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Lower and Upper Bounds of the Forgotten Topological Index

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Dedicated to Prof. Fuji Zhang on the occasion of his 80th birthday

Abstract

In a 2015 paper [8] by Furtula and Gutman, the sum of cubes of vertex degrees of a molecular graph G is called the forgotten topological index and denoted by F(G). Authors of [8] establish lower and upper bounds of F(G) and show that F(G) can play a significant role in some physico-chemical applications.

In this paper, we provide new lower and upper bounds of the forgotten topological index F(G) in terms of graph irregularity, Zagreb indices, graph size, and maximum/minimum vertex degrees. We characterize all graphs that attain the new bounds of F(G) and show that the new bounds are better than the bounds given in [8] for all benzenoid systems with more than one hexagon. As corollaries, various upper bounds of F(G) easily follow. Moreover, upper bounds of F(G) for connected K_{r+1} -free graphs are also presented.

1 Introduction

In 2015, Furtula and Gutman [8] named the sum of cubes of vertex degrees of a molecular graph G as the forgotten topological index, and denoted it as F(G). Both the forgotten topological index and the first Zagreb index were employed in the formulas for total π electron energy in a 1972 paper [11] by Gutman and Trinajstić, as a measure of branching extent of the carbon-atom skeleton of the underlying molecule. Since then the first Zagreb index has eventually become one of the most popular and extensively studied graphbased molecular structure descriptors (for more details, see surveys [9, 10, 15]). However, the forgotten topological index has not yet been given special attention to and fully investigated. In the recent paper [8], Furtula and Gutman pointed out the importance of F(G) that it can be used to obtain a high accuracy of the prediction of logarithm of the octanol-water partition coefficient; see also [1]. By the weighted average inequality and Cauchy-Schwarz inequality, they obtained the following lower bounds on the forgotten topological index for any graph with m edges:

(1)
$$F(G) \ge \frac{M_1^2(G)}{2m}$$
.
(2) $F(G) \ge \frac{M_1^2(G)}{m} - 2M_2(G)$.

They pointed out that both bounds are attained in the case of regular graphs.

In the same paper, they also give an upper bound of F(G) for any graph G with n vertices and m edges:

(3) $F(G) \leq 2M_2(G) + m(n-2)^2$, where equality holds if and only if G is a star.

Note that in the above (3) we have corrected a typo in the upper bound given in their paper [8] where it appears as $F(G) \leq 2M_2(G) + m(n-2)$ with the error that the square for (n-2) is missing.

In this paper, we apply Cauchy-Schwarz inequality and Jensen's inequality (see [13]), and the variance bound inequality by Bhatia and Davis [3] to obtain new lower and upper bounds on the forgotten topological index in terms of graph irregularity, Zagreb indices, graph size, and extremal vertex degrees. Graphs that attain our bounds of F(G) are characterized. Moreover, various other upper bounds of F(G) are obtained as corollaries. Finally, we show that our new bounds are better than the bounds given in [8] for all benzenoid systems with more than one hexagon although they are incomparable for general graphs.

2 Preliminaries

All graphs considered in this paper are finite connected simple graphs. The set of all vertices of a graph G is denoted by V(G) and its cardinality |V(G)| is called the order of G. The set of all edges of a graph G is denoted by E(G) and its cardinality |E(G)| is called the size of G. The degree of a vertex u of G is the number of vertices adjacent to u in G and denoted by $d_G(u)$, and it will be written as d(u) briefly when no confusion can occur. A graph G is called regular if all vertices of G have the same vertex degree. A graph G is called bi-degreed if it has two distinct vertex degrees. A benzenoid system

is a 2-connected plane graph such that its each inner face is a regular hexagon with unit side length. So any benzenoid system with more than one hexagon is bi-degreed with two distinct vertex degrees: 2 and 3.

We now recall some vertex-degree-related topological indices that appear in the paper. They are the two Zagreb indices [4,12], the Forgotten Topological index [8], edge imbalance and irregularity of a graph [2].

The first Zagreb index $M_1(G)$ is the sum of squares of vertex degrees of G. It is well known that

$$M_1(G) = \sum_{u \in V(G)} d^2(u) = \sum_{uv \in E(G)} (d(u) + d(v))$$

The second Zagreb index $M_2(G)$ of G is the sum of the products of two end vertex degrees over all edges of G, that is,

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v) \ .$$

The forgotten topological index F(G) is the sum of cubes of vertex degrees of G. It is well known that

$$F(G) = \sum_{u \in V(G)} d^3(u) = \sum_{uv \in E(G)} \left(d^2(u) + d^2(v) \right) \ .$$

The edge imbalance of an edge is the absolute value of the difference of its two end vertex degrees. The irregularity of the graph G, denoted as irr(G), is the sum of all edge imbalances of G, that is,

$$irr(G) = \sum_{uv \in E(G)} |d(u) - d(v)| .$$

Note that a graph with constant edge imbalance is not necessary to be a bi-degreed graph, and that a bi-degreed graph is not necessary to have constant edge imbalance either.

Definition 2.1 [16] A connected graph G is called a bi-regular graph if G is a bipartite graph with two partite sets A and B such that each vertex in A has degree Δ and each vertex in B has degree δ .

Note: (i) Bi-regular graphs are called semi-regular bipartite graphs in [7].

(ii) In the above definition, Δ and δ are not restricted to be distinct. So, regular bipartite graphs are special cases of bi-regular graphs.

(iii) A bi-regular graph is a special type of bi-degreed bipartite graph, which has constant edge imbalance. A bi-degreed bipartite graph is not necessary to be bi-regular. One easy example is any benzenoid system with more than one hexagon.

In the following lemma, we give necessary and sufficient conditions for non-regular graphs to be bi-regular. This result has its own right in graph theory.

Lemma 2.2 Let G be a connected non-regular graph. Then the following statements are equivalent:

- (i) G is bi-regular.
- (ii) G is bi-degreed and |d(u) d(v)| > 0 is constant for all edges uv of G.
- (iii) d(u) + d(v) is constant for all edges uv of G.

Proof. Clearly, (i) implies (ii).

Now we prove that (ii) implies (iii). Since G is bi-degreed, we may write the two distinct vertex degrees as Δ and δ . Note that |d(u) - d(v)| > 0 is constant for all edges uv of G. Then $\{d(u), d(v)\} = \{\Delta, \delta\}$ for all edges uv of G, and so (iii) holds.

To show that (iii) implies (i), we first see that if d(u) + d(v) is constant for all edges uv of G, then any two vertices joined by a path of even length in G must have the same vertex degree. We now show that G is bipartite by contradiction. Suppose that G is not bipartite. Then G has an odd cycle C. Let a, b be two adjacent vertices on C. Then C contains a path of even length connecting a and b. Hence, d(a) = d(b) = s for some positive integer s. For any vertex x of G, there is a path P between a and x, since G is connected. By (iii), each edge e on the path P has the property that the sum of the two end vertex degrees of e is 2s since d(a) + d(b) = 2s for the edge ab of G. Recall that d(a) = s. Then each vertex on the path P has vertex degree s and so does x. It follows that G is regular. This contradicts the assumption that G is not regular. Hence, G is bipartite. Furthermore, any two vertices u, v in the same partite set of G are joined by a path of even length, and so d(u) = d(v). Therefore, G is bi-regular. This shows that (iii) implies (i). Thus, the proof of the proposition is complete.

We conclude this section with some inequalities to be used in the paper.

• Cauchy-Schwarz inequality (see [13]):

Let a_i and b_i be real numbers for all $1 \leq i \leq n$. Then

$$\left(\sum_{i=1}^n a_i b_i\right)^2 \le \left(\sum_{i=1}^n a_i^2\right) \left(\sum_{i=1}^n b_i^2\right) \ .$$

Equality holds if and only if $a_i b_j = a_j b_i$ for all $1 \le i, j \le n$.

• Jensen's inequality (see [13]):

Let f be a real continuous convex function over an interval I (i.e., the second derivative $f''(x) \ge 0$ for all $x \in I$). Then

$$f\left(\sum_{i=1}^{n} p_i x_i\right) \le \sum_{i=1}^{n} p_i f(x_i)$$

where $x_i \in I$ for all $1 \leq i \leq n$, and $0 < p_i < 1$ such that $\sum_{i=1}^n p_i = 1$. Equality holds if and only if $x_1 = x_2 = \cdots = x_n$ or f is linear.

• Chebyshev's sum inequality (see [13]):

Let $a_1 \ge a_2 \ge \cdots \ge a_n$ and $b_1 \ge b_2 \ge \cdots \ge b_n$ be real numbers. Then

$$\frac{1}{n}\sum_{i=1}^{n}a_{i}b_{i} \ge \left(\frac{1}{n}\sum_{i=1}^{n}a_{i}\right)\left(\frac{1}{n}\sum_{i=1}^{n}b_{i}\right) \ge \frac{1}{n}\sum_{i=1}^{n}a_{i}b_{n+1-i}$$

Each equality holds if and only if $a_1 = a_2 = \cdots = a_n$ or $b_1 = b_2 = \cdots = b_n$.

• Bhatia and Davis's bound on variance [3]:

Let a_1, \dots, a_n be real numbers such that $a \leq a_i \leq A$ for all $1 \leq i \leq n$ and $\mu = \frac{\sum_{i=1}^n a_i}{n}$. Then

$$\frac{\sum_{i=1}^{n} (a_i - \mu)^2}{n} \le (A - \mu)(\mu - a),$$

where equality holds if and only if each a_i is either A or a.

3 New lower bounds of F(G)

Proposition 3.1 Let G be a connected graph with m edges. Then

$$F(G) \ge \frac{irr^2(G)}{m} + 2M_2(G),$$

where equality holds if and only if |d(u) - d(v)| is constant for all edges uv of G.

Proof.

$$\begin{split} F(G) &= \sum_{uv \in E(G)} [d^2(u) + d^2(v)] \\ &= \sum_{uv \in E(G)} \left[d^2(u) - 2d(u)d(v) + d^2(v) \right] + 2\sum_{uv \in E(G)} d(u)d(v) \\ &= \left(\sum_{uv \in E(G)} |d(u) - d(v)|^2 \right) + 2M_2(G) \\ &= \left(\sum_{uv \in E(G)} |d(u) - d(v)|^2 \right) \cdot \left(\frac{1}{m} \sum_{uv \in E(G)} 1^2 \right) + 2M_2(G) \; . \end{split}$$

By Cauchy-Schwarz inequality,

$$F(G) \ge \frac{1}{m} \left(\sum_{uv \in E(G)} |d(u) - d(v)| \right)^2 + 2M_2(G) = \frac{irr^2(G)}{m} + 2M_2(G) ,$$

where equality holds if and only if |d(u) - d(v)| is constant for all edges uv.

The graphs that attain the above lower bound are regular graphs or a kind of bipartite graphs which are described in the following proposition.

Proposition 3.2 Let G be a connected non-regular graph. Then |d(u) - d(v)| = t > 0is constant for all edges uv of G if and only if G is a bipartite graph with the following properties: (i) The set of vertex degrees is $\{\delta, \delta + t, \dots, \delta + st\}$ where $\Delta = \delta + st$ for some positive integer s. (ii) Let A_j ($0 \le j \le s$) be the set of vertices of G with vertex degree $\delta + jt$. Then A_j is a nonempty independent set of G, and any edge of G is an edge between A_{j-1} and A_j for some $1 \le j \le s$.

Proof. Sufficiency is trivial. To show necessity, we first prove that G is bipartite by contradiction. Suppose that G has an odd cycle C. Let v be a vertex on C whose vertex degree is the smallest among all vertices of C. Let a, b be the two neighbors of v on C. Then they must have the same degree. Let P be the path between a and b along cycle C that is different from the path avb. Write P as $a(=v_0)v_1v_2\cdots v_{m-1}(v_m =)b$. For each $1 \leq i \leq m$, color edge $v_{i-1}v_i$ red if $d(v_i) - d(v_{i-1}) = t$, and blue if $d(v_i) - d(v_{i-1}) = -t$. Then the number of edges in red must be the same as the number of edges in blue since a and b have the same vertex degree. So, P must have an even number of edges. This

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contradicts the assumption that C is an odd cycle. Therefore, G is bipartite. Properties (i) and (ii) follow immediately since G has constant edge imbalance.

Now, we give another lower bound of F(G) below.

Proposition 3.3 Let G be a connected graph with m edges. Then

$$F(G) \ge \frac{irr^2(G) + M_1^2(G)}{2m}$$
,

where equality holds if and only if G is regular or bi-regular.

Proof. By Jensen's inequality, $\left[\sum_{uv \in E(G)} (d(u) + d(v))\right]^2 \le m \sum_{uv \in E(G)} (d(u) + d(v))^2$. Then we have

$$\begin{split} 2mF(G) - M_1^2(G) &= 2m \sum_{uv \in E(G)} \left(d^2(u) + d^2(v) \right) - \left[\sum_{uv \in E(G)} (d(u) + d(v)) \right]^2 \\ &\geq 2m \sum_{uv \in E(G)} \left(d^2(u) + d^2(v) \right) - m \sum_{uv \in E(G)} (d(u) + d(v))^2 \\ &= m \sum_{uv \in E(G)} |d(u) - d(v)|^2 \,, \end{split}$$

where equality holds if and only if d(u) + d(v) is constant for all edges uv of G.

By Jensen's inequality,

$$2mF(G) - M_1^2(G) \ge \left[\sum_{uv \in E(G)} |d(u) - d(v)|\right]^2 = irr^2(G),$$

where equality holds if and only if |d(u) - d(v)| is constant all edges uv of G.

Hence,

$$F(G) \ge \frac{irr^2(G) + M_1^2(G)}{2m}$$

Moreover, by Lemma 2.2, we see that equality holds if and only if G is regular or bi-regular.

4 New upper bounds of F(G)

Lemma 4.1 Let a_1, \dots, a_k be real numbers such that $a \le a_i \le A$ for all $1 \le i \le k$ and $\mu = \frac{\sum_{i=1}^k a_i}{k}$. Then $\sum_{i=1}^k a_i^2 \le k[\mu(A+a) - Aa]$. Moreover, equality holds if and only if each a_i is either A or a.

Proof. By Bhatia and Davis's bound on variance, $\frac{\sum_{i=1}^{k}(a_i-\mu)^2}{k} \leq (A-\mu)(\mu-a)$, where equality holds if and only if each a_i is either A or a.

Note that $\frac{\sum_{i=1}^{k}(a_i-\mu)^2}{k} = \frac{\sum_{i=1}^{k}a_i^2}{k} - \mu^2$. Then $\sum_{i=1}^{k}a_i^2 \leq k[\mu(A+a) - Aa]$, where equality holds if and only if each a_i is either A or a.

Proposition 4.2 Let G be a connected graph with n vertices and m edges. Let Δ and δ denote the maximum and the minimum of the vertex degrees of G, respectively. Then

$$F(G) \leq (\Delta + \delta)M_1(G) + \frac{1}{2}(\Delta - \delta)irr(G) - 2m\Delta\delta$$
,

where the equality holds if and only if G is regular.

Proof. Let $a_i = d(u_i) + d(v_i)$ where $E(G) = \{u_i v_i | 1 \le i \le m\}$. Then $\mu = \frac{\sum_{i=1}^m a_i}{m} = \frac{M_1(G)}{m}$ and $2\delta \le a_i \le 2\Delta$ for all $1 \le i \le m$. By Lemma 4.1,

(a)
$$\sum_{i=1}^{m} (d(u_i) + d(v_i))^2 \le m \left[\frac{M_1(G)}{m} (2\Delta + 2\delta) - 4\Delta \delta \right] = 2(\Delta + \delta)M_1(G) - 4m\Delta\delta,$$

where equality holds if and only if $d(u_i) + d(v_i)$ is either 2Δ or 2δ for each edge $u_i v_i$ of G.

Let $a_i = |d(u_i) - d(v_i)|$ where $E(G) = \{u_i v_i | 1 \le i \le m\}$. Then $\mu = \frac{\sum_{i=1}^m a_i}{m} = \frac{irr(G)}{m}$ and $0 \le a_i \le \Delta - \delta$ for all $1 \le i \le m$. By Lemma 4.1,

(b)
$$\sum_{i=1}^{m} \left(d(u_i) - d(v_i) \right)^2 \le m \left[\frac{irr(G)}{m} (\Delta - \delta + 0) - (\Delta - \delta) \cdot 0 \right] = (\Delta - \delta)irr(G),$$

where equality holds if and only if $|d(u_i) - d(v_i)|$ is either $\Delta - \delta$ or 0 for each edge $u_i v_i$ of G.

Take (1/2)((a)+(b)), we obtain $F(G) \leq (\Delta + \delta)M_1(G) + \frac{1}{2}(\Delta - \delta)irr(G) - 2m\Delta\delta$, where equality holds if and only if G is regular.

The following result will be used to obtain a corollary of Proposition 4.2. It is Theorem 4.3 in [6] for which we give a different proof here.

Proposition 4.3 [6] Let G be a connected graph with n vertices and m edges. Let Δ and δ denote the maximum and the minimum of the vertex degrees of G, respectively. Then $M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta$, where equality holds if and only if G is regular or bi-degreed. **Proof.** Let $V(G) = \{x_i | 1 \leq i \leq n\}$. Then $\mu = \frac{\sum_{i=1}^n d(x_i)}{n} = \frac{2m}{n}$ and $\delta \leq d(x_i) \leq \Delta$ for all $1 \leq i \leq n$. By Lemma 4.1,

$$M_1(G) = \sum_{x_i \in V(G)} d^2(x_i) \le n \left[\frac{2m}{n} (\Delta + \delta) - \Delta \delta \right] = 2m(\Delta + \delta) - n\Delta \delta \,,$$

where equality holds if and only if G is regular or bi-degreed.

Corollary 4.4 Let G be a connected graph with n vertices and m edges. Let Δ and δ denote the maximum and the minimum of the vertex degrees of G, respectively. Then

$$F(G) \le (\Delta + \delta)[2m(\Delta + \delta) - n\Delta\delta] + \frac{1}{2}(\Delta - \delta)\sqrt{mn[2m(\Delta + \delta) - n\Delta\delta] - 4m^3} - 2m\Delta\delta,$$

where equality holds if and only if G is regular.

Proof. Note that $M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta$ in [6], where equality holds if and only if G is regular or bi-degreed; and $irr(G) \leq \sqrt{m[nM_1(G) - 4m^2]}$ in [18], where equality holds if and only if G has constant edge imbalance. Then $irr(G) \leq \sqrt{mn[2m(\Delta + \delta) - n\Delta\delta] - 4m^3}$. By Lemma 2.2, equality holds if and only if G is regular or bi-regular.

The result is proved by bringing the above bounds of $M_1(G)$ and irr(G) into Proposition 4.2. Moreover, the necessary and sufficient condition for the equality is valid, since the equality of Proposition 4.2 holds if and only if G is regular.

Corollary 4.5 Let G be a connected K_{r+1} -free graph with n vertices and $m \ge 1$ edges, where $r \ge 2$. Let Δ and δ denote the maximum and the minimum of the vertex degrees of G, respectively. Then

$$F(G) \le (\Delta+\delta)\frac{2r-2}{r}nm + \frac{1}{2}(\Delta-\delta)m\sqrt{\frac{2r-2}{r}n^2 - 4m} - 2m\Delta\delta$$

where equality holds if and only if G is a regular complete r-partite graph for $r \ge 2$.

Proof. It is known [18] that for a connected K_{r+1} -free graph G of n vertices and $m \ge 1$ edges, $M_1(G) \le \frac{2r-2}{r}nm$ and $irr(G) \le m\sqrt{\frac{2r-2}{r}n^2 - 4m}$, where $2 \le r \le n-1$ and each equality holds if and only if G is a complete bipartite graph for r = 2 and a regular complete r-partite graph for $r \ge 3$.

The inequality is shown by bringing the above bounds on $M_1(G)$ and irr(G) into Proposition 4.2. Moreover, the necessary and sufficient condition for the equality is valid, since the equality of Proposition 4.2 holds if and only if G is regular.

We can obtain another upper bound of F(G) for connected K_{r+1} -free graphs in terms of r, graph order and graph size by using some results from [17].

Proposition 4.6 Let G be a connected K_{r+1} -free graph with n vertices and m edges.. Then

$$F(G) \le \frac{(r-1)m}{r} \left[\frac{r^2 + 2r - 4}{r} n^2 - 4m \right],$$

where the equality holds if and only if G is a complete bipartite graph for r = 2 and a regular complete r-partite graph for $r \ge 3$.

Proof. By Theorem 1 from [17] and its proof, one can see the following three inequalities.

(1)
$$F(G) = \sum_{u \in V(G)} d^{3}(u) \leq 2M_{2}(G) + nM_{1}(G) - 4m^{2}$$

(2)
$$M_{1}(G) \leq \frac{2r - 2}{2}nm$$

(3)
$$M_{2}(G) \leq \frac{2}{r}m^{2} + \frac{(r - 1)(r - 2)}{r^{2}}n^{2}m$$

The equalities hold if and only if G is a complete bipartite graph for r = 2 and a regular complete r-partite graph for $r \ge 3$. By bringing inequalities (2) and (3) into inequality (1), we obtain the desired upper bound of F(G).

5 Comparison of the bounds of F(G)

It is pointed out in [8] that two lower bounds $L_1 = \frac{M_1^2(G)}{2m}$ and $L_2 = \frac{M_1^2(G)}{m} - 2M_2(G)$ are incomparable for molecular graphs 1,2-diethylcyclobutane and 1,3-diethylcyclobutane. In Proposition 3.1 and Proposition 3.3, we obtain new lower bounds $L = \frac{irr^2(G)}{m} + 2M_2(G)$ and $L' = \frac{irr^2(G) + M_1^2(G)}{2m}$.

It is natural to do comparison of these bounds for general connected graphs. For the interest of applications, we also do comparison of these bounds for benzenoid systems with more than one hexagon, which will be called *nontrivial benzenoid systems* for representational simplicity.

(i) To compare L and L', we calculate $M_1^2(G) - irr^2(G)$ that appears in L - L'.

$$\begin{split} M_1^2(G) - irr^2(G) &= \left[\sum_{uv \in E(G)} (d(u) + d(v))\right]^2 - \left[\sum_{uv \in E(G)} |d(u) - d(v)|\right]^2 \\ &= \left[\sum_{uv \in E(G)} d(u) + d(v) + |d(u) - d(v)|\right] \cdot \left[\sum_{uv \in E(G)} d(u) + d(v) - |d(u) - d(v)|\right] \\ &= \left[\sum_{uv \in E(G)} 2\max\{d(u), d(v)\}\right] \cdot \left[\sum_{uv \in E(G)} 2\min\{d(u), d(v)\}\right] \\ &= 4\left[\sum_{uv \in E(G)} \max\{d(u), d(v)\}\right] \cdot \left[\sum_{uv \in E(G)} \min\{d(u), d(v)\}\right] \end{split}$$

Write $E(G) = \{u_i v_i | \text{ where } d(u_i) \ge d(v_i) \text{ for all } 1 \le i \le m \}$. Then

$$M_1^2(G) - irr^2(G) = 4\sum_{i=1}^m d(u_i) \sum_{i=1}^m d(v_i)$$

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$$L - L' = \left(\frac{irr^2(G)}{m} + 2M_2(G)\right) - \left(\frac{irr^2(G) + M_1^2(G)}{2m}\right)$$
$$= \frac{4mM_2(G) - (M_1^2(G) - irr^2(G))}{2m}$$
$$= \frac{4\left(m\sum_{i=1}^m d(u_i)d(v_i) - \sum_{i=1}^m d(u_i)\sum_{i=1}^m d(v_i)\right)}{2m}$$

Case 1. Either $d(u_1) = d(u_2) = \dots = d(u_m)$ or $d(v_1) = d(v_2) = \dots = d(v_m)$. Then L = L' since $m \sum_{i=1}^m d(u_i) d(v_i) - \sum_{i=1}^m d(u_i) \sum_{i=1}^m d(v_i) = 0$.

For example, let G be the graph obtained by identifying the center of a copy of a star to each vertex of a regular graph. Then two new lower bounds L and L' are the same.

Case 2. None of the above two groups of equalities holds. Without loss of generality, we can assume that $(d(u_1) \ge d(u_2) \ge \cdots \ge d(u_m))$ is non-increasing.

Subcase 2.1. $(d(v_1) \ge d(v_2) \ge \cdots \ge d(v_m))$ is also non-increasing. Then L > L' since by Chebysev's sum inequality, $m \sum_{i=1}^{m} d(u_i) d(v_i) - \sum_{i=1}^{m} d(u_i) \sum_{i=1}^{m} d(v_i) > 0.$

For example, if G is bi-degreed with two distinct vertex degrees $\Delta > \delta$, then E(G) contains at most three types of edges uv such that $(d(u), d(v)) = (\Delta, \Delta)$ or (Δ, δ) or (δ, δ) . Therefore, for any bi-degreed graph G with all three types of edges, the lower bound L is better than the lower bound L'. In particular, any nontrivial benzenoid system is bi-degreed (degree 2 and degree 3) with all three types of edges (d(u), d(v)) = (3, 3) or (3, 2) or (2, 2). So the lower bound L is better than the lower bound L'. For subgraphs G of a benzenoid system, there are examples where L > L', L = L', or L < L'. However, as long as G has no pendant edges with a vertex of degree 3, it always holds that L > L'.

Subcase 2.2. Sequence $(d(v_1) \le d(v_2) \le \cdots \le d(v_m))$ is non-decreasing. Then L < L' since by Chebysev's sum inequality, $m \sum_{i=1}^{m} d(u_i)d(v_i) - \sum_{i=1}^{m} d(u_i) \sum_{i=1}^{m} d(v_i) < 0$.

Subcase 2.3. Sequence $(d(v_1), d(v_2), \dots, d(v_m))$ is not monotonic. Then L and L' are incomparable.

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We observe some special examples for this case. If G is non-regular with the constant edge imbalance $d(u_i) - d(v_i) = c > 0$ for any edge $u_i v_i$ $(1 \le i \le m)$. Then it is easy to check that $m \sum_{i=1}^{m} d(u_i) d(v_i) - \sum_{i=1}^{m} d(u_i) \sum_{i=1}^{m} d(v_i) = 0$. So L = L'. Thus, for any non-regular graph G with constant edge imbalance, two lower bounds L and L' are the same.

(ii) To compare L with L_1 and L_2 , we do similar analysis as part (i).

$$\begin{split} L - L_1 &= \frac{irr^2(G)}{m} + 2M_2(G) - \frac{M_1^2(G)}{2m} \\ &= \frac{2irr^2(G) + 4mM_2(G) - M_1^2(G)}{2m} \\ &= \frac{4mM_2(G) - (M_1^2(G) - irr^2(G)) + irr^2(G)}{2m} \\ &= \frac{4\left(m\sum_{i=1}^m d(u_i)d(v_i) - \sum_{i=1}^m d(u_i)\sum_{i=1}^m d(v_i)\right) + \left(\sum_{i=1}^m (d(u_i) - d(v_i))\right)^2}{2m} \\ L - L_2 &= \left(\frac{irr^2(G)}{m} + 2M_2(G)\right) - \left(\frac{M_1^2(G)}{m} - 2M_2(G)\right) \\ &= \frac{4mM_2(G) - (M_1^2(G) - irr^2(G))}{m} \\ &= \frac{4\left(m\sum_{i=1}^m d(u_i)d(v_i) - \sum_{i=1}^m d(u_i)\sum_{i=1}^m d(v_i)\right)}{m} \\ \end{split}$$

(iii) Comparing L' with L_1 , it is clear that $L' \ge L_1$ with equality for regular graphs only. To compare L' and L_2 we do similar analysis as part (i).

$$L' - L_2 = \left(\frac{irr^2(G) + M_1^2(G)}{2m}\right) - \left(\frac{M_1^2(G)}{m} - 2M_2(G)\right)$$
$$= \frac{4mM_2(G) - (M_1^2(G) - irr^2(G))}{2m}$$
$$= \frac{4\left(m\sum_{i=1}^m d(u_i)d(v_i) - \sum_{i=1}^m d(u_i)\sum_{i=1}^m d(v_i)\right)}{2m}.$$

Then, from the above analysis, we get the following

Proposition 5.1 (i) The lower bounds $L = \frac{irr^2(G)}{m} + 2M_2(G)$ given in Proposition 3.1 and $L' = \frac{irr^2(G)+M_1^2(G)}{2m}$ given in Proposition 3.3 are incomparable for general grpahs. But L is better than L' for all nontrivial benzenoid systems. (ii) The lower bound L is incomparable with the two lower bounds $L_1 = \frac{M_1^2(G)}{2m}$ and $L_2 = \frac{M_1^2(G)}{m} - 2M_2(G)$ given in [8] for general graphs. But L is better than both L_1 and L_2 for all nontrivial benzenoid systems.

(iii) The lower bound L' is better than the lower bound L_1 except the case when they are equal for regular graphs; L' is incomparable with the lower bound L_2 given in [8] for general graphs, but L' is better than L_2 for all nontrivial benzenoid systems.

Comparing our new upper bound with the upper bound given in [8], we have the following.

Proposition 5.2 The upper bound $U = (\Delta + \delta)M_1(G) + \frac{1}{2}(\Delta - \delta)irr(G) - 2m\Delta\delta$ given in Proposition 4.2 is incomparable with the upper bound $U_1 = 2M_2(G) + m(n-2)^2$ given in [8] for general graphs. But U is better than U_1 for all benzenoid systems.

Proof.

$$\begin{split} U - U_1 &= (\Delta + \delta)M_1(G) + \frac{1}{2}(\Delta - \delta)irr(G) - 2m\Delta\delta - 2M_2(G) - m(n-2)^2 \\ &= (\Delta + \delta)\sum_{uv \in E(G)} (d(u) + d(v)) + \frac{1}{2}(\Delta - \delta)\sum_{uv \in E(G)} |d(u) - d(v)| - 2m\Delta\delta \\ &- 2\sum_{uv \in E(G)} (d(u)d(v)) - m(n-2)^2 \\ &\leq (\Delta + \delta)m(2\Delta) + \frac{1}{2}(\Delta - \delta)m(\Delta - \delta) - 2m\Delta\delta - 2m\delta^2 - m(n-2)^2 \\ &= m(\Delta - \delta)(\frac{5}{2}\Delta + \frac{3}{2}\delta) - m(n-2)^2 \end{split}$$

Any benzenoid system has $\Delta \geq 2$ and $\delta = 2$. It follows that $U - U_1 < 0$, and so U is better than U_1 if G is a benzenoid system.

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