MODIFIED ZAGREB INDICES OF BRIDGE GRAPHS

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Definitions

- For a graph $G = (V(G), E(G))$, the first and the second Zagreb indices are defined as $M_1(G) = \sum_{v \in V(G)} (d(v))^2$ and $M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$ respectively, where $d(v)$ denotes the degree of the vertex v in G.

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- The first and the second modified Zagreb index were defined as ${}^mM_1(G) = \sum_{v \in V(G)} \frac{1}{(d(v))^2}$ and ${}^mM_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}$ respectively, where $d(v)$ is the degree of the vertex v in G.

Bridge Graph B_1

Let $\{G_i\}_{i=1}^{k}$ be a set of finite pairwise disjoint graphs with distinct vertices $u_i, v_i \in V(G_i)$ such that u_i and v_i are not adjacent in G_i. The bridge graph $B_1 = B_1(G_1, G_2, ..., G_k; u_1, v_1, u_2, v_2, u_3, v_3, ..., u_k, v_k)$ of $\{G_i\}_{i=1}^{k}$ with respect to the vertices $\{u_i, v_i\}_{i=1}^{k}$ is the graph obtained from the graphs $G_1, G_2, ..., G_k$ by connecting the vertices v_i and u_{i+1} by an edge for all $i = 1, 2, ..., k-1$ as shown in the following Figure.

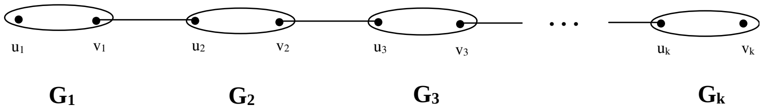

Figure: The bridge graph $B_1 = B_1(G_1, G_2, ..., G_k; u_1, v_1, u_2, v_2, ..., u_k, v_k)$

Bridge Graph B_2

Let $\{G_i\}_{i=1}^{k}$ be a set of finite pairwise disjoint graphs with vertices $v_i \in V(G_i)$. The bridge graph $B_2 = B_2(G_1, G_2, ..., G_k; v_1, v_2, v_3, ..., v_k)$ of $\{G_i\}_{i=1}^{k}$ with respect to the vertices $\{v_i\}_{i=1}^{k}$ is the graph obtained from the graphs $G_1, G_2, ..., G_k$ by connecting the vertices v_i and v_{i+1} by an edge for all $i = 1, 2, ..., k-1$ as shown in the following Figure.

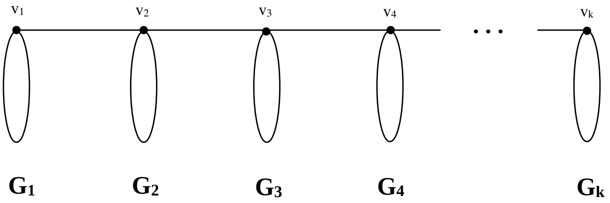

Figure: $B_2 = B_2(G_1, G_2, ..., G_k; v_1, v_2, v_3, ..., v_k)$

Modified Zagreb Indices of Bridge Graph B_1

Theorem

The first modified Zagreb index of the bridge graph $B_1, k \geq 2$ is given by

$$ {}^{m}M_1(B_1) = \sum_{i=1}^{k}({}^{m}M_1(G_i)) - \Bigg\{ \sum_{i=1,k} \frac{2d(u_i)+1}{d(u_i)^2(d(u_i)+1)^2} + 4\sum_{i=2}^{k-1}\Bigg\{ \frac{d(u_i)+1}{d(u_i)^2(d(u_i)+2)^2} + \frac{d(v_i)+1}{d(v_i)^2(d(v_i)+2)^2} \Bigg\} \Bigg\} $$

Proof.

Using the definition of first modified Zagreb index, we have

$$
\begin{aligned}
{}^{m}M_1(B_1) &= \sum_{i=1}^{k}({}^{m}M_1(G_i)) - \sum_{i=1}^{k-1}\frac{1}{d(v_i)^2} - \sum_{i=2}^{k}\frac{1}{d(u_i)^2} + \sum_{i=2}^{k-1}\frac{1}{(d(v_i)+2)^2} \\
&\quad + \sum_{i=2}^{k-1}\frac{1}{(d(u_i)+2)^2} + \frac{1}{(d(v_1)+1)^2} + \frac{1}{(d(u_k)+1)^2} \\
&= \sum_{i=1}^{k}({}^{m}M_1(G_i)) - \Bigg\{\frac{2d(v_1)+1}{d(v_1)^2(d(v_1)+1)^2} + \frac{2d(u_k)+1}{d(u_k)^2(d(u_k)+1)^2} \\
&\quad + 4\sum_{i=2}^{k-1}\Bigg\{\frac{d(u_i)+1}{d(u_i)^2(d(u_i)+2)^2} + \frac{d(v_i)+1}{d(v_i)^2(d(v_i)+2)^2}\Bigg\}\Bigg\}
\end{aligned}
$$

∎

Corollary

If $G_i = G$ *for all* $i = 1, 2, ..., k$ *and* $u, v \in V(G)$*, then*

$$
{}^{m}M_1(B_1) = k\,{}^{m}M_1(G) - \left\{ \frac{2d(u)+1}{d(u)^2(d(u)+1)^2} + \frac{2d(v)+1}{d(v)^2(d(v)+1)^2} \right. \\
\left. + 4(k-2)\left\{ \frac{d(u)+1}{d(u)^2(d(u)+2)^2} + \frac{d(v)+1}{d(v)^2(d(v)+2)^2} \right\} \right\}
$$

Theorem

The second modified Zagreb index of the bridge graph $B_1, k \geq 2$ is given by

$$
{}^{m}M_2(B_1) = \sum_{i=1}^{k} ({}^{m}M_2(G_i)) - \left\{ \sum_{i=1}^{k-1} \sum_{w \in N(v_i)} \frac{1}{d(v_i)[d(v_i)+1]d(w)} + \sum_{i=2}^{k} \sum_{w \in N(u_i)} \frac{1}{d(u_i)[d(u_i)+1]d(w)} - \sum_{i=1}^{k-1} \frac{1}{[d(v_i)+1][d(u_{i+1})+1]} \right\}
$$

Proof.

By the definition of second modified Zagreb index, ${}^mM_2(B_2)$ is equal to the sum of $\dfrac{1}{d_{B_2}(x)d_{B_2}(y)}$, where the summation is taken over all edges $xy \in E(B_2)$. From the definition of the bridge graph B_1, $E(B_1) = E(G_1) \cup E(G_2) \cup \ldots \cup E(G_k) \cup \{v_i u_{i+1}; 1 \leq i \leq k-1\}$. In order to compute ${}^mM_2(B_1)$, we partition our sum into four sums as follows.

The first sum S_1 is taken over all edges $xy \in E(G_1)$.

$$S_1 =^m M_2(G_1) - \sum_{w \in N(v_1)} \frac{1}{d(v_1)(d(v_1)+1)d(w)}$$

The second sum S_2 is taken over all edges $xy \in E(G_k)$.

$$S_2 =^m M_2(G_1) - \sum_{w \in N(u_k)} \frac{1}{d(u_k)(d(u_k)+1)d(w)}$$

The third sum S_3 is taken over all edges $xy \in E(G_i)$ for all $i = 2, 3, ..., k-1$.

$$S_3 = \sum_{i=2}^{k-1}({}^{m}M_2(G_i)) - \sum_{i=2}^{k-1}\left\{ \sum_{w \in N(u_i)} \frac{1}{d(u_i)(d(u_i)+1)d(w)} + \sum_{w \in N(v_i)} \frac{1}{d(v_i)(d(v_i)+1)d(w)} \right\}$$

The last sum S_4 is taken over all edges $v_i u_{i+1}$ for all $i = 1, 2, ..., k-1$.

$$S_4 = \sum_{i=1}^{k-1} \frac{1}{(d(v_i)+1)(d(u_{i+1}+1)}$$

Now ${}^{m}M_2(B_1)$ is obtained by adding S_1, S_2, S_3, S_4.

Corollary

If $G_i = G$ *for all* $i = 1, 2, ..., k$ *and* $u, v \in V(G)$, *then*

$$
{}^{m}M_2(B_1) = k({}^{m}M_2(G)) - (k-1)\left\{ \sum_{w \in N(u)} \frac{1}{[d(u)][d(u)+1]d(w)} + \sum_{w \in N(v)} \frac{1}{[d(v)][d(v)+1]d(w)} - \frac{1}{[d(u)+1][d(v)+1]} \right\}
$$

Modified Zagreb Indices of Bridge Graph B_2

Theorem

The first modified Zagreb index of the bridge graph $B_2, k \geq 2$ is given by

$$^{m}M_1(B_2) = \sum_{i=1}^{k} H(G_i) - \left\{ \sum_{i=1}^{k} \frac{1}{[d(v_i)^2]} + \sum_{i=2}^{k-1} \frac{1}{[d(v_i)+2]^2} + \sum_{i=1,k} \frac{1}{[d(v_i)\ \cdots}\right.$$

Using the definition of first modified Zagreb index, we get the result.

Corollary

If $G_i = G$ for all $i = 1, 2, ..., k$ and $u, v \in V(G)$, then

$$^{m}M_1(B_2) = k^{m}M_1(G) - \left\{ \frac{k}{[d(v)^2]} + \frac{k-2}{[d(v)+2]^2} + \frac{2}{[d(v)+1]^2} \right\}$$

Theorem

The second modified Zagreb index of the bridge graph $B_2, k \geq 2$ is given by

$$
\begin{aligned}
{}^mM_2(B_2) = \sum_{i=1}^{k}({}^mM_2(G_i)) - \Bigg\{ \sum_{i=1,k} \sum_{w \in N(v_i)} \frac{1}{d(v_i)(d(v_i)+1)d(w)} \\
+ \sum_{i=2}^{k-1} \sum_{w \in N(v_i)} \frac{1}{d(v_i)(d(v_i)+2)d(w)} - \frac{1}{(d(v_i)+1)(d(v_i)+2)} \\
- \sum_{i=2}^{k-1} \frac{1}{(d(v_i)+2)(d(v_{i+1})+2)} - \frac{1}{(d(v_{k-1})+2)(d(v_k)+1)} \Bigg\}
\end{aligned}
$$

Proof.

By the definition of second modified Zagreb index, ${}^mM_2(B_2)$ is equal to the sum of $\dfrac{2}{d_{B_2}(x)d_{B_2}(y)}$, where the summation is taken over all edges $xy \in E(B_2)$. From the definition of the bridge graph B_2, $E(B_2) = E(G_1) \cup E(G_2) \cup \ldots \cup E(G_k) \cup \{v_i u_{i+1}; 1 \leq i \leq k-1\}$. In order to compute ${}^mM_2(B_2)$, we partition our sum into four sums as follows.

The first sum S_1 is taken over all edges $xy \in E(G_1)$.

$$S_1 =^m M_2(G_1) - \sum_{w \in N(v_1)} \frac{1}{d(v_1)(d(v_1)+1)d(w)}$$

The second sum S_2 is taken over all edges $xy \in E(G_k)$.

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The third sum S_3 is taken over all edges $xy \in E(G_i)$ for all $i = 2, 3, ..., k-1$.

$$S_3 = \sum_{i=2}^{k-1} ({}^{m}M_2(G_i)) - \sum_{i=2}^{k-1} \left\{ \sum_{w \in N(v_i)} \frac{2}{d(v_i)(d(v_i)+2)d(w)} \right\}$$

The last sum S_4 is taken over all edges $v_i u_{i+1}$ for all $i = 1, 2, ..., k-1$.

$$S_4 = \frac{1}{(d(v_1)+1)(d(v_2)+2)} + \frac{1}{(d(v_{k-1})+2)(d(v_k)+1)} + \sum_{i=1}^{k-2} \frac{1}{(d(v_i)+2)(d(v_{i+1})+2)}$$

Now ${}^{m}M_2(B_2)$ is obtained by adding S_1, S_2, S_3, S_4.

Corollary

If $G_i = G$ *for all* $i = 1, 2, ..., k$ *and* $u, v \in V(G)$*, then*

$$^{m}M_2(B_2) = k(^{m}M_2(G)) - \Bigg\{ 2 \sum_{w \in N(v)} \frac{1}{d(v)(d(v)+1)d(w)} + (k-2) \sum_{w \in N(v)} \frac{1}{d(v)(d(v)+2)d(w)} - \frac{1}{(d(v)+2)} \left[\frac{k-2}{(d(v)+2)} + \frac{2}{d(v)+1} \right] \Bigg\}$$

Polyphenyl Chains O_h, M_h and L_h

Two vertices u and v of a hexagon H are said to be in ortho-position if they are adjacent in H. If two vertices u and v are at distance two, they are said to be in meta-position and if two vertices u and v are at distance three, they are said to be in para-position. Examples of vertices in the above three types of positions are shown in figure 3.

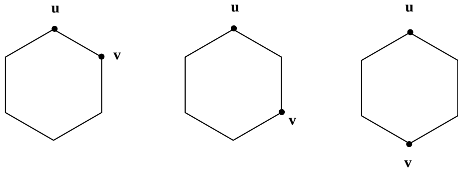

Figure: Ortho-, meta- and para-positions of vertices in hexagon

An internal hexagon H in a polyphenyl chain is said to be an ortho-hexagon, mete-hexagon and para-hexagon, respectively if two vertices of H incident with two edges which connect other two hexagons are in ortho-, meta- and para-position. A polyphenyl chain of h hexagons is $ortho - PPC_h$, denoted by O_h, if all its internal hexagons are ortho-hexagons. Similarly we define $meta - PPC_h$ (denoted by M_h) and $para - PPC_h$ (denoted by L_h), (see figure 4).

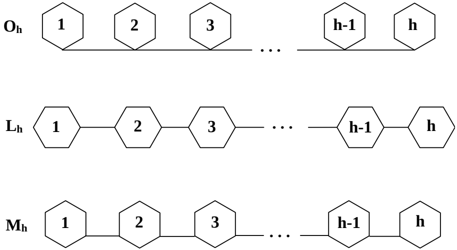

Figure: Ortho-, para- and meta-polyphenyl chanins with h hexagons

The polyphenyl chains M_h and L_h can be viewed as the bridge graphs $B_1(C_6, C_6, ..., C_6; u, v, u, v, ..., u, v)$ (h times) where C_6 is the cycle on six vertices and u and v are the vertices shown in figure 3. Since ${}^mM_1(C_6) = {}^m M_2(C_6) = 3/2$, using corollaries 1 and 2 we obtain

$$
\begin{aligned}
{}^mM_1(M_h) = {}^m M_1(L_h) &= \frac{69h + 22}{48} \\
{}^mM_2(M_h) = {}^m M_2(L_h) &= \frac{23h + 4}{18}
\end{aligned}
$$

The polyphenyl chains O_h can be viewed as the bridge graph $B_2(C_6, C_6, ..., C_6; v, v, ..., v)$($h$ times). Using corollaries 3 and 4,

$$
\begin{aligned}
{}^mM_1(O_h) &= \frac{189h + 14}{144} \\
{}^mM_2(O_h) &= \frac{75h - 2}{48}
\end{aligned}
$$

- Azari M, Iranmanesh A, Gutman I, Zagreb Indices of Bridge and Chain Graphs, MATCH Commun. Math. Comput. Chem.70(2013) 921-938.
- Balakrishnan R, Ranganathan K, A Textbook of Graph Theory(second edition), Springer-Verlog, New York, 2012.
- Ghorbani M, Hosseinzadeh M.A, A note on Zagreb indices of nanostar dendrimers, Optoelectron.Adv. Mater., 4 (2010) 1887-1880.
- Ghorbani M, Hosseinzadeh M.A, A new version of Zagreb indices, Filomat, 26 (2012) 93-100.
- Gutman I, Ruščić B, Trinajstić N, Wilcox C F, Graph theory and molecular orbitals. XII. Acyclic polyenes, J. Chem. Phys. 62 (1975) 3399-3405.

- Gutman I, Trinajstić N, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535-538.
- Gutman I, Das K C, The first Zagreb index 30 years after, MATCH Commun. Math. Comput. Chem. 50 (2004) 83-92.
- Hao J, Theorems about Zagreb indices and modified Zagreb indices, MATCH Commun. Math. Comput. Chem. 65 (2011) 659-670.
- Hao J, The modified Zagreb Indices of Nanotubes and Dendrimer Nanostars, Journal of Computational and Theoretical Nanoscience, Vol 9, (2012) 727-730.
- Li X, Yang X, Wang G, Hu R, The vertex PI and Szeged indices of chain graphs, MATCH Commun. Math. Comput. Chem.68(2012) 349-356.

- Li X, Yang X, Wang G, Hu R, The vertex PI and Szeged indices of chain graphs, MATCH Commun. Math. Comput. Chem.68(2012) 349-356.
- Mansour T, Schork M, Wiener, hyper-Wiener, detour and hyper-detour indices of bridge and chain graphs, J. Math. Chem. 581(2009) 59-69.
- Milicevic A, Nikolic S, On variable Zagreb indices, Croat. Chem. Acta 77 (2004) 97101.
- Nikolić S, Kovačević G, Milićević A, Trinajstić N, The Zagreb indices 30 years after, Croat, Chem. Acta 76 (2003) 113-124.
- Vukicevic D, Trinajstic N, Modified Zagreb M2 index comparison with the Randic connectivity index for benzenoid systems, Croat. Chem. Acta 76 (2003).

- Zhang S, Wang W, Cheng T. C. E, Bicyclic graphs with the first three smallest and largest values of the first general Zagreb index, MATCH Commun. Math. Comput. Chem. 56 (2006) 579-592.
- Zhang H, Zhang S, Unicyclic graphs with the first three smallest and largest first general first Zagreb index, MATCH. Commun. Math. Comput. Chem. 55 (2006) 427-438.

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