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New upper bounds for the symmetric division deg index of graphs

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Abstract

We find a new upper bound for the symmetric division deg index $SDD(G)$ of a graph G with n vertices, in terms of the inverse degree index, that is attained by all regular, all complete multipartite graphs, $K_{p_1,p_2,\dots,p_r}$, and all $(n-1,d)$-regular graphs of order n, where $1 \le d < n-1$. This upper bound allows us to find further upper bounds in terms of other indices and other parameters. Along the way, we review some maximal results and upper bounds, and conjecture other results for c-cyclic graphs when $c \ge 3$.

Keywords: symmetric division deg index; inverse degree index; multipartite graphs; mixed degree-Kirchhoff index; Kirchhoff index.

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1. Introduction

Let $G = (V, E)$ be a finite simple connected graph with vertex set $V = \{1, 2, \dots, n\}$, edge set E and degrees $\Delta = d_1 \ge d_2 \ge \cdots \ge d_n = \delta$. A graph is d-regular if all its vertices have degree d; a graph is (a, b)-regular if its vertices have degree either a or b. (Beware: no bipartiteness is required in our definition of (a, b)-regular graph. For all graph theoretical terms the reader is referred to reference [15]).

The symmetric division deg index of G, defined by

$$SDD(G) = \sum_{(i,j)\in E} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right),$$

was introduced by Vukičević and Gašperov in [14] as one of the 148 so-called Adriatic indices, with a good predictive power for the total surface area of polychlorobiphenyls. More qualitative characteristics of this index relative to other indices can be found in [8].

In [13] several lower and upper bounds are found for $SDD(G)$, in particular

$$SDD(G) \le n\Delta \le n^2 - n, \tag{1}$$

where the equality is attained by all regular graphs. In this reference they also find that the maximum for the SDD index among trees of order n is $n^2 - 2n + 2$, attained by the star graph, and the maximum value among unicyclic graphs of order n is

$$n^2 - 3n + 5 + \frac{2}{n-1}, \tag{2}$$

attained by the graph constructed by connecting two leaves of the n-star with an extra edge.

Further upper and lower bounds for $SDD(G)$ were found in [9] and [10], specifically for our interests:

$$SDD(G) \le |E| \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta} \right), \tag{3}$$

where the equality in (3) is attained by all regular graphs and the star graph. Also,

$$SDD(G) \le p \left(\Delta + \frac{1}{\Delta} \right) + (|E| - p) \left(\frac{\Delta}{\delta_1} + \frac{\delta_1}{\Delta} \right),$$

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where p is the number of pendant vertices and δ_1 is the smallest degree larger than 1. The equality is attained by all regular graphs and the star graph. Additionally, more upper and lower bounds are found in terms of the Hyper-Zagreb index $HM(G) = \sum_{(i,j)\in E}(d_i + d_j)^2$ such as

$$SDD(G) \le p\left(\Delta + \frac{1}{\Delta}\right) + \frac{1}{\delta_1^2}\left[HM(G) - p(1+\delta_1^2)\right] - 2(|E| - p),$$

where the equality is attained by all regular graphs and the star graph.

In reference [9], the authors go on to obtain some Nordhaus-Gaddum type results, and they also identify the unicyclic graphs of order n with largest and second largest values of $SDD(G)$. They quote the largest value as

$$\frac{1}{2(n-1)}(2n^3 - 7n^2 + 10n + 3), \tag{4}$$

which is not correct and should be replaced with (2). Indeed, it is immediate to compute that for G the 3-cycle with an extra vertex attached with an extra edge to any of the vertices of the cycle we get $SDD(G) = \frac{29}{3}$, directly by the definition and through (2), whereas (4) produces $\frac{59}{6}$.

Reference [10] is concerned with the SSD index of operations of graphs in terms of the indices of the original graphs.

In [12] the authors give an upper bound for chemical trees and also they determine the graphs with the second, third and fourth minimum values of $SSD(G)$ for trees and unicyclic graphs, and the first, second and third minimum values for byciclic graphs.

Yang *et al.* define in [16] the *extended adjacency index* $EA(G)$, that turns out to be equal to $\frac{1}{2}SDD(G)$ and proceed to find maximal and minimal values of the index among trees, unicyclic and bicyclic graphs, effectively revisiting some results of [9, 12, 13]. They give an incorrect lower bound in the bicyclic case that should be $n + \frac{4}{3}$ (their quoted value would be the *second* smallest value among bicyclic graphs) as can be seen checking that for the graphs G_n which consist of the n-cycle with an extra edge between two non-adjacent vertices, one has $SDD(G_n) = 2n + \frac{8}{3}$, and thus $EA(G_n) = n + \frac{4}{3}$. (See Theorem 5(i) in [12]) . Their only new contribution seems to be the upper bound for the bicyclic graphs of order n, which for the SDD index would say:

$$SDD(G) \le n^2 - \frac{11}{3}n + 8 + \frac{4}{n-1}, \tag{5}$$

for all bicyclic graphs, where the equality is attained by the graph with degree sequence $(n-1, 3, 2^2, 1^{n-4})$ (here the powers represent the number of times the specific degree is repeated).

In [3] we considered a descriptor related to the SDD index, the mixed degree-Kirchhoff index defined as

$$\hat{R}(G) = \sum_{i<j}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right)R_{ij},$$

where R_{ij} is the effective resistance between vertices i and j when the graph is thought of as an electrical network. The index $\hat{R}(G)$ suggests a number of other different potential descriptors, where R_{ij} could be replaced with other functions of the edges, like the distance $d(i,j)$ in the graph between vertices i and j, and where the summation could be expanded from $(i,j) \in E$ to $i < j$, etc. Lemma 2 in the next section remind us that one of these possible descriptors is actually an affine transformation of the inverse degree index, of paramount importance in this article and defined as

$$I(G) = \sum_{i=1}^{n}\frac{1}{d_i}.$$

We point out finally that the SDD index is the subject of active contemporary research as attested by the very recent articles [1] (where among other things the authors correct an upper bound for the SDD index of molecular trees given in the recent article [12]) and [7].

2. The bounds

2.1 Upper bounds in terms of the inverse degree

We first present a couple of lemmas.

Lemma 2.1.

$$\frac{d_i}{d_j} + \frac{d_j}{d_i} \ge 2,$$

and the equality is attained if and only if $d_i = d_j$.

The following result was noted in passing in [4], without a proof that we include here for completeness

Lemma 2.2. *For any G we have*

$$\sum_{i<j}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)=2|E|I(G)-n.$$

Proof.

$$\sum_{i<j}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)=\sum_i\frac{1}{d_i}\sum_{j\neq i}d_j=\sum_i\frac{1}{d_i}(2|E|-d_i)=2|E|I(G)-n.$$

□

Now we can prove the main result of this note: an upper bound for $SDD(G)$ which is attained by a family of graphs larger than in any other similar upper bound found in the literature.

Proposition 2.1. *For any n vertex graph G we have*

$$SDD(G)\leq 2|E|(1+I(G))-n^2. \tag{6}$$

The equality in (6) is attained if and only if $d_i=d_j$ for every pair of non-adjacent vertices i and j of G, in particular by d-regular graphs, complete multipartite $K_{p_1,p_2,\ldots,p_r}$ graphs and $(n-1,d)$-regular graphs, for $1\leq d<n-1$.

Proof. For any G we have

$$\begin{aligned}SSD(G)&=\sum_{(i,j)\in E}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)=\sum_{i<j}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)-\sum_{(i,j)\notin E}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)\\&\leq\sum_{i<j}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)-\sum_{(i,j)\notin E}2 \qquad (7)\\&=2|E|I(G)-n-2\left(\binom{n}{2}-|E|\right)=2|E|(1+I(G))-n^2.\end{aligned}$$

For regular graphs it is clear that the inequality in (7) becomes an equality. The same happens for the complete multipartite graphs $K_{p_1,p_2,\ldots,p_r}$ because all pairs of vertices which are not at the endpoints of an edge have the same degree $\sum_{i\neq 1}p_i$ or the same degree $\sum_{i\neq 2}p_i$..., etc., making the expression $\frac{d_i}{d_j}+\frac{d_j}{d_i}$ equal to 2; a similar reasoning works for $(n-1,d)$-regular graphs: pairs of vertices which are not connected by an edge have the same degree d.

□

It is possible to find examples of $(n-1,d)$-regular graphs which are not complete multipartite: if we consider the n-wheel graph for $n\geq 6$ (for $n=5$, the wheel is equal to $K_{1,2,2}$), this is an $(n-1,3)$-regular graph which is easy to see is not multipartite on account of the single vertex with degree $n-1$, which must be one of the elements of the partition, and the remaining $n-1$ vertices cannot be partitioned in any way to make the graph multipartite without forcing some vertices to having degree greater than 3.

The strength of the bound (6) is that there are many known results for $I(G)$ that can be applied in order to get additional results for $SDD(G)$. In that regard, one may consult the review paper [2]. For instance, we can show the following

Proposition 2.2. *For all G we have*

$$SDD(G)\leq 2|E|\left(1+\left(\frac{1}{\delta}-\frac{1}{\Delta}\right)\left(n-1-\frac{2|E|}{n}\right)\right). \tag{8}$$

The equality is attained by all regular graphs.

Proof. Direct from (6) and the bound

$$I(G)\leq\frac{n^2}{2|E|}+\left(\frac{1}{\delta}-\frac{1}{\Delta}\right)\left(n-1-\frac{2|E|}{n}\right). \tag{9}$$

□

Remark 2.1. *It is stated in the review [2] and the original article [6] that in bound (9), besides by regular graphs, the equality is attained by the star graph. This is clearly not the case, because when G is the star graph, (9) becomes*

$$\frac{n^2}{2(n-1)}+\frac{(n-2)^2}{n}\neq n-1+\frac{1}{n-1}.$$

When we compare bound (8) with bound (3), the one in the literature that uses similar parameters, we observe that they are not comparable. Indeed, (3) attains the equality for the star graph, whereas (8) does not. On the other hand, if we consider the graph G_n to be the complete graph K_n minus one edge, for $n \geq 3$, it is clear that $\delta = n-2$ and $\Delta = n-1$, so that

$$\frac{\Delta}{\delta} + \frac{\delta}{\Delta} = \frac{n-1}{n-2} + \frac{n-2}{n-1} = 2 + \frac{1}{(n-1)(n-2)},$$

and (3) becomes

$$n(n-1) - 2 + \frac{n(n-1)-2}{2(n-1)(n-2)},$$

whereas (8) becomes

$$n(n-1) - 2 + \frac{4[n(n-1)-2]}{n(n-1)(n-2)},$$

so that (8) outperforms (3) for $n \geq 8$ (notice that these two bounds are better than the universal bound (1), so this discussion is not vacuous).

We can also exhibit a tight bound for $SDD(G)$ in terms of the Kirchhoff index $Kf(G)$ as follows:

Proposition 2.3. *For any G we have*

$$SDD(G) \leq 2|E|\left(\frac{Kf(G)+n}{n-1}\right) - n^2.$$

The equality is attained by the complete graph K_n and the complete bipartite graphs $K_{r,n-r}$, for $1 \leq r \leq \lceil \frac{n}{2} \rceil$.

Proof. In [17] it is shown that

$$I(G) \leq \frac{Kf(G)+1}{n-1},$$

where the equality is attained by K_n and by the complete bipartite graphs $K_{r,n-r}$, for $1 \leq r \leq \lceil \frac{n}{2} \rceil$.

□

We can also establish an upper bound for trees in terms of the diameter d using the fact (see [11]) that if T is a tree then $I(T) \leq \frac{3n}{2} - d$, where the equality is attained for all paths P_n, and the fact that the path P_3 also attains the equality in (6):

Proposition 2.4. *For any tree T of order n and diameter d, we have*

$$SDD(T) \leq 2(n-1)\left(1 + \frac{3n}{2} - d\right) - n^2,$$

where the equality is attained by the path P_3.

In a similar way, we could derive upper bounds for $SDD(G)$ in terms of the atom-bond connectivity, the harmonic and the Narumi-Katayama indices, using ad hoc upper bounds for $I(G)$ reviewed in reference [2], to which we direct the interested reader.

2.2 Upper bounds for c-cyclic graphs, $0 \leq c \leq 2$

In [5], using majorization, we found among other things the maximum values of the inverse degree index for c-cyclic graphs where $0 \leq c \leq 6$. This means that if we insert those values in (6) we will get upper bounds for the value of $SDD(G)$ among these c-cyclic graphs. The problem is that we do not get meaningful bounds for $c \geq 3$ because in those cases they exceed the universal upper bound (1). For $c \leq 2$ we obtain the following result.

Proposition 2.5. *The following upper bounds hold for $SDD(G)$ when G is*

a tree: $n^2 - 2n + 2$;

unicyclic: $n^2 - 2n + 2 + \dfrac{2}{n-1}$;

bicyclic: $n^2 - \dfrac{4}{3}n - \dfrac{4}{3} + \dfrac{4}{n-1}$.

3. Closing Remarks

The upper bound for the trees in Proposition 5 is attained by the star graph, because such graph is $(n-1,1)$-regular, so it provides an alternative way to prove that the maximum for $SDD(T)$ among trees T occurs for the star graph. For unicyclic and bicyclic graphs we obtain bounds that are slightly larger than the actual values (2) and (5) because the maximal graphs for $I(G)$ are not (n,d)-regular, though close enough (in the unicyclic case the bounds coincide for $n=3$, in the bicyclic for $n=4$). It is worth remarking that after comparing the results in [5] with those in [9,12,13,16], one can see that the graphs where the maximum and minimum values are attained for $I(G)$ coincide with those where the same extremal values are attained for $SDD(G)$, in the case of c-cyclic graphs for $0 \le c \le 2$, which leads us to propose the following conjecture.

Conjecture 3.1. *The extremal values of $I(G)$ and $SDD(G)$ in the set of c-cyclic graphs of order n, $3 \le c \le 6$, are attained by the same graph G.*

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