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General Sombor index of graphs and trees

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Abstract

Topological indices such as the general Sombor index are studied because of their extensive applications. For $c, g \in \mathbb{R}$, the general Sombor index for a graph H is $SO_{c,g}(H) = \sum_{vw \in E(H)} ([d_H(v)]^c + [d_H(w)^c])^g$, where $E(H)$ is the set of edges of H, and $d_H(v)$ and $d_H(w)$ are the degrees of vertices v and w. Trees of given order with the largest $SO_{c,g}$ for $c \geq 1$ and $g > 0$, trees of given order with the smallest $SO_{c,g}$ for $c \geq 1$ and $g \geq 1$, bipartite graphs of prescribed matching number and order with the largest $SO_{c,g}$ for $c \geq 1$ and $g \geq 0$ are presented. We also obtain several corollaries including bounds for the classical Sombor index and forgotten index.

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1. Introduction

In a graph H, the notation $d_H(v)$ represents the degree of a vertex v. H with the vertex set $V(H) = S_1 \cup S_2$, where $S_1 \cap S_2 = \emptyset$, is bipartite, if no two vertices of S_1 are joined and no two vertices of S_2 are joined. Moreover, if each vertex of S_1 is joined to each vertex in S_2, where $|S_1| = z_1$ and $|S_2| = z_2$, then H is called complete bipartite and it is denoted by K_{z_1,z_2}. The path with z vertices is denoted by P_z. We denote the matching number of H by m, edge cover number by β', vertex cover number by β and independence number by α.

The general Sombor index

$$SO_{c,g}(H) = \sum_{vw\in E(H)} ([d_H(v)]^c + [d_H(w)]^c)^g$$

of a graph H, where $E(H)$ is the edge set of H, is a new index defined by Hernández et al. [9] for $c, g \in \mathbb{R}$. From $SO_{c,g}(H)$ we get the forgotten index $FI(H)$ if $c = 2$ and $g = 1$ (see [6]) and the classical Sombor index if $c = 2$ and $g = \frac{1}{2}$. The Sombor index was defined in [7] a few years ago and it has been extensively investigated.

In [9] and [12], the authors obtained some extremal results on $SO_{c,g}$, and investigated relations between $SO_{c,g}$ and other indices. Some results on the Sombor index can be found in [1, 3, 4, 8, 10, 14, 15, 17, 19, 20] and results on other indices in [2, 5, 11, 13].

2. Main results

First, we investigate trees which are graphs without cycles and such graphs can represent various chemical structures.

Theorem 1: *Let $c \geq 1$ and $g > 0$. For a tree A with z vertices, where $z \geq 4$,*

$$SO_{c,g}(A) \leq (z-1)[(z-1)^c + 1]^g.$$

The extremal tree is $K_{1,z-1}$.

Proof: Let vw be any edge of A with $d_A(w) \leq d_A(v)$. Clearly, $z \geq d_A(v) + d_A(w)$ for trees, which gives $z - d_A(w) \geq d_A(v)$. Thus for $c \geq 1$, $[z - d_A(w)]^c \geq [d_A(v)]^c$. So

$$([d_A(v)]^c + [d_A(w)]^c)^g \leq ([d_A(w)]^c + [z - d_A(w)]^c)^g = f(d_A(w))$$

where $\left\lfloor \frac{z}{2} \right\rfloor \geq d_A(w) \geq 1$ for $g > 0$ and $c \geq 1$. Then

$$f'(d_A(w)) = cg([d_A(w)]^{c-1} - (z-[d_A(w)])^{c-1})[[d_A(w)]^c + (z-[d_A(w)])^c]^{g-1}.$$

For $a>1$ (and $g>0$), we obtain $f'(d_A(w))<0$, so $f(d_A(w))$ is strictly decreasing on $1 \le d_A(w) \le \lfloor \frac{z}{2} \rfloor$. Thus

$$\begin{aligned}([d_A(v)]^c + [d_A(w)]^c)^g &\le ([d_A(w)]^c + [z-d_A(w)]^c)^g = f(d_A(w)) \\ &\le f(1) = [(z-1)^c + 1]^g,\end{aligned}$$

where the first inequality is equality only for $d_A(w)+d_A(v)=z$. The second inequality is equality only for $d_A(w)=1$. We obtain

$$\begin{aligned}SO_{c,g}(A) &= \sum_{vw\in E(A)} ([d_A(v)]^c + [d_A(w)]^c)^g \\ &\le (z-1)[(z-1)^c+1]^g,\end{aligned}$$

giving equality only if $d_A(v)=z-1$ and $d_A(w)=1$ for every $vw\in E(A)$ which implies that $A \cong K_{1,z-1}$.

For $c=1$ (and $g>0$),

$$([d_A(w)]^c + [d_A(v)]^c)^g \le z^g$$

and

$$SO_{c,g}(A) = \sum_{vw\in E(A)} [d_A(v)+d_A(w)]^g \le (z-1)z^g,$$

giving equality only if $d_A(v)+d_A(w)=z$ for each edge $vw\in E(A)$ which implies that $A \cong K_{1,z-1}$.

Let us present a lemma from [16] which is useful for Theorems 2 and 3.

Lemma 1: *Let* $c>1$, $x\ge 1$, $c_1>0$ *and* $k_1>0$. *Then*

$$x^c + (x+c_1+k_1)^c > (x+c_1)^c + (x+k_1)^c.$$

Lemma 2 is also useful for Theorem 2.

Lemma 2: *For* $c\ge 1$ *and* $g\ge 1$,

$$f(x) = (x^c+2^c)^g - [(x-1)^c + 2^c]^g$$

is non-decreasing for $x\ge 2$.

Proof: We get

$$\begin{aligned} f'(x) &= g(x^c+2^c)^{g-1}cx^{c-1} - cg[(x-1)^c+2^c]^{g-1}(x-1)^{c-1} \\ &= cg[(x^c+2^c)^{g-1}x^{c-1} - (x-1)^{c-1}[(x-1)^c+2^c]^{g-1}] \\ &\geq 0 \end{aligned}$$

if $g \geq 1$ and $c \geq 1$, since $[(x-1)^c+2^c]^{g-1} \leq (x^c+2^c)^{g-1}$, $(x-1)^c < x^c$, $(x-1)^{c-1} \leq x^{c-1}$.

Theorem 2: *Let $c \geq 1$ and $g \geq 1$. For any tree A having z vertices, where $z \geq 4$,*

$$SO_{c,g}(A) \geq (z-3)2^{(c+1)g} + 2(2^c+1)^g.$$

The extremal graph is P_z.

Proof: We denote a tree having z vertices and the smallest $SO_{c,g}$ for $c \geq 1$ and $g \geq 1$ by A. Let us show that $A \cong P_z$.

By contradiction, assume that $A \ncong P_z$. Let $P: v_0v_1v_2\ldots v_D$ be a longest path in A. Let k be the smallest natural number where $d_A(v_k) \geq 3$. So, $k \geq 1$, $d_A(v_k) = p \geq 3$, $d_A(v_0) = 1$ and $d_A(v_1) = \ldots = d_A(v_{k-1}) = 2$. Let w, w_1, w_2, $\ldots$, w_{p-3} be the vertices adjacent to v_k not being in P. We define $A' = A - v_kw + v_0w$. Then v_0 and v_k are the only vertices with distinct degrees in A and A'. We obtain $d_{A'}(v_0) = 2$ and $d_{A'}(v_k) = p-1$.

If $k \geq 2$, then

$$\begin{aligned} &SO_{c,g}(A) - SO_{c,g}(A') \\ &= \sum_{i=1}^{p-3}[([d_A(v_k)]^c + [d_A(w_i)]^c)^g - ([d_{A'}(v_k)]^c + [d_{A'}(w_i)]^c)^g] \\ &\quad + ([d_A(v_k)]^c + [d_A(w)]^c)^g - ([d_{A'}(v_0)]^c + [d_{A'}(w)]^c)^g \\ &\quad + ([d_A(v_k)]^c + [d_A(v_{k+1})]^c)^g - ([d_{A'}(v_k)]^c + [d_{A'}(v_{k+1})]^c)^g \\ &\quad + ([d_A(v_{k-1})]^c + [d_A(v_k)]^c)^g - ([d_{A'}(v_{k-1})]^c + [d_{A'}(v_k)]^c)^g \\ &\quad + ([d_A(v_0)]^c + [d_A(v_1)]^c)^g - ([d_{A'}(v_0)]^c + [d_{A'}(v_1)]^c)^g \\ &= \sum_{i=1}^{p-3}[(p^c + [d_A(w_i)]^c)^g - ([p-1]^c + [d_A(w_i)]^c)^g] \\ &\quad + (p^c + [d_A(w)]^c)^g - (2^c + [d_A(w)]^c)^g \\ &\quad + (p^c + [d_A(v_{k+1})]^c)^g - ([p-1]^c + [d_A(v_{k+1})]^c)^g \\ &\quad + (2^c + p^c)^g - (2^c + [p-1]^c)^g \\ &\quad + (2^c + 1^c)^g - (2^c + 2^c)^g \\ &> (2^c + p^c)^g - (2^c + [p-1]^c)^g + (2^c + 1^c)^g - (2^c + 2^c)^g \\ &\geq (2^c + 3^c)^g - (2 \cdot 2^c)^g + (2^c + 1^c)^g - (2^c + 2^c)^g \\ &\geq 0, \end{aligned}$$

since by Lemma 2,

$$(2^c+2^c)^g-(2^c+1^c)^g \le (2^c+3^c)^g-(2\cdot 2^c)^g \le (2^c+p^c)^g-(2^c+[p-1]^c)^g$$

for $c,g\ge 1$.

If $k=1$, then instead of considering two edges v_0v_1 and $v_{k-1}v_k$, we need to consider only one edge v_0v_1. We obtain

$$\begin{aligned}
&SO_{c,g}(A)-SO_{c,g}(A')\\
&>([d_A(v_0)]^c+[d_A(v_1)]^c)^g-([d_{A'}(v_0)]^c+[d_{A'}(v_1)]^c)^g\\
&=(1^c+p^c)^g-(2^c+[p-1]^c)^g\\
&\ge 0
\end{aligned}$$

for $c,g\ge 1$, since by Lemma 1, we have $1^c+p^c>2^c+[p-1]^c$ for $c>1$.

So $SO_{c,g}(A)>SO_{c,g}(A')$, therefore A does not have the smallest $SO_{c,g}$, a contradiction. Thus $A\cong P_z$ and

$$SO_{c,g}(P_z)=(z-3)(2^c+2^c)^g+2(2^c+1)^g=(z-3)2^{(c+1)g}+2(2^c+1)^g.$$

Lemma 3 is useful for Theorem 3.

Lemma 3: *Let u_1,u_2 be two vertices which are not adjacent in a graph H. For $c\ge 1$ and $g\ge 0$,*

$$SO_{c,g}(H)<SO_{c,g}(H+u_1u_2).$$

Proof: Let us denote the graph $H+u_1u_2$ by H'. We get $d_{H'}(w)\ge d_H(w)$ and $d_{H'}(v)\ge d_H(v)$ for each $vw\in E(H)$. So

$$([d_{H'}(w)]^c+[d_{H'}(v)]^c)^g\ge([d_H(w)]^c+[d_H(v)]^c)^g$$

for $c\ge 1$ and $g\ge 0$. We have $d_{H'}(u_1)\ge 1$ and $d_{H'}(u_2)\ge 1$, thus

$$([d_{H'}(u_1)]^c+[d_{H'}(u_2)]^c)^g>0$$

for $c\ge 1$ and $g\ge 0$. Hence

$$\begin{aligned}
SO_{c,g}(H')&=\sum_{vw\in E(H')}([d_{H'}(w)]^c+[d_{H'}(v)]^c)^g\\
&=([d_{H'}(u_1)]^c+[d_{H'}(u_2)]^c)^g+\sum_{vw\in E(H)}([d_{H'}(w)]^c+[d_{H'}(v)]^c)^g\\
&>\sum_{vw\in E(H)}([d_{H'}(w)]^c+[d_{H'}(v)]^c)^g\ge\sum_{vw\in E(H)}([d_H(w)]^c+[d_H(v)]^c)^g\\
&=SO_{c,g}(H).
\end{aligned}$$

For every graph with z vertices, $1 \le m \le \lfloor \frac{z}{2} \rfloor$. where $m = 1$ only for stars. So, we present a bound for $m \ge 2$.

Theorem 3: *Let $c \ge 1$ and $g \ge 0$. For any graph H having matching number m and z vertices which is bipartite such that $2 \le m \le \lfloor \frac{z}{2} \rfloor$, we have*

$$SO_{c,g}(H) \le m(z-m)(m^c + (z-m)^c)^g.$$

The extremal graph is $K_{m,z-m}$.

Proof: Considering all the graphs given z and m, we denote a graph having the maximum $SO_{c,g}$ by H'. We can assume that $|S_1| \le |S_2|$, where S_1 and S_2 are the partite sets of H'.

By contradiction, we prove that H' is $K_{m,z-m}$. Suppose that H' is not $K_{m,z-m}$. Note that $|S_1| \ge m$ (if $|S_1| \le m-1$, then H' would have the matching number at most $m-1$). Clearly $H' \not\subseteq K_{m,z-m}$, (otherwise if $H' \subseteq K_{m,z-m}$, then $SO_{c,g}(H') < SO_{c,g}(K_{m,z-m})$ from Lemma 3. Thus $m < |S_1| \le |S_2|$.

Let M' denote any matching of H' having m edges. Let $S_1^m \subseteq S_1$ and $S_2^m \subseteq S_2$ such that S_1^m and S_2^m contain m vertices incident with the edges of M'. We obtain $|S_1| = m + r'$ and $|S_2| = m + t'$, where $r', t' \ge 1$ (and $2m + r' + t' = z$). Note that $u_1 \in S_1 \setminus S_1^m$ is not adjacent to $u_2 \in S_2 \setminus S_2^m$, otherwise H' would contain the matching $M' \cup \{u_1u_2\}$ with $m+1$ edges.

Let F' denote a graph with $V(F') = V(H')$, where every $v \in S_1^m$ and every $w \in S_2^m$ are adjacent, every $v \in S_1^m$ and every $w' \in S_2 \setminus S_2^m$ are adjacent, and every $w \in S_1 \setminus S_1^m$ and every $w \in S_2^m$ are adjacent. So $H' \subseteq F'$, thus $SO_{c,g}(H') < SO_{c,g}(F')$ from Lemma 3. However, the matching number of F' is greater than m. We obtain $d_{F'}(u) = t' + m$ for $u \in S_1^m$, $d_{F'}(u') = r' + m$ for $u' \in S_2^m$, and $d_{F'}(u'') = m$ for $u'' \in V(F') \setminus (S_1^m \cup S_2^m)$. We have $z - m = m + r' + t'$. Then

$$\begin{aligned}
&SO_{c,g}(K_{m,z-m}) - SO_{c,g}(F') \\
&= \sum_{vw \in E(K_{m,z-m})} ([d_{K_{m,z-m}}(v)]^c + [d_{K_{m,z-m}}(w)]^c)^g \\
&\quad - \sum_{vw \in E(F')} ([d_{F'}(v)]^c + [d_{F'}(w)]^c)^g \\
&= m(z-m)((z-m)^c + m^c)^g - mm([m+t']^c + [m+r']^c)^g \\
&\quad - mr'([m+r']^c + m^c)^g - mt'([m+t']^c + m^c)^g \\
&= m^2[([m+r'+t']^c + m^c)^g - ([m+t']^c + [m+r']^c)^g] \\
&\quad + mr'[([m+r'+t']^c + m^c)^g - ([m+r']^c + m^c)^g] \\
&\quad + mt'[([m+r'+t']^c + m^c)^g - ([m+t']^c + m^c)^g].
\end{aligned}$$

By Lemma 1, for $c > 1$,

$$[m+r']^c + [m+t']^c < [m+r'+t']^c + m^c.$$

Thus, for $c \geq 1$ and $g \geq 0$,

$$([m+r']^c + [m+t']^c)^g \leq ([m+r'+t']^c + m^c)^g.$$

We have $m+r' < m+r'+t'$ and $m+t' < m+r'+t'$, thus for $c \geq 1$,

$$[m+r']^c < [m+r'+t']^c \text{ and } [m+t']^c < [m+r'+t']^c.$$

So, for $c \geq 1$ and $g \geq 0$,

$$([m+r']^c + m^c)^g \leq ([m+r'+t']^c + m^c)^g$$

and

$$([m+t']^c + m^c)^g \leq ([m+r'+t']^c + m^c)^g.$$

Therefore $SO_{c,g}(K_{m,z-m}) - SO_{c,g}(F') \geq 0$. We have $SO_{c,g}(K_{m,z-m}) \geq SO_{c,g}(F') > SO_{c,g}(H')$, hence H' does not have the maximum $SO_{c,g}$, a contradiction. So H' is $K_{m,z-m}$ and

$$SO_{c,g}(K_{m,z-m}) = m(z-m)(m^c + (z-m)^c)^g.$$

3. Corollaries

By [18], for every graph having z vertices,

$$\alpha + \beta = z.$$

For graphs without isolated vertices,

$$m + \beta' = z.$$

For bipartite graphs having no isolated vertices,

$$\alpha = \beta', \text{ thus } m = \beta;$$

see [18]. Therefore, Corollary 1 follows from Theorem 3.

Corollary 1: *Let $c \geq 1$ and $g \geq 0$. For any bipartite graph H having z vertices and vertex cover number β such that $2 \leq \beta \leq \lfloor \frac{z}{2} \rfloor$,*

$$SO_{c,g}(H) \leq \beta(z-\beta)(\beta^c + (z-\beta)^c)^g.$$

The extremal graph is $K_{\beta,z-\beta}$.

We have $2 \le m \le \lfloor \frac{z}{2} \rfloor$ in Theorem 3, so

$$z-2 \ge \beta' \ge \left\lceil \frac{z}{2} \right\rceil.$$

Using $m+\beta' = z$, Theorem 3 says that for a bipartite graph H having matching number $z-\beta'$ and z vertices,

$$SO_{c,g}(H) \le (z-\beta)\beta((z-\beta)^c + \beta^c)^g.$$

Thus, we obtain Corollary 2.

Corollary 2: *Let $c \ge 1$ and $g \ge 0$. For a bipartite graph H having z vertices and independence number/edge cover number α such that $\lceil \frac{z}{2} \rceil \le \alpha \le z-2$, we have*

$$SO_{c,g}(H) \le \alpha(z-\alpha)(\alpha^c + (z-\alpha)^c)^g.$$

The extremal graph is $K_{\alpha, z-\alpha}$.

We use $c=2$ and $g=\frac{1}{2}$ in Theorem 3 and Corollary 1 to get a bound on the classical Sombor index. Similarly, we use $c=2$ and $g=1$ to obtain a bound on the forgotten index.

Corollary 3: *For any bipartite graph H having z vertices and matching number/vertex cover number m such that $2 \le m \le \lfloor \frac{z}{2} \rfloor$, we have*

$$SO(H) \le m(z-m)\sqrt{z^2+2m^2-2zm}$$

and

$$FI(H) \le m(z^3 - 3z^2m + 4zm^2 - 2m^3).$$

The extremal graph is $K_{m,z-m}$.

Corollary 4 for the Sombor index and forgotten index follows from Corollary 2.

Corollary 4: *For a bipartite graph H having z vertices and independence number/edge cover number α such that $\lceil \frac{z}{2} \rceil \le \alpha \le z-2$, we have*

$$SO(H) \le \alpha(z-\alpha)\sqrt{z^2-2z\alpha+2\alpha^2}$$

and

$$FI(H) \le \alpha(z^3 - 3z^2\alpha + 4z\alpha^2 - 2\alpha^3).$$

The extremal graph is $K_{\alpha, z-\alpha}$.

We use $c = 2$ and $g = \frac{1}{2}$ in Theorem 1 to get Corollary 5 on the classical Sombor index. This result was given also in [7].

Corollary 5: *For a tree A containing z vertices, where* $z \geq 4$,

$$SO(A) \leq (z-1)\sqrt{z^2 - 2z + 2}.$$

The extremal graph is $K_{1,z-1}$.

We get Corollary 6 on the forgotten index when using $c = 2$ and $g = 1$ in Theorems 1 and 2.

Corollary 6: *For a tree A having z vertices, where* $z \geq 4$,

$$8z - 14 \leq FI(A) \leq z^3 - 3z^2 + 4z - 2.$$

The graph with the smallest and largest FI are P_z and $K_{1,z-1}$, respectively.

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