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REMARK ON FORGOTTEN TOPOLOGICAL INDEX OF A LINE GRAPHS

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Abstract. Let G be a simple connected graph with n vertices and m edges and let $d(e_1) \geqslant d(e_2) \geqslant \cdots \geqslant d(e_m)$ be edge degree sequence of graph G. Denote by $EF = \sum_{i=1}^{m} d(e_i)^3$ reformulated forgotten index of G. Lower and upper bounds for the invariant EF are obtained.

1. Introduction

Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be a simple connected graph with n vertices and m edges. Denote by $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n > 0$, $d_i = d(i)$, and $d(e_1) \geqslant d(e_2) \geqslant \cdots \geqslant d(e_m)$, sequences of vertex and edge degrees, respectively. In this paper we use standard notation: $\Delta_e = d(e_1) + 2$, $\Delta_{e_2} = d(e_2) + 2$, $\delta_e = d(e_m)+2$, $\delta_{e_2} = d(e_{m-1})+2$. If i-th and j-th vertices (e_i and e_j edges) are adjacent, it is denoted as $i \sim j$ ($e_i \sim e_j$). As usual, $L(G)$ denotes a line graph of a graph G.

In [**7**] vertex-degree-based topological indices, named as the first and the second Zagreb indices, M_1 and M_2, were defined as

$$M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2 \quad \text{and} \quad M_2 = M_2(G) = \sum_{i \sim j} d_i d_j.$$

It is noticed that the first Zagreb index satisfies the identity [**5**]

$$M_1 = \sum_{i \sim j} (d_i + d_j). \tag{1.1}$$

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In [**6**] forgotten topological index F was defined as (see also [**8**])

$$F = F(G) = \sum_{i=1}^{n} d_i^3.$$

By analogy to M_1, invariant F can be written in the following way

$$F = \sum_{i\sim j}(d_i^2 + d_j^2) = \sum_{i\sim j}(d_i + d_j)^2 - 2M_2. \tag{1.2}$$

Details on topological indices M_1, M_2, and F can be found in [**2**,**3**,**5**,**8**–**11**,**15**].

A vertex-degree-based topological index, named as harmonic index, H, was defined as [**19**]

$$H = H(G) = \sum_{i\sim j} \frac{2}{d_i + d_j}. \tag{1.3}$$

In [**14**], the edge-degree graph topological indices, named the first and the second reformulated Zagreb indices, EM_1 and EM_2, were introduced by

$$EM_1 = EM_1(G) = \sum_{i=1}^{m} d(e_i)^2 \quad \text{and} \quad EM_2 = EM_2(G) = \sum_{e_i\sim e_j} d(e_i)d(e_j).$$

Apparently, EM_1 and EM_2 are not new topological indices, since they are the first and the second Zagreb indices for a line graph of graph G, so we have that $EM_1(G) = M_1(L(G))$ and $EM_2(G) = M_2(L(G))$. According to this, we can define reformulated forgotten index, i.e. forgotten index of a line graph as [**12**]

$$EF = EF(G) = \sum_{i=1}^{m} d(e_i)^3.$$

All the above mentioned topological indices find their applications in chemistry as molecular structure descriptors, as molecules are usually modeled as undirected graphs (see for example [**2**,**3**,**6**–**11**,**14**,**19**]). Very often in chemistry the aim is the construction of chemical compounds with certain properties, which not only depend on the chemical formula but also strongly on the molecular structure. That's where various topological indices come into consideration. Considering the fact that obtaining the exact and easy to compute formulas for these indices is not always possible, it is useful to know approximating expressions, i.e. to determine upper and lower bounds of the corresponding indices in terms of number vertices (atoms), number of edges (bonds), maximum vertex degree (valency), etc.

In [**16**] it was shown that topological indices M_1 and F can be also represented in terms of edge-degrees of graph, i.e. as

$$M_1 = \sum_{i=1}^{m}(d(e_i) + 2) \quad \text{and} \quad F + 2M_2 = \sum_{i=1}^{m}(d(e_i) + 2)^2 .$$

It turns out that such definitions enable to obtain better lower bounds for F.

In this paper we first prove that for topological index EF holds

$$EF = \sum_{i=1}^{m} (d(e_i)+2)^3 - 6(F + 2M_2) + 12M_1 - 8m.$$

Then, similarly as in [**16**], we use appropriate analytical inequalities to approximate $\sum_{i=1}^{m}(d(e_i)+2)^3$ and determine the bounds for EF.

2. Preliminaries

In this section we recall some inequalities for sequences of real numbers that will be used in proofs of theorems.

Let $p = (p_i)$, $i = 1, 2, \ldots, m$, be positive real number sequence. Let $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, \ldots, m$, be sequences of non-negative real numbers of similar monotonicity. By $T_m(a, b; p)$ we denote the expression

$$T_m(a,b;p) = \sum_{i=1}^{m} p_i \sum_{i=1}^{m} p_i a_i b_i - \sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} p_i b_i. \tag{2.1}$$

In [**18**] the following inequality was proved

$$T_m(a,b;p) \geqslant T_{m-1}(a,b;p). \tag{2.2}$$

Let $a = (a_i)$, $i = 1, 2, \ldots, m$, be positive real number sequence with the property $0 < r \leqslant a_i \leqslant R < +\infty$. In [**13**] (see also [**1, 4**]) the following inequality was proved

$$\sum_{i=1}^{m} a_i \sum_{i=1}^{m} \frac{1}{a_i} \leqslant m^2 \left(1 + \alpha(m)\left(\sqrt{\frac{R}{r}} - \sqrt{\frac{r}{R}}\right)^2\right), \tag{2.3}$$

where

$$\alpha(m) = \frac{1}{4}\left(1 - \frac{(-1)^{m+1}+1}{2m^2}\right). \tag{2.4}$$

Let $p = (p_i)$, and $a = (a_i)$, $i = 1, 2, \ldots, m$, be positive real number sequences. Then for any α, $\alpha \leqslant 0$ or $\alpha \geqslant 1$, we have

$$\left(\sum_{i=1}^{m} p_i\right)^{\alpha-1} \sum_{i=1}^{m} p_i a_i^{\alpha} \geqslant \left(\sum_{i=1}^{m} p_i a_i\right)^{\alpha}. \tag{2.5}$$

If $0 \leqslant \alpha \leqslant 1$, then opposite inequality is valid in (2.5).

Inequality (2.5) is known in the literature as Jensen's inequality (see for example [**17**]).

3. Main results

The following theorem establishes lower bound for topological index EF in terms of invariants M_1, M_2, F, and graph parameters m, Δ_e, Δ_{e_2}.

THEOREM 3.1. *Let G be a simple connected graph with n vertices and $m \geqslant 2$ edges. Then*

$$EF \geqslant \frac{(F+2M_2-3M_1)^2 + M_1(3M_1-8m) + \Delta_e\Delta_{e_2}(\Delta_e-\Delta_{e_2})^2}{M_1}. \tag{3.1}$$

Equality holds if and only if $L(G)$ is a regular graph.

PROOF. According to (2.2) we have that $T_m \geqslant T_2$, i.e.

$$\sum_{i=1}^{m} p_i \sum_{i=1}^{m} p_i a_i b_i - \sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} p_i b_i \geqslant p_1 p_2 (a_1-a_2)(b_1-b_2).$$

For $p_i = a_i = b_i = d(e_i)+2$, $i = 1, 2, \dots, n$, this inequality becomes

$$\sum_{i=1}^{m}(d(e_i)+2)\sum_{i=1}^{m}(d(e_i)+2)^3 - \left(\sum_{i=1}^{m}(d(e_i)+2)^2\right)^2 \geqslant \Delta_e\Delta_{e_2}(\Delta_e-\Delta_{e_2})^2. \tag{3.2}$$

Having in mind (1.1) and (1.2) we obtain the following identities

$$M_1 = \sum_{i=1}^{m}(d(e_i)+2) \quad \text{and} \quad F + 2M_2 = \sum_{i=1}^{m}(d(e_i)+2)^2.$$

According to these equalities, inequality (3.2) becomes

$$M_1 \sum_{i=1}^{m}(d(e_i)+2)^3 - (F+2M_2)^2 \geqslant \Delta_e\Delta_{e_2}(\Delta_e-\Delta_{e_2})^2. \tag{3.3}$$

On the other hand, we have

$$\begin{aligned}\sum_{i=1}^{m}(d(e_i)+2)^3 &= \sum_{i=1}^{m}\big(d(e_i)^3 + 6(d(e_i)+2)^2 - 12(d(e_i)+2) + 8\big)\\ &= EF + 6(F+2M_2) - 12M_1 + 8m,\end{aligned}$$

i.e.

$$EF = \sum_{i=1}^{m}(d(e_i)+2)^3 - 6(F+2M_2) + 12M_1 - 8m. \tag{3.4}$$

By combining relations (3.3) and (3.4) we get the inequality (3.1).

Equality in (3.2) holds if and only if $\Delta_e = d(e_1)+2 = \cdots = d(e_m)+2 = \delta_e$, therefore equality in (3.1) holds if and only if $L(G)$ is a regular graph. $\square$

In a similar way we can prove the next theorem.

THEOREM 3.2. *Let G be a simple connected graph with n vertices and $m \geqslant 3$ edges. Then*

$$EF \geqslant \delta_e^3 + \frac{(F+2M_2-\delta_e^2)^2 + \Delta_e\Delta_{e_2}(\Delta_e-\Delta_{e_2})^2}{M_1-\delta_e} - 6(F+2M_2) + 12M_1 - 8m,$$

with equality if and only if $L(G)$ is regular.

In the following theorem we determine upper bound for EF in terms of invariants M_1, M_2, F, H, and graph parameters m, Δ_e, δ_e.

THEOREM 3.3. *Let G be a simple connected graph with n vertices and m, $m \geqslant 2$, edges. Then*

$$EF \leqslant \frac{8m^4}{H^3}\left(1+\alpha(m)\frac{(\Delta_e^3-\delta_e^3)^2}{\Delta_e^3\delta_e^3}\right) - 6(F+2M_2)+12M_1-8m, \tag{3.5}$$

where $\alpha(m)$ is given by (2.4)*. Equality holds if and only if $L(G)$ is regular.*

PROOF. For $a_i = (d(e_i)+2)^3$, $i=1,2,\dots,m$, $r=\delta_e^3$ and $R=\Delta_e^3$, the inequality (2.3) transforms into

$$\sum_{i=1}^{m}(d(e_i)+2)^3\sum_{i=1}^{m}\frac{1}{(d(e_i)+2)^3} \leqslant m^2\left(1+\alpha(m)\left(\sqrt{\frac{\Delta_e^3}{\delta_e^3}}-\sqrt{\frac{\delta_e^3}{\Delta_e^3}}\right)^2\right). \tag{3.6}$$

For $\alpha=3$, $p_i=1$, $a_i=\frac{1}{d(e_i)+2}$, $i=1,2,\dots,m$, the inequality (2.5) becomes

$$\sum_{i=1}^{m}\frac{1}{(d(e_i)+2)^3} \geqslant \frac{\left(\sum_{i=1}^{m}\frac{1}{d(e_i)+2}\right)^3}{m^2}. \tag{3.7}$$

According to (1.3) we easily get

$$H=\sum_{i\sim j}\frac{2}{d_i+d_j}=\sum_{i=1}^{m}\frac{2}{d(e_i)+2},$$

wherefrom the inequality (3.7) becomes

$$\sum_{i=1}^{m}\frac{1}{(d(e_i)+2)^3} \geqslant \frac{H^3}{8m^2}. \tag{3.8}$$

From (3.8) and (3.6) it follows

$$\frac{H^3}{8m^2}\sum_{i=1}^{m}(d(e_i)+2)^3 \leqslant m^2\left(1+\alpha(m)\frac{(\Delta_e^3-\delta_e^3)^2}{\Delta_e^3\delta_e^3}\right).$$

Finally, from (3.4) and the previous inequality we have that

$$EF+6(F+2M_2)-12M_1+8m \leqslant \frac{8m^4}{H^3}\left(1+\alpha(m)\frac{(\Delta_e^3-\delta_e^3)^2}{\Delta_e^3\delta_e^3}\right),$$

wherefrom (3.5) is obtained. □

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