



Combinatorics

On the edge Szeged index of bridge graphs

Sur l'indice de Szeged d'arête de graphes pontés

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ABSTRACT

In this Note, we introduce a formula for the edge Szeged index of bridge graphs. Using this formula, the edge Szeged indices of several graphs are computed.

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RÉSUMÉ

Nous présentons une formule pour l'indice de Szeged pour les arêtes de graphes pontés. Nous calculons également, grâce à cette formule, les indices de Szeged d'arête de plusieurs graphes.

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1. Introduction and preliminaries

Topological indices are numerical graph invariants that quantitatively characterize molecular structure. The Wiener index is one of the oldest topological indices [13,15]. The Szeged index is closely related to the Wiener index.

We consider simple graphs. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, denote by $d_G(u, v)$ or $d(u, v)$ the distance between vertices u and v in G , i.e., the length of a shortest path in G connecting u and v . If e is an edge of G connecting vertices u and v , then we write $e = uv$ or $e = vu$. For $e = uv \in E(G)$, let $n_u(e|G)$ and $n_v(e|G)$ be respectively the number of vertices of G lying closer to vertex u than to vertex v and the number of vertices of G lying closer to vertex v than to vertex u , i.e.,

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

and

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

The Szeged index of G , proposed by Gutman [3], is defined as

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e|G)n_v(e|G).$$

If G is a tree, then $Sz(G)$ is equal to the Wiener index of G [15]. The Szeged index is a graph invariant that has been extensively studied, see, e.g., [2,5–7,9,12,16,17].

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For $w \in V(G)$ and $e = uv \in E(G)$, the distance between vertex w and edge e is defined as the minimum of the distances between w and the ends of e , i.e., $d_G(w, e) = d(w, e) = \min\{d_G(w, u), d_G(w, v)\}$. For $e = uv \in E(G)$, let

$$m_u(e|G) = |\{f \in E(G) \mid d_G(u, f) < d_G(v, f)\}|$$

and

$$m_v(e|G) = |\{f \in E(G) \mid d_G(v, f) < d_G(u, f)\}|.$$

The edge Szeged index of G , proposed by Gutman and Ashrafi [4], is defined as

$$Sz_e(G) = \sum_{e=uv \in E(G)} m_u(e|G)m_v(e|G).$$

Some properties of the edge Szeged index may be found in [1,8,14].

Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise vertex-disjoint connected graphs with $v_i \in V(G_i)$. The bridge graph $B(G_1, G_2, \dots, G_d) = B(G_1, G_2, \dots, G_d; v_1, v_2, \dots, v_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is the graph obtained from the graphs G_1, G_2, \dots, G_d by connecting the vertices v_i and v_{i+1} by an edge for all $i = 1, 2, \dots, d-1$.

In [10], Mansour and Schork introduced formulas for the vertex PI index and Szeged index of bridge graphs, and used the formulas to compute the vertex PI indices and Szeged indices of several graphs. Work on other graph invariants of bridge graphs may be found in [11]. In this note, we use the techniques from [10] to find a formula for the edge Szeged index of bridge graphs, and by using this formula, the edge Szeged indices of several graphs are computed.

2. Main results

For a graph G with $v \in V(G)$, let $Q_v(G)$ be the set of edges xy of G such that $d_G(v, x) = d_G(v, y)$.

In a bridge graph $B(G_1, G_2, \dots, G_d)$, for $i = 1, 2, \dots, d$, let $L(G_i)$ be the set of edges $e = uv$ in $E(G_i) \setminus Q_{v_i}(G_i)$ such that $d_G(u, v_i) < d_G(v, v_i)$ and $R(G_i)$ the set of edges $e = uv$ in $E(G_i) \setminus Q_{v_i}(G_i)$ such that $d_G(u, v_i) > d_G(v, v_i)$. To make this well defined, we choose an arbitrary direction on the edges of G_i (which is fixed for all the following computations); the results do not depend on the direction chosen.

Theorem 2.1. The edge Szeged index of bridge graph $G = B(G_1, G_2, \dots, G_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is given by

$$Sz_e(G) = \sum_{i=1}^d Sz_e(G_i) + \sum_{i=1}^d (|E(G)| - |E(G_i)|)(l_i + r_i) + \sum_{i=1}^{d-1} \alpha_i (|E(G)| - 1 - \alpha_i),$$

where

$$l_i = \sum_{e=uv \in L(G_i)} m_v(e|G_i), \quad r_i = \sum_{e=uv \in R(G_i)} m_u(e|G_i), \quad \alpha_i = \sum_{j=1}^i |E(G_j)| + i - 1$$

for all $i = 1, 2, \dots, d$.

Proof. Let $G = B(G_1, G_2, \dots, G_d)$. Note that $E(G_i) = Q_{v_i}(G_i) \cup L(G_i) \cup R(G_i)$ for $i = 1, 2, \dots, d$. From the definition of the edge Szeged index, we have

$$\begin{aligned} Sz_e(G) &= \sum_{e=uv \in E(G)} m_u(e|G)m_v(e|G) = \sum_{i=1}^d \sum_{e=uv \in Q_{v_i}(G_i)} m_u(e|G)m_v(e|G) + \sum_{i=1}^d \sum_{e=uv \in L(G_i) \cup R(G_i)} m_u(e|G)m_v(e|G) \\ &\quad + \sum_{i=1}^{d-1} m_{v_i}(v_i v_{i+1}|G)m_{v_{i+1}}(v_i v_{i+1}|G). \end{aligned}$$

For $i = 1, 2, \dots, d$, if $e = uv \in Q_{v_i}(G_i)$, then $d(v_i, u) = d(v_i, v)$, and thus for any $f \in E(G) \setminus E(G_i)$, we have $d(u, f) = d(v, f)$, implying that $m_u(e|G) = m_u(e|G_i)$, $m_v(e|G) = m_v(e|G_i)$, and then

$$\sum_{e=uv \in Q_{v_i}(G_i)} m_u(e|G)m_v(e|G) = \sum_{e=uv \in Q_{v_i}(G_i)} m_u(e|G_i)m_v(e|G_i).$$

For $i = 1, 2, \dots, d$, if $e = uv \in L(G_i)$, then $d(u, v_i) < d(v, v_i)$, and thus

$$\begin{aligned} m_u(e|G)m_v(e|G) &= \left(m_u(e|G_i) + d - 1 + \sum_{\substack{1 \leq j \leq d \\ j \neq i}} |E(G_j)| \right) m_v(e|G_i) \\ &= m_u(e|G_i)m_v(e|G_i) + (|E(G)| - |E(G_i)|)m_v(e|G_i), \end{aligned}$$

and if $e = uv \in R(G_i)$, then $d(v, v_i) < d(u, v_i)$, and thus

$$\begin{aligned} m_u(e|G)m_v(e|G) &= m_u(e|G_i) \left(m_v(e|G_i) + d - 1 + \sum_{\substack{1 \leq j \leq d \\ j \neq i}} |E(G_j)| \right) \\ &= m_u(e|G_i)m_v(e|G_i) + (|E(G)| - |E(G_i)|)m_u(e|G_i). \end{aligned}$$

Thus

$$\begin{aligned} \sum_{e=uv \in L(G_i) \cup R(G_i)} m_u(e|G)m_v(e|G) &= \sum_{e=uv \in L(G_i)} m_u(e|G)m_v(e|G) + \sum_{e=uv \in R(G_i)} m_u(e|G)m_v(e|G) \\ &= \sum_{e=uv \in L(G_i)} [m_u(e|G_i)m_v(e|G_i) + (|E(G)| - |E(G_i)|)m_v(e|G_i)] \\ &\quad + \sum_{e=uv \in R(G_i)} [m_u(e|G_i)m_v(e|G_i) + (|E(G)| - |E(G_i)|)m_u(e|G_i)] \\ &= \sum_{e=uv \in L(G_i) \cup R(G_i)} m_u(e|G_i)m_v(e|G_i) \\ &\quad + (|E(G)| - |E(G_i)|) \left(\sum_{e=uv \in L(G_i)} m_v(e|G_i) + \sum_{e=uv \in R(G_i)} m_u(e|G_i) \right). \end{aligned}$$

For $i = 1, 2, \dots, d-1$, obviously,

$$m_{v_i}(v_i v_{i+1}|G)m_{v_{i+1}}(v_i v_{i+1}|G) = \left(\sum_{j=1}^i |E(G_j)| + i - 1 \right) \left[\sum_{j=i+1}^d |E(G_j)| + d - (i+1) \right].$$

Now it follows that

$$\begin{aligned} Sz_e(G) &= \sum_{i=1}^d \sum_{e=uv \in Q_{v_i}(G_i)} m_u(e|G_i)m_v(e|G_i) + \sum_{i=1}^d \sum_{e=uv \in L(G_i) \cup R(G_i)} m_u(e|G_i)m_v(e|G_i) + \sum_{i=1}^d (|E(G)| - |E(G_i)|) \\ &\quad \times \left(\sum_{e=uv \in L(G_i)} m_v(e|G_i) + \sum_{e=uv \in R(G_i)} m_u(e|G_i) \right) + \sum_{i=1}^{d-1} \left(\sum_{j=1}^i |E(G_j)| + i - 1 \right) \left(\sum_{j=i+1}^d |E(G_j)| + d - i - 1 \right) \\ &= \sum_{i=1}^d \sum_{e=uv \in E(G_i)} m_u(e|G_i)m_v(e|G_i) + \sum_{i=1}^d (|E(G)| - |E(G_i)|)(l_i + r_i) + \sum_{i=1}^{d-1} \alpha_i(|E(G)| - 1 - \alpha_i), \end{aligned}$$

as desired. \square

For a connected graph H with vertex v , let $G_d(H, v) = B(\underbrace{H, \dots, H}_{d \text{ times}}; \underbrace{v, \dots, v}_{d \text{ times}})$. Obviously, $G_1(H, v) = H$. As a corollary of Theorem 2.1, we have

Corollary 2.1. Let H be a connected graph with m edges, and let $v \in V(H)$. Then

$$Sz_e(G_d(H, v)) = dSz_e(H) + (m+1)d(d-1)(l_H + r_H) + (d-1) \left(\frac{(m+1)d(md+m+d-5)}{6} + 1 \right),$$

where $l_H = \sum_{e=xy \in L(H)} m_y(e|H)$ and $r_H = \sum_{e=xy \in R(H)} m_x(e|H)$.

Proof. Setting $G_i = H$ and $v_i = v$ with $i = 1, 2, \dots, d$ in Theorem 2.1, we have $|E(G_d(H, v))| = d|E(H)| + d - 1 = md + d - 1$, and then

$$\begin{aligned}
Sz_e(G_d(H, v)) &= \sum_{i=1}^d Sz_e(H) + \sum_{i=1}^d (|E(G_d(H, v))| - |E(H)|)(l_H + r_H) + \sum_{i=1}^{d-1} \alpha_i (|E(G_d(H, v))| - 1 - \alpha_i) \\
&= d Sz_e(H) + (m+1)d(d-1)(l_H + r_H) + \sum_{i=1}^{d-1} \alpha_i (|E(G_d(H, v))| - 1 - \alpha_i),
\end{aligned}$$

where $\alpha_i = \sum_{j=1}^i |E(H)| + i - 1 = (m+1)i - 1$. Note that

$$\begin{aligned}
\sum_{i=1}^{d-1} \alpha_i (|E(G_d(H, v))| - 1 - \alpha_i) &= \sum_{i=1}^{d-1} [(m+1)i - 1][(m+1)d - (m+1)i - 1] \\
&= \sum_{i=1}^{d-1} [-(m+1)^2 i^2 + (m+1)^2 di - (m+1)d + 1] \\
&= -\frac{(m+1)^2 d(d-1)(2d-1)}{6} + \frac{(m+1)^2 d^2(d-1)}{2} - [(m+1)d - 1](d-1).
\end{aligned}$$

The result follows easily. \square

Let $P_n = u_1 u_2 \dots u_n$ be the path on n vertices. Obviously, $P_n = G_n(P_1, u_1)$. By Corollary 2.1,

$$Sz_e(P_n) = (n-1) \left(\frac{n(n-5)}{6} + 1 \right) = \binom{n-1}{3}.$$

Let $A_{d,n} = G_d(P_n, u_1)$. Obviously, $A_{d,1} = P_d$ and $A_{1,n} = P_n$.

Corollary 2.2. The edge Szeged index of $A_{d,n}$ is given by

$$Sz_e(A_{d,n}) = d \binom{n-1}{3} + 6 \binom{d}{2} \binom{n}{3} + n^2 \binom{d+1}{3} - (nd-1)(d-1).$$

Proof. By Corollary 2.1, we have

$$\begin{aligned}
Sz_e(A_{d,n}) &= d Sz_e(P_n) + nd(d-1)(l_{P_n} + r_{P_n}) + (d-1) \left(\frac{nd[(n-1)d + (n-1) + d - 5]}{6} + 1 \right) \\
&= d Sz_e(P_n) + nd(d-1)(l_{P_n} + r_{P_n}) + n^2 \cdot \frac{(d+1)d(d-1)}{6} - (nd-1)(d-1).
\end{aligned}$$

Note that $Sz_e(P_n) = \binom{n-1}{3}$ and $l_{P_n} + r_{P_n} = \sum_{i=1}^{n-2} i = \binom{n-1}{2}$. Then the result follows easily. \square

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References

- [1] X. Cai, B. Zhou, Edge Szeged index of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* 63 (2010) 133–144.
- [2] A.A. Dobrynin, Graphs having maximal value of the Szeged index, *Croat. Chem. Acta* 70 (1997) 819–825.
- [3] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes N. Y.* 27 (1994) 9–15.
- [4] I. Gutman, A.R. Ashrafi, The edge version of the Szeged index, *Croat. Chem. Acta* 81 (2008) 263–266.
- [5] A. Ilić, Note on PI and Szeged indices, *Math. Comput. Modelling* 52 (2010) 1570–1576.
- [6] P.V. Khadikar, N.V. Deshpande, P.P. Kale, A.A. Dobrynin, I. Gutman, G. Dömötör, The Szeged index and an analogy with the Wiener index, *J. Chem. Inf. Comput. Sci.* 35 (1995) 547–550.
- [7] P.V. Khadikar, S. Karmarkar, V.K. Agrawal, J. Singh, A. Shrivastava, I. Lukovits, M.V. Diudea, Szeged index – Applications for drug modeling, *Lett. Drug Design Discov.* 2 (2005) 606–624.
- [8] M.H. Khalifeh, H. Yousefi-Azari, A.R. Ashrafi, I. Gutman, The edge Szeged index of product graphs, *Croat. Chem. Acta* 81 (2008) 277–281.
- [9] S. Klavžar, A. Rajapakse, I. Gutman, The Szeged and the Wiener index of graphs, *Appl. Math. Lett.* 9 (1996) 45–49.
- [10] T. Mansour, M. Schork, The vertex PI index and Szeged index of bridge graphs, *Discrete Appl. Math.* 157 (2009) 1600–1606.
- [11] T. Mansour, M. Schork, Wiener, hyper-Wiener, detour and hyper-detour indices of bridge and chain graphs, *J. Math. Chem.* 47 (2010) 72–98.
- [12] S. Simić, I. Gutman, V. Baltić, Some graphs with extremal Szeged index, *Math. Slovaca* 50 (2000) 1–15.
- [13] N. Trinajstić, *Chemical Graph Theory*, 2nd edn., CRC Press, Boca Raton, FL, 1992.
- [14] D. Vukičević, Note on the graphs with the greatest edge-Szeged index, *MATCH Commun. Math. Comput. Chem.* 61 (2009) 673–681.
- [15] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* 69 (1947) 17–20.
- [16] J. Žerovnik, Szeged index of symmetric graphs, *J. Chem. Inf. Comput. Sci.* 39 (1999) 77–80.
- [17] B. Zhou, X. Cai, Z. Du, On Szeged indices of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* 63 (2010) 113–132.