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Sombor Index of Hypergraphs

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Abstract

Recently, the Sombor index of a graph was defined, and a large amount of study was conducted quite quickly. It has been proposed to generalise the idea of vertex degree-based topological indices from graphs to hypergraphs. We give the bounds for the Sombor index of hypergraphs and bipartite hypergraphs using the total number of vertices in the graph. Hypertrees are the connected hypergraph, where the removal of any hyperedge disconnects the hypergraph. A k-uniform hypergraph is a hypergraph with k vertices in every hyperedge and a linear hypergraph is a hypergraph where any two hyperedges can have at most one vertex in common. We give the extremal hypergraphs among the class of uniform, linear and general hypertrees. The expected generalisation of some vertex degree based topological indices from graphs to hypergraphs has been listed.

1 Introduction

Despite the fact that the Sombor index was recently defined in 2020, it has received extensive research due to its wide range of applications [1, 2, 8]. Topological indices play an important role in predicting the properties of molecules and materials, which aids drug design and materials science.

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They enable quantitative structure-activity relationship (QSAR) studies, which guide compound optimisation for desired activities. Sombor index is a vertex degree based topological index defined for graphs and hence, provides information about the spatial arrangement of atoms within a molecule, which helps to explain structure-property relationships. Regardless of having so many applications, the vertex degree based topological indices has only been studied for simple graphs and recently for graphs with self-loops [24], and it has not been considered for hypergraphs to our knowledge, whereas the Wiener index has been considered [23].

Hypergraphs find application in chemistry when modeling molecules or chemical reactions involving multiple atoms bonding simultaneously. Unlike graphs, hypergraphs can represent interactions involving more than two atoms, which is particularly relevant for reactions with complex bonding patterns or in capturing molecular properties that arise from multiple atom groupings. Hypergraphs offer a more accurate depiction of certain chemical scenarios, such as transition states in reactions, which involve multiple atoms simultaneously changing their bonding configurations. The lack of a convenient representation for molecules with delocalized polycentric bonds is the main draw back of the structure theory. Hence these problems can be resolved by hypergraph respresentation of the molecules, which is known as molecular hyppergraphs. The model for an organometallic compound, where the hyperedges with two vertices represent covalent bond and with more than two vertices represent delocalised polycentric bonds, was studied in [14].

Let $\mathcal{H} = (V, E)$ be a hypergraph on the non-empty finite vertex set V, with the (hyper) edge set E, which contains the subsets (called hyperedges) of V. If $\mathcal{H}$ does not contain multiple hyperedges, then E is the subset of the power set of V. Let v be a vertex and e be a hyperedge in $\mathcal{H}$ and, if $v \in e$ then we say e contains v or v is contained in e. The degree of any vertex v in $\mathcal{H}$ denoted by d_v, is the number of hyperedges that contain v. The degree of a hyperedge e is the number of vertices that are contained in e. In this article, we consider the hypergraph $\mathcal{H}$ that does not contain any multiple hyperegdes or empty hyperedges or hyperedges of degree one. A hypergraph $\mathcal{H}$ is said to be linear, if any two hyperedges in $\mathcal{H}$ have at most one vertex in common.

A walk in a hypergraph is a sequence of vertices and hyperedges, $(v_0, e_1, v_1, e_2, v_2, \ldots, e_t, v_t)$ with $v_{i-1}v_i \in e_i$ and $v_{i-1} \neq v_i$. A walk w in a hypergraph $\mathcal{H}$ is called a path in $\mathcal{H}$ if all e_i's and all v_i's are distinct in w and, is called a cycle if all e_i's and v_i's are distinct except $v_0 = v_t$. A hypergraph is connected, if there exist a path between any two vertices in the hypergraph. A hypertree [20] $\mathcal{T}$ is a connected hypergraph in which removal of any hyperedge in $\mathcal{T}$ disconnects the hypergraph and it is important to note that a hypertree can contain cycle. Two hyperedges in a hypergraph are said to be adjacent if they have at least one vertex in common. A vertex u in a hypergraph is called a pendant vertex, if degree of the vertex u is one. A hyperedge e in a hypergraph is said to be a pendant hyperedge at a vertex $v \in e$ of degree greater than or equal two, if degree of every *other* vertex in e is of degree one. A hypergraph with degrees of its every hyperedge is k is known as a k-uniform hypergraph. A sunflower hypergraph $\mathcal{S}(m, k, h)$ is a h uniform hypergraph, with $m > 0$, and $0 < k < h$ is defined [4] as follows. Let $\mathcal{A}$ be a set of k vertices called seeds and define m disjoint sets $\{\mathcal{B}_i\}_{i=1}^{m}$ of $h-k$ vertices each, called petals. Now, hyperedges of the sunflower are $\mathcal{A} \cup \{\mathcal{B}_i\}, 1 \leq i \leq m$. A bipartite hypergraph $\mathcal{H}(V = V_1 \cup V_2, E)$ is a hypergraph whose vertex set V can be partitioned into non-empty subsets V_1 and V_2 such that, every hyperedge in E contains at least one vertex from each of the partition V_1 and V_2.
The Sombor index of a graph G is defined as

$$SO(G) = \sum_{\{u,v\} \in E} \sqrt{d_u^2 + d_v^2},$$

where d_u and d_v are the degrees of the vertices u and v respectively. We define the Sombor index for the hypergraph $\mathcal{H}$ as

$$SO(\mathcal{H}) = \sum_{e_i \in E} \sqrt{\sum_{u \in e_i} d_u^2},$$

where the summation inside runs over all the vertices u in e_i and the summation outside runs over all the edges e_i in E. To avoid confusion, several of the terms used in the subsequent sections are defined here.

A hypergraph on the vertex set V (which has at least two vertices) with edge set being the collection of all possible subsets of V which are non-empty is known as a complete hypergraph and is denoted by $\mathcal{H}_{K_n}$. The hypergraph which is obtained by removing all the hyperedges of degree one from $\mathcal{H}_{K_n}$, is denoted by $\mathcal{H}^*_{K_n}$.

A complete bipartite hypergraph denoted by $\mathcal{H}_{K_{p,q}}$ can be defined as the bipartite hypergraph $\mathcal{H}(V_1 \cup V_2, E)$, with *all possible hyperedges* such that, every hyperedge in E contains at least one vertex from each of the partition V_1 and V_2.

In a hypertree, if the degree of every vertex is at most two and a hyperedge is adjacent to at most two other hyperedges then we call it as a hyperpath. A hyperstar can be defined as a hypertree whose all hyperedges are pendant hyperedges. In [21], the authors defined uniform hypertree (or hyperpath or hyperstar) as the power graph of tree (or path graph or star graph), which was later studied as a general hypertrees.

For any other undefined terminologies one can refer to [3].

The bounds for the Sombor index of a hypergraph and hypertrees are discussed in this article.

2 Hypergraph and bipartite hypergraph

This section deals with the bounds for the Sombor index of a hypergraph and a bipartite hypergraph.

Theorem 1. *Let $\mathcal{H}$ be a connected hypergraph with no single element subset as a hyperedge, on $n \geq 2$ vertices. Then*

$$\sqrt{n} \leq SO(\mathcal{H}) \leq \left(2^{n-1} - 1\right) \sum_{i=2}^{n} \sqrt{i} \binom{n}{i},$$

where the lower bound is attained by the hypergraph, whose edge set $E = \{V\}$ and the upper bound is attained by the hypergraph $\mathcal{H}^*_{K_n}$.

Proof. Since the hypergraph $\mathcal{H}$ is connected, the lower bound is trivial and is attained when $\mathcal{H}$ has only one hyperedge which contains all the vertices of $\mathcal{H}$.

It is easy to observe that the upper bound is attained by $\mathcal{H}^*_{K_n}$. Since $\mathcal{H}$ can not contain empty edges or multiple edges or edges of degree one, in $\mathcal{H}^*_{K_n}$ of order $n \geq 2$, there will be $\binom{n}{i}, 2 \leq i \leq n$ hyperedges of degree i. Here $\mathcal{H}^*_{K_n}$ is regular and the degree of any vertex u in $\mathcal{H}^*_{K_n}$ is given by

$$d_u = \binom{n-1}{1} + \binom{n-1}{2} + \cdots + \binom{n-1}{n-1} = 2^{n-1} - 1.$$

Now,

$$\begin{aligned}
SO(\mathcal{H}^*_{K_n}) &= \sum_{e_i \in E} \sqrt{\sum_{u \in e_i} d_u^2} \\
&= \sum_{\substack{e_i \in E \\ |e_i|=2}} \sqrt{\sum_{u \in e_i} d_u^2} + \sum_{\substack{e_i \in E \\ |e_i|=3}} \sqrt{\sum_{u \in e_i} d_u^2} + \cdots + \sum_{\substack{e_i \in E \\ |e_i|=n}} \sqrt{\sum_{u \in e_i} d_u^2} \\
&= \sum_{\substack{e_i \in E \\ |e_i|=2}} \sqrt{2d_u^2} + \sum_{\substack{e_i \in E \\ |e_i|=3}} \sqrt{3d_u^2} + \cdots + \sum_{\substack{e_i \in E \\ |e_i|=n}} \sqrt{nd_u^2} \\
&= \binom{n}{2}\sqrt{2}d_u + \binom{n}{3}\sqrt{3}d_u + \cdots + \binom{n}{n}\sqrt{n}d_u \\
&= \left(2^{n-1} - 1\right) \sum_{i=2}^{n} \sqrt{i}\binom{n}{i}.
\end{aligned}$$

■

Corollary. *Let $\mathcal{H}$ be a connected hypergraph on $n \geq 1$ vertices. (i.e. if $\mathcal{H}$ contains single element subset as a hyperedge, then*

$$SO(\mathcal{H}) \leq 2^{n-1} \sum_{i=1}^{n} \sqrt{i}\binom{n}{i},$$

where the equality is attained by the complete hypergraph, $\mathcal{H}_{K_n}$.

Let $\mathcal{H}^{(k)}_{K_n}$ be the k-uniform hypergraph on n vertices with all possible k-element subset of the vertex set as the edge set.

Theorem 2. *Let $\mathcal{H}$ be a connected k-uniform hypergraph on $n \geq 2$ vertices. Then*

$$SO(\mathcal{H}) \leq \sqrt{k}\binom{n}{k}\binom{n-1}{k-1}$$

where the equality is attained by the hypergraph $\mathcal{H}^{(k)}_{K_n}$.

Theorem 3. *Let* $\mathcal{H} = \mathcal{H}(V_1 \cup V_2, E)$ *be a connected bipartite hypergraph on* $n = p + q$ *vertices, where* $|V_1| = p$ *and* $|V_2| = q$*. Then*

$$\sqrt{n} \leq SO(\mathcal{H}) \leq \sum_{j=2}^{n} \sum_{i=1}^{j-1} \binom{p}{i} \binom{q}{j-i} \sqrt{i d_u^2 + (j-i) d_v^2},$$

(*if* $s > t$, $\binom{t}{s} = 0$), *where* $d_u = 2^{p-1}(2^q - 1)$ *and* $d_v = 2^{q-1}(2^p - 1)$*. Here, the upper bound is attained by the complete bipartite hypergraph* $\mathcal{H}_{K_{p,q}}$.

Proof. Let V_1 and V_2 be the bipartition of the vertex set V of the bipartite hypergraph, $\mathcal{H}$ with $|V_1| = p$ and $|V_2| = q$.
The lower bound is direct and the maximum number of possible hyperedges in a bipartite hypergraph $\mathcal{H}(V_1 \cup V_2, E)$ is attained by the complete bipartite hypergraph, $\mathcal{H}_{K_{p,q}}$. Therefore, the degree of any vertex $u \in V_1$ is given by,

$$\begin{aligned} d_u &= (2^q - 1) + (p-1)(2^q - 1) + \binom{p-1}{2}(2^q - 1) + \cdots \\ &\quad + \binom{p-1}{p-1}(2^q - 1) = (2^q - 1)(2^{p-1}). \end{aligned}$$

Similarly, the degree of any vertex $v \in V_2$ is $d_v = (2^p - 1)(2^{q-1})$. Let E be the edge set of the complete bipartite hypergraph $\mathcal{H}_{K_{p,q}}$. Then,

$$\begin{aligned} SO(\mathcal{H}_{K_{p,q}}) &= \sum_{e_i \in E} \sqrt{\sum_{x \in e_i} d_x^2} \\ &= \sum_{\substack{e_i \in E \\ |e_i| = 2}} \sqrt{\sum_{x \in e_i} d_x^2} + \sum_{\substack{e_i \in E \\ |e_i| = 3}} \sqrt{\sum_{x \in e_i} d_x^2} + \cdots + \sum_{\substack{e_i \in E \\ |e_i| = n}} \sqrt{\sum_{x \in e_i} d_x^2} \end{aligned}$$

Here, $\sum\limits_{\substack{e_i \in E \\ |e_i| = 2}} \sqrt{\sum\limits_{x \in e_i} d_x^2} = \sum\limits_{\substack{e_i \in E \\ |e_i| = 2}} \sqrt{d_u^2 + d_v^2} = pq\sqrt{d_u^2 + d_v^2}$, where $u \in V_1, v \in V_2$.

$$\sum_{\substack{e_i\in E\\|e_i|=3}} \sqrt{\sum_{x\in e_i} d_x^2} = q\binom{p}{2}\sqrt{2d_u^2+d_v^2} + p\binom{q}{2}\sqrt{d_u^2+2d_v^2}$$

$$= \sum_{i=1}^{2}\binom{p}{i}\binom{q}{3-i}\sqrt{id_u^2+(3-i)d_v^2}.$$

For an arbitrary j, where $2 \leq j \leq n$, we have

$$\sum_{\substack{e_i\in E\\|e_i|=j}} \sqrt{\sum_{x\in e_i} d_x^2} = \sum_{i=1}^{j-1}\binom{p}{i}\binom{q}{j-i}\sqrt{id_u^2+(j-i)d_v^2},$$

provided $\binom{t}{s} = 0$, if $s > t$. On taking the summation from $j = 2$ to $j = n$,

$$SO(\mathcal{H}) \leq \sum_{j=2}^{n}\sum_{i=1}^{j-1}\binom{p}{i}\binom{q}{j-i}\sqrt{id_u^2+(j-i)d_v^2}. \qquad \blacksquare$$

Let $\mathcal{H}^{(k)}_{K_{p,q}}$ be the bipartite hypergraph with bipartition $V = V_1 \cup V_2$ and edge set as all possible k-element subsets of V such that every subset contain at least one element from each of V_1 and V_2.

Theorem 4. *Let $\mathcal{H} = \mathcal{H}(V_1 \cup V_2, E)$ be a connected k-uniform bipartite hypergraph on $n = p + q$ vertices, where $|V_1| = p$ and $|V_2| = q$. Then*

$$SO(\mathcal{H}) \leq \sum_{j=1}^{r}\binom{p}{j}\binom{q}{k-j}\sqrt{jD_1^2+(k-j)D_2^2}$$

(if $s > t$, $\binom{t}{s} = 0$), where $D_1 = \sum_{i=0}^{r}\binom{p-1}{i}\binom{q}{k-1-i}$ and $D_2 = \sum_{i=0}^{r}\binom{q-1}{i}\binom{p}{k-1-i}$, where $r = \min\{k-1, p, q\}$. The upper bound is attained by the k-uniform bipartite hypergraph $\mathcal{H}^{(k)}_{K_{p,q}}$.

3 Extremal hypertrees

The bounds for the Sombor index of a hypertree is discussed in this section.

Theorem 5. *Let $\mathcal{T}$ be a hypertree on n vertices. Then*

$$\sqrt{n} \leq SO(\mathcal{T}) \leq (n-1)\sqrt{(n-1)^2+1},$$

where the equality in the upper bound holds if and only if $\mathcal{T}$ is star graph on n vertices.

Proof. The lower bound is direct because a hyperedge containing all the vertices of the hypergraph is a hypertree. Among n vertex hypertrees the maximum number of hyperedges possible is $n-1$ and is attained when all the hyperedges of the hypertrees are of degree two. That is, the tree on n vertices. But, in [10] authors have shown that the star graph S_n has the maximum value of Sombor index among all trees of order n and

$$SO(S_n) = \sum_{e_i \in E} \sqrt{\sum_{u \in e_i} d_u^2} = \sum_{e_i \in E} \sqrt{(n-1)^2+1} = (n-1)\sqrt{(n-1)^2+1}.$$

■

Theorem 6. *Let $\mathcal{P}_n$ be a hyperpath on $n \geq 3$ vertices. Then*

$$\sqrt{n} \leq SO(\mathcal{P}_n) \leq 2\sqrt{5} + 2\sqrt{2}(n-3),$$

where the equality in the upper bound holds if and only if $\mathcal{P}_n$ is a path graph on n vertices.

Proof. Since the degree of any vertex in the hyperpath is either one or two, maximising the number of edges in a hypergraph along with maximising the number of vertices having degree equal to two, maximises the $SO(\mathcal{P}_n)$. The maximum number of edges possible in a hyperpath is $n-1$ as well as the maximum number of vertices having degree equal to two is $n-2$ and both are attained by path graph P_n. Therefore,

$$SO(P_n) = 2\sqrt{2^2+1} + (n-3)\sqrt{2.2^2} = 2\sqrt{5} + 2\sqrt{2}(n-3).$$ ■

Let $\mathcal{P}_n^*$ be a linear hyperpath on n vertices and $n > m \geq 3$ hyperedges such that all hyperedges are of degree two, except one non-pendant hyperedge whose degree is greater than or equal to two. A hyperpath $\mathcal{P}_n^*$ is shown in Figure 1.

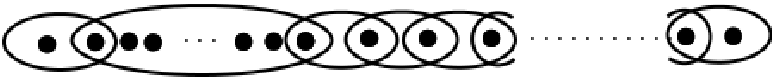

Figure 1. The hyperpath $\mathcal{P}_n^*$

Lemma 1. *Let $\mathcal{P}_n$ be a hyperpath on $n = m+k, k \geq 1$ vertices with $m \geq 3$ hyperedges. Then*

$$2\sqrt{5} + (m-3)\sqrt{8} + \sqrt{k+7} \leq SO(\mathcal{P}_n)$$

where the equality holds if and only if $\mathcal{P}_n$ is isomorphic to $\mathcal{P}_n^*$.

Proof. Since the number of vertices and hyperedges are fixed, in order to minimise $SO(\mathcal{P}_n)$, the number vertices of degree two must be minimum. Let $a_i > 0, 1 \leq i \leq m$, be a positive integer and $0 \leq \alpha \leq 1$ be a real, then

$$\left(\sum a_i\right)^{\alpha} \leq \sum a_i^{\alpha}. \tag{1}$$

Therefore, all the vertices of degree one are to be contained in least possible number of hyperedges. Let $a < b$ and $k > 0$ be reals, then we have

$$\sqrt{a+k} - \sqrt{a} > \sqrt{b+k} - \sqrt{b}. \tag{2}$$

Therefore, except one vertex of degree one in each of the two pendant hyperedges all the remaining vertices of degree one are to be contained in any one of the non-pendant hyperedges. Hence,

$$\begin{aligned} SO(\mathcal{P}_n^*) &= 2\sqrt{2^2+1} + \sqrt{2.2^2 + (k-1).1^2} + (m-3)\sqrt{2.2^2} \\ &= 2\sqrt{5} + \sqrt{7+k} + (m-3)\sqrt{8}. \end{aligned}$$ ■

Theorem 7. *Let $\mathcal{T}$ be a hypertree on $n = m+k, k \geq 1$ vertices, with $m \geq 3$ hyperedges. Then*

$$2\sqrt{5} + (m-3)\sqrt{8} + \sqrt{k+7} \leq SO(\mathcal{T}) \leq m\sqrt{km^2+1},$$

where the equality in the lower bound and upper bound holds if and only if $\mathcal{T}$ is isomorphic to the hyperpath $\mathcal{P}_n^*$, and the sunflower $\mathcal{S}(m, k, k+1)$ respectively.

Proof. The lower bound follows from Lemma 1. In order to obtain the upper bound, maximum number of vertices should have the maximum degree and these vertices has to be included uniformly among all the hyperedges. In a hypertree on $n = m + k, k \geq 1$ vertices, with m hyperedges, it is crucial to observe that a hyperedge can have a maximum degree of $k+1$ and it is trivial that a vertex can have maximum degree of m. In the extremal hypergraph $\mathcal{S}(m, k, k+1)$, each hyperedge is of degree $k+1$ (maximum among all hypertrees) and in each hyperedge k vertices (out of $k+1$, which is also maximum among all hypertrees) have degree equal to the maximum degree, m. ■

The sunflower hypergraph $\mathcal{S}(4, 7, 8)$ on 11 vertices and 4 hyperedges as shown in Figure 2, has the Sombor index value equal to $4\sqrt{7(4^2)+1}$.

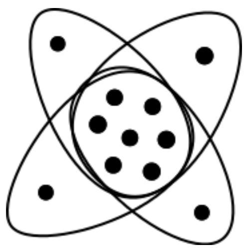

Figure 2. The sunflower hypergraph $\mathcal{S}(4, 7, 8)$.

$\mathcal{S}_n^*$ is a hyperstar on $n = m+k$ vertices, where $k = 1+m(r-1)+t, r \geq 1, 0 \leq t \leq m-1$, with m hyperedges such that t out of m hyperedges are of degree $r+2$ and $m-t$ hyperedges are of degree $r+1$. Figure 3 represents the hyperstar $\mathcal{S}_{21}^*$ with 6 hyperedges.

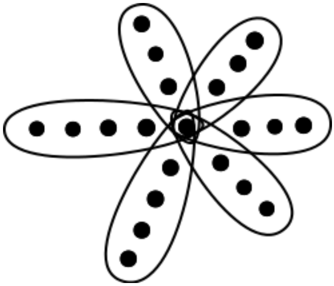

Figure 3. The hyperstar $\mathcal{S}_{21}^*$ with $m = 6$.

$\mathcal{S}_n^\dagger$ is a hyperstar on $n = m+k, k \geq 1$ vertices, with m hyperedges, such that $m-1$ hyperedges contain one pendant vertex each, and one hyperedge contain k pendant vertices. The hyperstar $\mathcal{S}_{11}^\dagger$ having 6 hyperedges is shown in Figure 4.

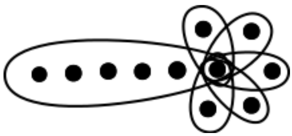

Figure 4. The hyperstar $\mathcal{S}_{11}^\dagger$ with 6 hyperedges

Lemma 2. *Let $\mathcal{S}_n$ be a hyperstar on $n = m + k$ vertices, where $k = 1 + m(r-1) + t, r \geq 1, 0 \leq t \leq m-1$, with m hyperedges. Then*

$$(m-1)\sqrt{m^2+1} + \sqrt{m^2+k} \leq SO(\mathcal{S}_n) \leq t\sqrt{m^2+r+1} + (m-t)\sqrt{m^2+r},$$

where the equality in the lower bound holds if and only if $\mathcal{S}_n$ is isomorphic to $\mathcal{S}_n^\dagger$ and equality in the upper bound holds if and only if $\mathcal{S}_n$ is isomorphic to $\mathcal{S}_n^*$.

Proof. In a hyperstar, as every hyperedge is a pendant hyperedge, degree of every vertex except the central vertex, is one. Therefore, the variation in $SO(\mathcal{S}_n)$ is due to assignment of these $n-1$ pendant vertices among the m pendant hyperedges. From the inequality (1), in order to minimise $SO(\mathcal{S}_n)$, maximum number of vertices among all these pendant vertices has to be included in a single hyperedge but each hyperedge in a hyperstar must contain atleast one pendant vertex. In $\mathcal{S}_n^\dagger$, $m-1$ hyperedges contain one pendant vertex each and remaining one hyperedge contain all the remaining k pendant vertices out of $n = m + k, k \geq 1$ vertices.

$$SO(\mathcal{S}_n^{\dagger}) = (m-1)\sqrt{m^2+1} + \sqrt{m^2+k}.$$

Now, in order to maximise $SO(\mathcal{S}_n)$, again by using the same inequality all these $m+k-1$ pendant vertices, where $k = 1 + m(r-1) + t, r \geq 1, 0 \leq t \leq m-1$, has to be included (almost) equally among all the hyperedges. Hence t out of m hyperedges will have the degree $r+2$ and $m-t$ hyperedges will have the degree $r+1$.

$$SO(\mathcal{S}_n^{*}) = t\sqrt{m^2+r+1} + (m-t)\sqrt{m^2+r}. \qquad \blacksquare$$

Theorem 8. *Let $\mathcal{T}$ be a hypertree on $n = m + k$ vertices, where $k = 1 + m(r-1) + t, r \geq 1, 0 \leq t \leq m-1$, with m hyperedges. Then*

$$SO(\mathcal{P}_n^{*}) \leq SO(\mathcal{T}) \leq SO(\mathcal{S}_n^{*}).$$

Theorem 9. *Let $\mathcal{T}$ be a k-uniform hypertree with m hyperedges. Then*

$$2\sqrt{k+3} + (m-2)\sqrt{k+6} \leq SO(\mathcal{T}) \leq m\sqrt{km^2+1},$$

with equality holds if and only if $\mathcal{T}$ is linear k-uniform hyperpath (lower bound) or $\mathcal{T}$ is isomorphic to the sunflower $\mathcal{S}(m, k, k+1)$ (upper bound).

Theorem 10. *Let $\mathcal{T}$ be a linear k-uniform hypertree with m hyperedges. Then*

$$2\sqrt{k+3} + (m-2)\sqrt{k+6} \leq SO(\mathcal{T}) \leq m\sqrt{m^2+k-1}$$

with equality if and only if $\mathcal{T}$ is linear k-uniform hyperpath or linear k-uniform hyperstar.

Theorem 11. *Let $\mathcal{P}_n$ be a hyperpath on $n = 2 + (m-1)r + t, r \geq 1, 0 \leq t \leq m-2$, vertices with m hyperedges. Then*

$$SO(\mathcal{P}_n) \le \begin{cases} 2\sqrt{4r+1} + 2\sqrt{2}(m-2), & if\ t=0 \\ \sqrt{4r+1} + \sqrt{4r+5} + 2\sqrt{2r+1} + 2\sqrt{2r}(m-3), & if\ t=1 \\ 2\sqrt{4r+5} + 4(t-1)\sqrt{2r+1} + 2\sqrt{2r}(m-2t), & if\ 2 \le t \le \left\lceil \frac{m-1}{2} \right\rceil \\ 2\sqrt{4r+5} + 2\left(2\left(t - \lceil \frac{m-1}{2} \rceil\right) - 1\right)\sqrt{2(r+1)} & \\ +2\left(m-1-2\left(t - \left\lceil \frac{m-1}{2} \right\rceil\right)\right)\sqrt{2r+1}, & if\ t\ is\ odd,\ and\ \left\lceil \frac{m-1}{2} \right\rceil + 1 \le t \le m-2 \\ 2\sqrt{4r+5} + 4\left(t - \left\lceil \frac{m-1}{2} \right\rceil\right)\sqrt{2r+2} & \\ +2\left(m-2-2\left(t - \left\lceil \frac{m-1}{2} \right\rceil\right)\right)\sqrt{2r+1}, & if\ t\ is\ even,\ and\ \left\lceil \frac{m-1}{2} \right\rceil + 1 \le t \le m-2 \end{cases}$$

Proof. Let m be the number of hyperedges and $n = 2 + (m-1)r + t, r \ge 1, 0 \le t \le m-2$ be the total number vertices in $\mathcal{P}_n$. As the total number of vertices and edges are fixed, in order to maximize $SO(\mathcal{P}_n)$, the number of vertices of degree two must be maximum and is equal to $n-2$. By using the inequality (1), it is important to note that the vertices of degree two has to be included equally in the intersection of hyperedges which are adjacent. That is, the difference between the number of vertices in the intersection of any two adjacent hyperedges with the number of vertices in the intersection of any other pair of adjacent hyperegdes of $\mathcal{P}_n$ is at most one. Now by using the inequality (2), the proof follows by characterising the extremal hypergraph $\mathcal{P}_n^\dagger$ by following cases.

Case 1. When $t = 0$, we have $n = (m-1)r + 2$ and the intersection of any two adjacent pairs of hyperedges contain r vertices. Figure 5, depicts the hyperpath $\mathcal{P}_n^\dagger$, when n is of the form $(m-1)r + 2$.

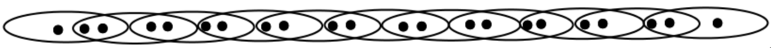

Figure 5. The hyperpath $\mathcal{P}_{22}^\dagger$ with $m = 11$

Therefore,

$$SO(\mathcal{P}_n^\dagger) = 2\sqrt{r\ (2^2) + 1} + (m-2)\sqrt{2r\ (2^2)}$$

$$= 2\sqrt{4r+1} + 2(m-2)\sqrt{2r}.$$

Case 2. When $t = 1$, the number of vertices $n = (m-1)r+3$. Now, again by using the inequality (2), except any one of the pendant hyperedges whose intersection with a non-pendant hyperedge contains $r+1$ vertices, all other adjacent pairs of hyperedges contain r vertices in their intersection. The hyperpath $\mathcal{P}_{23}^{\dagger}$ with $m = 11$ is shown in Figure 6.

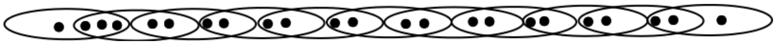

Figure 6. The hyperpath $\mathcal{P}_{23}^{\dagger}$ with $m = 11$

Hence, we have

$$\begin{aligned} SO(\mathcal{P}_n^{\dagger}) &= \sqrt{(r+1)2^2+1} + \sqrt{r\ (2^2)+1} + \sqrt{(2r+1)2^2} + (m-3)\sqrt{2r\ (2^2)} \\ &= \sqrt{4r+5} + \sqrt{4r+1} + 2\sqrt{(2r+1)} + 2(m-3)\sqrt{2r}. \end{aligned}$$

Case 3. When $2 \le t \le \lceil \frac{m-1}{2} \rceil$, two hyperedges each of which has only one adjacent hyperedge, will have $r+1$ vertices in the intersection with their adjacent pair of hyperedges. Now the vertices are to be included in the intersection of adjacent pair of hyperedges, in such a way that all the edges must have the degree either $2r$ or $2r+1$.
For this case, the example of the hyperpath $\mathcal{P}_n^{\dagger}$ on 24 and 27 vertices with 11 hyperedges and on 25 vertices with 10 hyperedges are shown in Figures 7, 8 and 9 respectively.

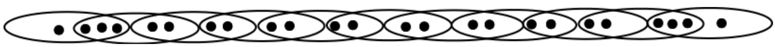

Figure 7. The hyperpath $\mathcal{P}_{24}^{\dagger}$ with $m = 11$

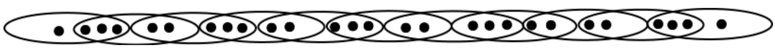

Figure 8. The hyperpath $\mathcal{P}_{27}^{\dagger}$ with $m = 11$

Figure 9. The hyperpath $\mathcal{P}_{25}^{\dagger}$ with $m = 10$

Now,

$$SO(\mathcal{P}_n^{\dagger}) = 2\sqrt{1+(r+1)2^2} + 2(t-1)\sqrt{(2r+1)2^2} + (m-2t)\sqrt{2r\ (2^2)}$$
$$= 2\sqrt{4r+5} + 4(t-1)\sqrt{2r+1} + 2(m-2t)\sqrt{2r}.$$

Case 4. When t is odd and $\lceil \frac{m-1}{2} \rceil + 1 \leq t \leq m-2$. Firstly, when $t = \lceil \frac{m-1}{2} \rceil + 1$, the vertex has to be included in the intersection of the unique hyperedge whose degree is $2r$, with any one of the adjacent hyperedges. Later, each vertex has to be included in the intersection of the adjacent hyperedges which contain r vertices until all the adjacent pairs of hyperedges has $r+1$ vertices in their intersection. Figure 10 depicts an example for Case 4.

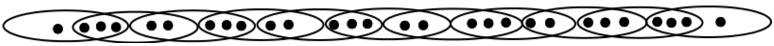

Figure 10. The hyperpath $\mathcal{P}_{28}^{\dagger}$ with $m = 11$

$$SO(\mathcal{P}_n^{\dagger}) = 2\sqrt{(r+1)2^2+1} + \left(2\left(t - \left\lceil \frac{m-1}{2} \right\rceil\right) - 1\right)\sqrt{2(r+1)2^2}$$
$$+ \left(m-1-2\left(t - \left\lceil \frac{m-1}{2} \right\rceil\right)\right)\sqrt{(2r+1)2^2}$$
$$= 2\sqrt{4r+5} + 2\left(2\left(t - \left\lceil \frac{m-1}{2} \right\rceil\right) - 1\right)\sqrt{2(r+1)}$$
$$+ 2\left(m-1-2\left(t - \left\lceil \frac{m-1}{2} \right\rceil\right)\right)\sqrt{2r+1}$$

Case 5. When t is even and $\lceil \frac{m-1}{2} \rceil + 1 \leq t \leq m-2$, the extremal hyperpath $\mathcal{P}_n^{\dagger}$, can be constructed similar to the previous case without much confusion and Figure 11 gives an example for $\mathcal{P}_n^{\dagger}$ on 26 vertices with 10 hyperedges.

Figure 11. The hyperpath $\mathcal{P}_{26}^{\dagger}$ with $m = 10$

$$SO(\mathcal{P}_n^{\dagger}) = 2\sqrt{(r+1)2^2+1} + 2\left(t - \left\lceil \frac{m-1}{2} \right\rceil\right)\sqrt{2(r+1)2^2}$$
$$+ 2\left(m-2-2\left(t - \left\lceil \frac{m-1}{2} \right\rceil\right)\right)\sqrt{2r+1}$$

$$= 2\sqrt{4r+5} + 4\left(t - \left\lceil\frac{m-1}{2}\right\rceil\right)\sqrt{2(r+1)}$$
$$+ 2\left(m - 2 - 2\left(t - \left\lceil\frac{m-1}{2}\right\rceil\right)\right)\sqrt{2r+1}$$

Figure 12. The hyperpath $\mathcal{P}^{\dagger}_{31}$ with $m = 11$

The hyperpath $\mathcal{P}^{\dagger}_{n}$ on $n = 2 + t + r(m-1)$ vertices with $t = m - 2$ will be of the above form, which has shown in Figure 12. ■

4 Conclusion

1). Some of the vertex degree based topological indices of graphs and the expected generalization to the hypergraphs have been listed.

Table 1. Expected generalizations for hypergraphs

Degree based indices	For graphs	For hypergraphs
First Zagreb [11]	$\sum_{\{u,v\}\in E} d_u + d_v$	$\sum_{e_i\in E}\sum_{u\in e_i} d_u$
Second Zagreb [12]	$\sum_{\{u,v\}\in E} d_u d_v$	$\sum_{e_i\in E}\prod_{u\in e_i} d_u$
First Hyper-Zagreb [25]	$\sum_{\{u,v\}\in E} (d_u + d_v)^2$	$\sum_{e_i\in E}\left(\sum_{u\in e_i} d_u\right)^2$
Second Hyper-Zagreb [28]	$\sum_{\{u,v\}\in E} (d_u d_v)^2$	$\sum_{e_i\in E}\left(\prod_{u\in e_i} d_u\right)^2$
Randić [22]	$\sum_{\{u,v\}\in E} \frac{1}{\sqrt{d_u d_v}}$	$\sum_{e_i\in E}\left(\prod_{u\in e_i} d_u\right)^{-\frac{1}{2}}$
Reciprocal Randić [13]	$\sum_{\{u,v\}\in E} \sqrt{d_u d_v}$	$\sum_{e_i\in E}\left(\prod_{u\in e_i} d_u\right)^{\frac{1}{2}}$
Sum-Connectivity [30]	$\sum_{\{u,v\}\in E} \frac{1}{\sqrt{d_u + d_v}}$	$\sum_{e_i\in E}\left(\sum_{u\in e_i} d_u\right)^{-\frac{1}{2}}$

Degree based indices	For graphs	For hypergraphs
Reciprocal Sum-Connectivity	$\sum_{\{u,v\}\in E} \sqrt{d_u + d_v}$	$\sum_{e_i\in E} \left(\sum_{u\in e_i} d_u\right)^{\frac{1}{2}}$
Forgotten [9]	$\sum_{\{u,v\}\in E} d_u^2 + d_v^2$	$\sum_{e_i\in E} \sum_{u\in e_i} d_u^2$
Inverse-degree [7]	$\sum_{\{u,v\}\in E} d_u^{-2} + d_v^{-2}$	$\sum_{e_i\in E} \sum_{u\in e_i} d_u^{-2}$
Geometric-Arithmetic [27]	$\sum_{\{u,v\}\in E} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$	$\sum_{e_i\in E} \frac{\lvert e_i\rvert \sqrt[\lvert e_i\rvert]{\prod_{u\in e_i} d_u}}{\sum_{u\in e_i} d_u}$
Arithmetic-Geometric [5]	$\sum_{\{u,v\}\in E} \frac{d_u + d_v}{2\sqrt{d_u d_v}}$	$\sum_{e_i\in E} \frac{\sum_{u\in e_i} d_u}{\lvert e_i\rvert \sqrt[\lvert e_i\rvert]{\prod_{u\in e_i} d_u}}$
Inverse Sum Indeg [26]	$\sum_{\{u,v\}\in E} \frac{d_u d_v}{d_u + d_v}$	$\sum_{e_i\in E} \frac{\prod_{u\in e_i} d_u}{\sum_{u\in e_i} d_u}$
Inverse degree [7]	$\sum_{\{u,v\}\in E} \frac{1}{d_u^2} + \frac{1}{d_v^2}$	$\sum_{e_i\in E} \sum_{u\in e_i} \frac{1}{d_u^2}$
First Gourava [15]	$\sum_{\{u,v\}\in E} d_u + d_v + (d_u d_v)$	$\sum_{e_i\in E} \sum_{u\in e_i} d_u + \prod_{u\in e_i} d_u$
Second Gourava [15]	$\sum_{\{u,v\}\in E} (d_u + d_v) d_u d_v$	$\sum_{e_i\in E} \left(\sum_{u\in e_i} d_u\right)\left(\prod_{u\in e_i} d_u\right)$
First Hyper-Gourava [16]	$\sum_{\{u,v\}\in E} (d_u + d_v + (d_u d_v))^2$	$\sum_{e_i\in E} \left(\sum_{u\in e_i} d_u + \prod_{u\in e_i} d_u\right)^2$
Second Hyper-Gourava [16]	$\sum_{\{u,v\}\in E} ((d_u + d_v)(d_u d_v))^2$	$\sum_{e_i\in E} \left(\left(\sum_{u\in e_i} d_u\right) \prod_{u\in e_i} d_u\right)^2$
Sum-Connectivity Gourava [17]	$\sum_{\{u,v\}\in E} \frac{1}{\sqrt{d_u + d_v + (d_u d_v)}}$	$\sum_{e_i\in E} \left(\sum_{u\in e_i} d_u + \prod_{u\in e_i} d_u\right)^{-\frac{1}{2}}$
Product-Connectivity Gourava [18]	$\sum_{\{u,v\}\in E} \sqrt{(d_u + d_v)(d_u d_v)}$	$\sum_{e_i\in E} \left(\left(\sum_{u\in e_i} d_u\right) \prod_{u\in e_i} d_u\right)^{\frac{1}{2}}$

Similarly, one can generalize the degree based multiplicative indices from graphs to hypergraphs.

2). The problem of finding maximum number of r-uniform hyperedges in a linear hypergraph on n vertices can be equated to the problem of finding the maximum number of edge disjoint complete subgraph K_r in the complete graph K_n (K_r decomposition of K_n for $r \leq n$, if exists).

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