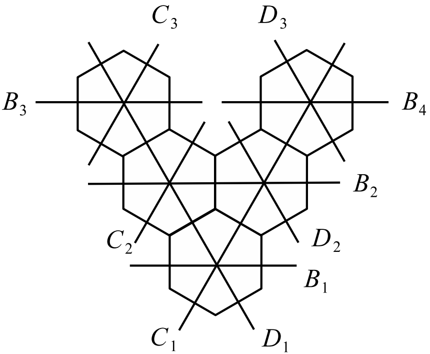

Figure: Elementary cuts of G.

Table: Contributions of pairs of elementary cuts.

Pair	$f(\cdot,\cdot)$	Pair	$f(\cdot,\cdot)$	Pair	$f(\cdot,\cdot)$	Pair	$f(\cdot,\cdot)$
B_1, B_2	28	B_1, C_3	4	B_4, C_2	14	C_2, D_1	40
B_1, B_3	4	B_2, C_1	36	B_4, C_3	4	C_2, D_2	49
B_1, B_4	4	B_2, C_2	42	C_1, C_2	42	C_2, D_3	14
B_2, B_3	16	B_2, C_3	16	C_1, C_3	12	C_3, D_1	14
B_2, B_4	16	B_3, C_1	12	C_2, C_3	32	C_3, D_2	14
B_3, B_4	4	B_3, C_2	32	C_1, D_1	25	C_3, D_3	4
B_1, C_1	14	B_3, C_3	20	C_1, D_2	40		
B_1, C_2	14	B_4, C_1	5	C_1, D_3	14		

$$WW_e(G) = 2 \cdot 1026 + 884 - 300 = 2636$$

The Steiner distance

Definition (Chartrand et. al.; 1989)

For a connected graph G and an non-empty set $S \subseteq V(G)$, the **Steiner distance** among the vertices of S, denoted by $d_G(S)$ or simply by $d(S)$, is the minimum size among all connected subgraphs whose vertex sets contain S.

Note that if H is a connected subgraph of G such that $S \subseteq V(H)$ and $|E(H)| = d(S)$, then H is a tree.

The Steiner k-Wiener index

Definition (X. Li, Y. Mao, I. Gutman; 2016)

Let G be a connected graph and k a positive integer such that $k \leq |V(G)|$. The **Steiner k-Wiener index** of G, denoted by $SW_k(G)$, is defined as

$$SW_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} d(S).$$

The Steiner k-hyper Wiener index

Definition

Let G be a connected graph and k a positive integer such that $k \leq |V(G)|$. The **Steiner k-hyper-Wiener index** of G, denoted by $SWW_k(G)$, is defined as

$$SWW_k(G) = \frac{1}{2} \sum_{\substack{S \subseteq V(G) \\ |S| = k}} d(S) + \frac{1}{2} \sum_{\substack{S \subseteq V(G) \\ |S| = k}} d(S)^2.$$

Modular graphs

A **median** of a triple of vertices u, v, w of G is a vertex m that lies on a shortest u, v-path, on a shortest u, w-path, and on a shortest v, w-path. A graph is a **median graph** if every triple of its vertices has a unique median. Moreover, a graph is called a **modular graph** if every triple of vertices has at least one median.

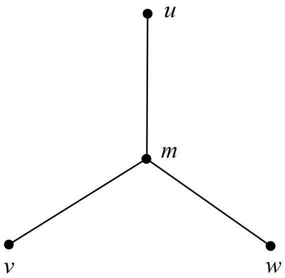

Figure: A median for u, v, w.

Lemma

Let G be a connected graph with at least three vertices. Three distinct vertices u, v, w have at least one median if and only if for the set $S = \{u, v, w\}$ it holds

$$2d(S) = d(u, v) + d(u, w) + d(v, w).$$

Theorem (M. Kovše)

Let G be a modular graph with at least three vertices. Then

$$SW_3(G) = \frac{|V(G)| - 2}{2} W(G).$$

The Steiner 3-hyper Wiener index of a modular graph

Theorem (N. Tratnik; 2018)

Let G be a modular graph with at least three vertices. Then

$$SWW_3(G) = \frac{|V(G)|-2}{4}W(G)+\frac{|V(G)|-2}{8}\overline{WW}(G)+\frac{1}{8}\widehat{WW}(G).$$

In the above theorem,

$$\overline{WW}(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v)^2,$$

$$\widehat{WW}(G) = \sum_{(u,v,w)\in O_3(G)} d(u,v)d(u,w),$$

where

$$O_3(G) = \{(u,v,w) \in V(G)^3 \mid u \neq v, u \neq w, v \neq w\}.$$

Additional notation

Let G be a partial cube with Θ-classes $E_1, \ldots, E_d$ and denote by U_i and U_i' the connected components of the graph $G - E_i$. For $i \neq j$, set

$$\begin{aligned} n_{ij}^{00} &= |V(U_i) \cap V(U_j)|, \\ n_{ij}^{01} &= |V(U_i) \cap V(U_j')|, \\ n_{ij}^{10} &= |V(U_i') \cap V(U_j)|, \\ n_{ij}^{11} &= |V(U_i') \cap V(U_j')|. \end{aligned}$$

Also, for $i \in \{1, \ldots, d\}$ let

$$n_i^0 = |V(U_i)|, \quad n_i^1 = |V(U_i')|.$$

Proposition (S. Klavžar, I. Gutman, B. Mohar; 1995)

Let G be a partial cube and let d be the number of its Θ-classes. Then

$$W(G) = \sum_{i=1}^{d} n_i^0 n_i^1 .$$

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Proposition (S. Klavžar; 2000)

Let G be a partial cube and let d be the number of its Θ-classes. Then

$$\overline{WW}(G) = \sum_{i=1}^{d} n_i^0 n_i^1 + 2 \sum_{i=1}^{d-1} \sum_{j=i+1}^{d} \left(n_{ij}^{00} n_{ij}^{11} + n_{ij}^{01} n_{ij}^{10} \right) .$$

Theorem (N. Tratnik; 2018)

Let G be a partial cube with at least three vertices and let d be the number of its Θ-classes. Then

$$
\begin{aligned}
\widehat{WW}(G) &= \sum_{i=1}^{d}\left(n_i^0 n_i^1 (n_i^1 - 1) + n_i^1 n_i^0 (n_i^0 - 1)\right)\\
&+ 2\sum_{i=1}^{d-1}\sum_{j=i+1}^{d}\Bigg(3n_{ij}^{00} n_{ij}^{01} n_{ij}^{10} + 3n_{ij}^{00} n_{ij}^{01} n_{ij}^{11}\\
&+ 3n_{ij}^{00} n_{ij}^{10} n_{ij}^{11} + 3n_{ij}^{01} n_{ij}^{10} n_{ij}^{11}\\
&+ n_{ij}^{00} n_{ij}^{11} (n_{ij}^{11} - 1) + n_{ij}^{01} n_{ij}^{10} (n_{ij}^{10} - 1)\\
&+ n_{ij}^{10} n_{ij}^{01} (n_{ij}^{01} - 1) + n_{ij}^{11} n_{ij}^{00} (n_{ij}^{00} - 1)\Bigg).
\end{aligned}
$$

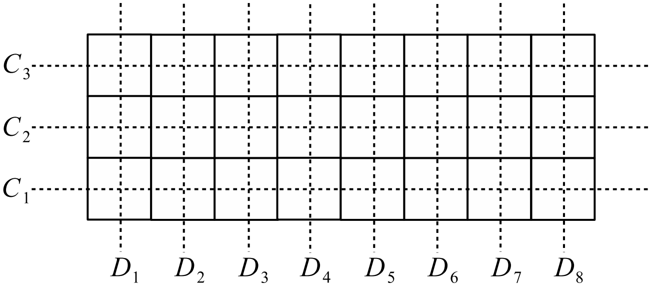

Figure: Grid graph $G_{9,4}$ with all the elementary cuts.

Theorem (N. Tratnik; 2018)

Let $G_{m,n}$ be a grid graph such that $m, n \geq 3$. Then

$$\begin{aligned} SWW_3(G_{m,n}) &= \frac{1}{360}\big(9m^5n^3 + 15m^4n^4 + 9m^3n^5 + 15m^4n^3 \\ &+ 15m^3n^4 - 30m^4n^2 - 50m^3n^3 - 30m^2n^4 \\ &+ 26m^3n - 45m^3n^2 - 45m^2n^3 + 45m^2n^2 \\ &+ 26mn^3 + 30m^2n + 30mn^2 - 20mn\big). \end{aligned}$$

Moreover, for any $n \geq 3$ it holds

$$SWW_3(G_{2,n}) = \frac{1}{15}\big(3n^5 + 10n^4 - 25n^2 + 12n\big).$$

THANK YOU!

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