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MATHEMATICAL PROPERTIES OF KG SOMBOR INDEX

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Abstract. Let $G = (\mathbf{V}, \mathbf{E})$ be a connected graph. A topological invariant named Sombor index was introduced by one of the present authors (I.G.) in 2021, defined as $SO(G) = \sum_{uv \in \mathbf{E}} \sqrt{d_u^2 + d_v^2}$, where d_u denotes the degree of the vertex $u \in \mathbf{V}$. The K Banhatti indices, introduced by another present author (V.R.K.) in 2016, are defined as $B_1(G) = \sum_{ue}(d_u + d_e)$ and $B_2(G) = \sum_{ue} d_u\, d_e$, where $\sum_{ue}$ indicates summation over vertices $u \in \mathbf{V}$ and the edges $e \in \mathbf{E}$ that are incident to u, and d_e is the degree of the edge e. In this paper, we introduce a novel topological graph invariant, named KG Sombor index, defined as $KG(G) = \sum_{ue} \sqrt{d_u^2 + d_e^2}$. Some basic properties of KG are established, as well as its relationships with other topological indices.

1. Introduction

All graphs considered in this paper are finite, connected, undirected, without loops and multiple edges. Let $G = (\mathbf{V}(G), \mathbf{E}(G))$ be a connected graph with $n = |\mathbf{V}(G)|$ vertices and $m = |\mathbf{E}(G)|$ edges. The degree d_u of a vertex $u \in \mathbf{V}(G)$ is the number of vertices adjacent to u. The degree of an edge $e = uv \in \mathbf{E}(G)$ is the number of edges incident to e. As well known, $d_e = d_u + d_v - 2$. We refer to [**9**] for undefined terms and notation.

A molecular graph is a graph whose vertices correspond to the atoms and the edges to the bonds of an underlying molecule. A single number that can be used to characterize some property of the molecule represented by a graph is called a topological index or (graph-based) molecular structure descriptor. Numerous such

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structure descriptors have been put forward in the recent literature, and found applications in theoretical chemistry, especially in QSPR/QSAR/QSTR research; for details see [**8, 11**] and the references cited therein.

The first and second Zagreb indices, defined as

$$M_1(G) = \sum_{uv \in \mathbf{E}(G)} (d_u + d_v)$$

and

$$M_2(G) = \sum_{uv \in \mathbf{E}(G)} d_u\, d_v$$

are two oldest and most detailed studied vertex-degree-based topological indices [**6, 7, 11**]. In the later consideration we shall need also the "forgotten" topological index [**4**]

$$F(G) = \sum_{uv \in \mathbf{E}(G)} (d_u^2 + d_v^2)\,.$$

Bearing in mind the algebraic form of the Zagreb indices, one of the present authors (V.R.K.) introduced the first and second K Banhatti indices as [**10**]

$$B_1(G) = \sum_{ue} (d_u + d_e) \tag{1.1}$$

and

$$B_2(G) = \sum_{ue} d_u\, d_e \tag{1.2}$$

where $\sum_{ue}$ indicates summation over vertices $u \in \mathbf{V}(G)$ and the edges $e \in \mathbf{E}(G)$ that are incident to u. Since the edge $e = uv$ is incident to both the vertices u and v, the Banhatti indices can be written as

$$B_1(G) = \sum_{uv \in \mathbf{E}(G)} \Big[\big[d_u + (d_u + d_v - 2)\big] + \big[d_v + (d_u + d_v - 2)\big] \Big] \tag{1.3}$$

$$B_2(G) = \sum_{uv \in \mathbf{E}(G)} \Big[\big[d_u (d_u + d_v - 2)\big] + \big[d_v (d_u + d_v - 2)\big] \Big]\,. \tag{1.4}$$

Recently, one of the present authors (I.G.) [**5**], invented a novel degree-based topological index, called Sombor index, inspired by a geometric interpretation of degree-radii of the edges. The Sombor index is defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}\,. \tag{1.5}$$

It attracted much attention of scholars, and its mathematical properties and chemical applicability was, and currently is, much investigated, see for instance [**1, 2, 3, 12, 15, 16, 17, 18, 19, 20, 21**].

Here, we initiate the study of new topological index named as *KG Sombor index*, defined as

$$KG = KG(G) = \sum_{ue} \sqrt{d_u^2 + d_e^2}\,. \tag{1.6}$$

Evidently, KG is a kind of combination between the original Sombor index, Eq. (1.5), and the K Banhatti indices, Eqs. (1.1) and (1.2). In the same way as relations (1.3) and (1.4) are obtained, we can express the KG index as

$$\begin{aligned} KG(G) &= \sum_{uv\in\mathbf{E}(G)} \left[\sqrt{d_u^2+(d_u+d_v-2)^2}+\sqrt{d_v^2+(d_u+d_v-2)^2}\right] \\ &= \sum_{uv\in\mathbf{E}(G)} \Big[\sqrt{2\,d_u^2+d_v^2+2d_u\,d_v-4(d_u+d_v)+4} \\ &+ \sqrt{d_u^2+2\,d_v^2+2d_u\,d_v-4(d_u+d_v)+4}\Big]. \end{aligned} \tag{1.7}$$

2. Specific families of graphs

THEOREM 2.1. *Let G be an r-regular graph of order n. Then*

$$KG(G)=nr\sqrt{5r^2-8r+4}. \tag{2.1}$$

PROOF. An r-regular graph has $m=nr/2$ edges and for each edge $d_e=2r-2$. By Eq. (1.6),

$$\begin{aligned} KG(G) &= \sum_{uv\in\mathbf{E}(G)} \left[\sqrt{d_u^2+d_e^2}+\sqrt{d_v^2+d_e^2}\right] \\ &= \frac{nr}{2}\left[\sqrt{r^2+(2r-2)^2}+\sqrt{r^2+(2r-2)^2}\right]=nr\sqrt{5r^2-8r+4}\,. \end{aligned}$$

□

COROLLARY 2.1.
(a) For the cycle C_n of size n, $KG(C_n)=4\sqrt{2n}$.

(b) For the complete graph K_n of order n, $KG(K_n)=n(n-1)\sqrt{5n^2-18n+17}$.

(c) For the k-hypercube Q_k of order 2^k, $KG(Q_k)=2^k\,k\sqrt{5k^2-8k+4}$.

(d) The generalized Petersen graph $GP\,(t,s)$ for $t\geqslant 3$ and $1\leqslant s\leqslant\lfloor(t-1)/2\rfloor$ is a connected cubic graph consisting of an inner star polygon $\{t,s\}$ with corresponding vertices in the inner and outer polygons connected by edges. Then $KG(GP(t,s))=30\,t$.

In an analogous manner, using Eq. (1.7), we arrive at:

THEOREM 2.2. *Let $K_{p,q}$ be the complete bipartite graph with $1\leqslant p\leqslant q$. Then*

$$KG(K_{p,q})=pq\left[\sqrt{p^2+(p+q-2)^2}+\sqrt{q^2+(p+q-2)^2}\right].$$

COROLLARY 2.2.
(a) For the regular bipartite graph $K_{p,p}$ of order $2p$, $KG(K_{p,p})=2p^2\sqrt{5p^2-8p+4}$.

(b) For the star $K_{1,q}$ or order $1+q$, $KG(K_{1,q})=q\left(\sqrt{q^2-2q+2}+\sqrt{2q^2-2q+1}\right)$.

THEOREM 2.3. *Let P_n be the path of order n. Then $KG(P_1) = 0$, $KG(P_2) = 2$, whereas for $n \geqslant 3$,*

$$KG(P_n) = 4\sqrt{2}(n-3) + 2(\sqrt{5} + \sqrt{2})\,.$$

3. Simple bounds

Let the minimum and maximum degree of a vertex in the graph G be denoted by δ and Δ, respectively.

THEOREM 3.1. *For any non-trivial connected graph G with m edges,*

$$2m\sqrt{5\delta^2 - 8\delta + 4} \leqslant KG(G) \leqslant 2m\sqrt{5\Delta^2 - 8\Delta + 4}.$$

The lower and upper bounds are attained if and only if G is regular.

PROOF. If $\delta \leqslant d_u, d_v \leqslant \Delta$, then $2(\delta - 1) \leqslant d_e \leqslant 2(\Delta - 1)$. Then from equation (1.6) we have

$$\begin{aligned} KG(G) &\leqslant \sum_{uv \in E(G)} \sqrt{\Delta^2 + 4(\Delta-1)^2} + \sum_{uv \in E(G)} \sqrt{\Delta^2 + 4(\Delta-1)^2} \\ &= 2m\sqrt{5\Delta^2 - 8\Delta + 4} \\ KG(G) &\geqslant \sum_{uv \in E(G)} \sqrt{\delta^2 + 4(\delta-1)^2} + \sum_{uv \in E(G)} \sqrt{\delta^2 + 4(\delta-1)^2} \\ &= 2m\sqrt{5\delta^2 - 8\delta + 4}\,. \end{aligned}$$

The equality case is evident from Eq. (2.1). □

THEOREM 3.2. *For any non-trivial connected graph G of order n,*

$$KG(P_n) \leqslant KG(G) \leqslant KG(K_n)\,.$$

The lower bound is attained if and only if $G \cong P_n$ and the upper bound is attained if and only if $G \cong K_n$. Expressions for $KG(P_n)$ and $KG(K_n)$ are found in Theorem 2.3 and Corollary 2.1(b).

The proof of Theorem 3.2 is fully analogous to the proof of Theorem 2 in Ref. [**5**]), and will not be repeated here.

4. Bounds in terms of other topological indices

We first recall an elementary auxiliary result.

LEMMA 4.1. *For any positive numbers a and b,*

$$\frac{1}{\sqrt{2}}(a+b) \leqslant \sqrt{a^2 + b^2} < a + b\,.$$

Equality on the left-hand side holds if and only if $a = b$.

Applying Lemma 4.1 to Eq. (1.6), we get

$$\frac{1}{\sqrt{2}}\sum_{ue}(d_u+d_e) \leqslant KG(G) < \sum_{ue}(d_u+d_e)$$

which in view of the definition of the first K Banhatti index, Eq. (1.1) implies

Theorem 4.1. *For any non-trivial connected graph G*

$$\frac{1}{\sqrt{2}}B_1(G) \leqslant KG(G) < B_1(G)$$

with equality on the left-hand side if G is regular of degree 2, i.e. if $G \cong C_n$.

Applying the same argument to Eq. (1.7), we get

$$\begin{aligned} KG(G) &< \sum_{uv\in \mathbf{E}(G)} \Big[[2\,d_u^2+d_v^2+2d_u\,d_v-4(d_u+d_v)+4] \\ &+ [d_u^2+2\,d_v^2+2d_u\,d_v-4(d_u+d_v)+4]\Big] \\ &= \sum_{uv\in \mathbf{E}(G)} \Big[3(d_u^2+d_v^2)-8(d_u+d_v)+4d_u\,d_v+8\Big] \end{aligned}$$

and

$$KG(G) \geqslant \frac{1}{\sqrt{2}}\sum_{uv\in \mathbf{E}(G)} \Big[3(d_u^2+d_v^2)-8(d_u+d_v)+4d_u\,d_v+8\Big]$$

which combined with the definitions of the first and second Zagreb index, and the forgotten index, yields

Theorem 4.2. *For any non-trivial connected graph G with m edges,*

$$\frac{1}{\sqrt{2}}\big[3F(G)-8M_1(G)+4M_2(G)+8m\big] \leqslant KG(G) < 3F(G)-8M_1(G)+4M_2(G)+8m\,.$$

It would be interesting to determine the conditions for equality in the left-hand side bound.

Theorem 4.3. *For any non-trivial connected graph G,*

$$\left[\frac{m\sqrt{5\Delta^2-8\Delta+4}}{\Delta(\Delta-1)}\right]B_2(G) \leqslant KG(G) \leqslant \left[\frac{m\sqrt{5\delta^2-8\delta+4}}{\delta(\delta-1)}\right]B_2(G)\,.$$

The lower and upper bounds are attained if and only if G is regular.

PROOF. From Eq. (1.6), we have

$$
\begin{aligned}
KG(G) &= \sum_{ue} d_u d_e \sqrt{\left(\frac{1}{d_u^2}+\frac{1}{d_e^2}\right)} = \left(\sum_{ue} d_u d_e\right)\left(\sum_{ue}\sqrt{\left(\frac{1}{d_u^2}+\frac{1}{d_e^2}\right)}\right) \\
&= B_2(G)\left[\sum_{uv\in E}\sqrt{\left(\frac{1}{d_u^2}+\frac{1}{d_e^2}\right)}+\sum_{uv\in E}\sqrt{\left(\frac{1}{d_u^2}+\frac{1}{d_e^2}\right)}\right] \qquad (4.1) \\
&\leqslant B_2(G)\left[\sum_{uv\in E}\sqrt{\left(\frac{1}{\delta^2}+\frac{1}{4(\delta-1)^2}\right)}+\sum_{uv\in E}\sqrt{\left(\frac{1}{\delta^2}+\frac{1}{4(\delta-1)^2}\right)}\right] \\
&\leqslant \left[\frac{m\sqrt{5\delta^2-8\delta+4}}{\delta(\delta-1)}\right] B_2(G)\,.
\end{aligned}
$$

In a similar manner, we get

$$KG(G) \geqslant B_2(G)\left[\frac{m\sqrt{5\Delta^2-8\Delta+4}}{\Delta(\Delta-1)}\right].$$

If G is regular, then the equality is evident from Theorem 2.1. □

The sum and product connectivity Banhatti indices are defined as

$$SB(G)=\sum_{ue}\frac{1}{\sqrt{d_u+d_e}} \qquad \text{and} \qquad PB(G)=\sum_{ue}\frac{1}{\sqrt{d_u\,d_e}}\,.$$

These indices are initiated by Kulli et al. [**13, 14**]. Analogously, the inverse version of the sum and product connectivity Banhatti indices of a graph G are defined as

$$ISB(G)=\sum_{ue}\sqrt{d_u+d_e} \qquad \text{and} \qquad IPB(G)=\sum_{ue}\sqrt{d_u\,d_e}\,.$$

By [**13, 14**], we have $PB(G)\leqslant SB(G)$ and hence $ISB(G)\leqslant IPB(G)$.

THEOREM 4.4. *For any non-trivial connected graph G,*

$$\sqrt{2}\,IPB(G)\leqslant KG(G)\leqslant m\,IPB(G)\left[\sqrt{\frac{\Delta^2+\theta}{\Delta(\Delta+\delta-2)}}+\sqrt{\frac{\delta^2+\theta}{\delta(\Delta+\delta-2)}}\right] \qquad (4.2)$$

where $\theta=(\Delta+\delta)^2-4(\Delta+\delta)+4$.

PROOF. From equation (1.6) one obtains

$$\begin{aligned}
KG(G) &= \sum_{ue}\sqrt{d_u\,d_e\left(\frac{d_u}{d_e}+\frac{d_e}{d_u}\right)} \leqslant \sum_{ue}\sqrt{d_u\,d_e}\left(\sum_{ue}\sqrt{\frac{d_u}{d_e}+\frac{d_e}{d_u}}\right)\\
&\leqslant IPB(G)\left[\sum_{ue}\sqrt{\frac{d_u}{d_u+d_v-2}+\frac{d_u+d_v-2}{d_u}}\right]\\
&\leqslant IPB(G)\Bigg[\sum_{uv\in E}\sqrt{\frac{\Delta}{\Delta+\delta-2}+\frac{\Delta+\delta-2}{\Delta}}\\
&+ \sum_{uv\in E}\sqrt{\frac{\delta}{\delta+\Delta-2}+\frac{\delta+\Delta-2}{\delta}}\Bigg]\\
&\leqslant m\,IPB(G)\left[\sqrt{\frac{\Delta^2+\theta}{\Delta(\Delta+\delta-2)}}+\sqrt{\frac{\delta^2+\theta}{\delta(\Delta+\delta-2)}}\right].
\end{aligned}$$

By the definitions of $KG(G)$ and $IPB(G)$, we have the $KG(G) \geqslant \sqrt{2}IPB(G)$.

Thus the relations (4.2) follow. □

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