Bounds and extremal graphs of second reformulated Zagreb index for graphs with cyclomatic number at most three

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Abstract

Miličević *et al.*, in 2004, introduced topological indices known as Reformulated Zagreb indices, where they modified Zagreb indices using the edge-degree instead of vertex degree. In this paper, we present a simple approach to find the upper and lower bounds of the second reformulated Zagreb index, $EM_2(G)$, by using six graph operations/transformations. We prove that these operations significantly alter the value of reformulated Zagreb index. We apply these transformations and identify those graphs with cyclomatic number at most 3, namely trees, unicyclic, bicyclic and tricyclic graphs, which attain the upper and lower bounds of second reformulated Zagreb index for graphs.

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1. Introduction

Topological indices play a crucial role in characterizing the properties of molecules in terms of physical, chemical and biological. Several types of topological indices exist in mathematical chemistry, such as the Wiener index (Wiener, 1947); Hyper Wiener index (Klein *et al.*, 1995); Hosoya index (Hosoya, 1971); Randić index (Randić, 1975); Augmented Zagreb index (Furtula *et al.*, 2010); Harmonic index (Fajtlowicz, 1987); to name a few. For more details on topological indices, we refer to some articles here (Basak, 2016; Devillers & Balaban, 2000; Gutman, 2013; Gutman *et al.*, 2014, 2020; Karelson, 2000; Narayankar *et al.*, 2020; Rada & Bermudo, 2019; Romero-Valencia *et al.*, 2019; Shang, 2016; Varmuza *et al.*, 2012).

Throughout this paper, we consider only non trivial simple connected graphs. Let a simple connected graph of n vertices be denoted by G = (V(G), E(G)), where V(G) and E(G) denote the set of vertices and set of edges of the graph respectively. Let $d_G(u)$ denote the *degree of the vertex u*, $d_G(e)$ denotes the *degree of the edge e*. $N_G(u) = \{v \in V(G) : uv \in E(G)\}$ denotes the set of all *neighbours* of vertex u in G, that is, $d_G(u) = |N_G(u)|$. The cyclomatic number of a graph is defined as cy(G) = |E(G)| - |V(G)| + 1. Trees have no cycles and hence has cyclomatic number to be 0. When m = n, G has cyclomatic number 1 and called as a *unicyclic graph*. When m = n + 1, G has cyclomatic number 2 and referred to as *bicyclic graph*. When m = n + 2, G has cyclomatic number 3 and referred to as *triyclic graph*. Let S_n , P_n , and C_n denoted the star graph, path graph, and cycle graph of n vertices. Other notations and definitions are taken from the book (Bondy *et al.*, 1976).

The Zagreb indices are one of the most important and well studied topological indices in the literature. It first appeared in 1972, during the study of π -energy of conjugate molecules. For a simple graph G, Zagreb indices (Gutman & Das, 2004; Gutman & Trinajstić, 1972) are defined as

$$M_1(G) = \sum_{u \in V(G)} d_G^2(u), \quad M_2(G) = \sum_{uv \in E(G)} d_G(u).d_G(v),$$

where $d_G(u)$ denotes the degree of the vertex $u \in V(G)$.

Motivated by the concept of line graph L(G) of a graph G, where the edges in G represents the vertices of line graph L(G), Miličević *et al.* (Miličević *et al.*, 2004) introduced a pair of topological indices in terms of edge-degree instead of vertex degree in Zagreb index and called it as Reformulated Zagreb index. For the simple graph G, first and second Reformulated Zagreb indices are defined as

$$EM_1(G) = \sum_{e \in E(G)} d_G^2(e), \quad EM_2(G) = \sum_{e \sim f} d_G(e).d_G(f),$$

where $e \sim f$ means the edge e and f are adjacent in graph G, i.e., the edge e and f have a common vertex. Further, if e = uv, then note that $d_G(e) = d_G(u) + d_G(v) - 2$.

Nowadays many researchers are interested in finding the bounds of topological indices of graphs, as well as characterizing the extremal graphs, see articles (Ali, Elumalai & Mansour, 2020; Ali, Milovanović, Matejić & Milovanović, 2020; Ali *et al.*, 2019; Borovicanin *et al.*, 2017; Deng, 2007; Ghalavand & Ashrafi, 2020; Gutman, 2013; Khalifeh *et al.*, 2009; Rajpoot & Selvaganesh, 2020; Xu & Das, 2012; Noureen *et al.*, 2020; Aouchiche *et al.*, 2020; Ali *et al.*, 2016; Ali & Bhatti, 2016). For the bounds of reformulated Zagreb indices we refer to (De, 2012; Ghalavand & Ashrafi, 2017; Ilić & Zhou , 2012; Ji *et al.*, 2014, 2015; Su *et al.*, 2011). In (Deng, 2007), the author proposes few graph operations which are useful in finding the bounds for Zagreb indices while in (Ji *et al.*, 2014, 2015) the authors discusses some graph operations to study the bounds of first reformulated Zagreb index.

In this paper, we focus on finding the bounds of second reformulated Zagreb index. In particular, we give the bounds for special graph classes, namely the trees, unicyclic graphs, bicyclic graphs and tricyclic graphs. In order to study the bounds for graphs, we propose to use certain transformations which help us in obtaining required results. Further, we also find the extremal graphs which attain these bounds.

The organization of the paper is as follows: In Section 2, we give three transformations which increases the value of the second reformulated Zagreb index. In Section 3, we give three transformations which decrease the value of EM_2 . In Section 4, we compute the bounds(both upper and lower) for $EM_2(G)$ when G is a tree, a unicyclic graph, a bicyclic graph, and a tricyclic graph. In this process, we also find the graphs which attain these bounds.

2. Three graph transformations which increase the second reformulated Zagreb index

In this section, we discuss three graph operations as defined in (Deng, 2007; Ji *et al.*, 2014) and show how they impact the second reformulated Zagreb index.

Transformation A: Let G_0 be a non-trivial graph and u be any vertex of G_0 . Let G_1 be a graph obtained from G_0 by joining u to the center of a star such that $d_{G_1}(v) \ge 2$, and $\{w_1, w_2, \ldots, w_t\}$ is the pendant neighbour of v in G_1 , see Figure 1. Here, we say that G_2 is obtained from G_1 by **transformation A** and write as $G_2 = G_1 - \{vw_1, vw_2, \ldots, vw_t\} + \{uw_1, uw_2, \ldots, uw_t\}$.



Fig. 1. Representation of transformation A.

Lemma 2.1 If G_2 is obtained by applying transformation A on G_1 , then $EM_2(G_1) < EM_2(G_2)$.

Proof: Let $N_{G_0}(u) = \{x \in V(G_0) : ux \in E(G_0)\}$. From the definition of $EM_2(G)$, we have

$$EM_{2}(G_{1}) = \sum_{e_{i},e_{j}\in E(G_{0}\setminus\{u\})} d_{G_{1}}(e_{i})d_{G_{1}}(e_{j}) + \sum_{x\in N_{G_{0}}(u)} \sum_{y\in N_{G_{0}}(x)\setminus\{u\}} d_{G_{1}}(ux)d_{G_{1}}(xy)$$
$$+ \sum_{x,y\in N_{G_{0}}(u)} d_{G_{1}}(xu)d_{G_{1}}(uy) + \sum_{x\in N_{G_{0}}(u)} d_{G_{1}}(xu)d_{G_{1}}(uv) + \sum_{i=1}^{t} d_{G_{1}}(uv)d_{G_{1}}(vw_{i})$$
$$+ \frac{t(t-1)}{2}(d_{G_{1}}(v)-1)^{2},$$

and

$$\begin{split} EM_2(G_2) &= \sum_{e_i, e_j \in E(G_0 \setminus \{u\})} d_{G_1}(e_i) d_{G_1}(e_j) + \sum_{x \in N_{G_0}(u)} \sum_{y \in N_{G_0}(x) \setminus \{u\}} (d_{G_1}(ux) + t) d_{G_1}(xy) \\ &+ \sum_{x, y \in N_{G_0}(u)} (d_{G_1}(xu) + t) (d_{G_1}(uy) + t) + \sum_{x \in N_{G_0}(u)} (d_{G_1}(xu) + t) d_{G_1}(uv) \\ &+ t \sum_{x \in N_{G_0}(u)} (d_{G_1}(xu) + t) (d_{G_1}(u) + t - 1) + \frac{t(t-1)}{2} (d_{G_1}(u) + t - 1)^2 \\ &+ t (d_{G_1}(u) + t - 1)^2. \end{split}$$

Then,

$$\begin{split} EM_2(G_2) - EM_2(G_1) &= \sum_{x \in N_{G_0}(u)} \sum_{y \in N_{G_0}(x) \setminus \{u\}} td_{G_1}(xy) + \sum_{x,y \in N_{G_0}(u)} t(d_{G_1}(xu) + d_{G_1}(uy) + t) \\ &+ \sum_{x \in N_{G_0}(u)} t(d_{G_1}(u) + t - 1)(d_{G_1}(xu) + t + 1) - t^2(d_{G_1}(u) + t - 1) \\ &+ \frac{t(t-1)}{2}((d_{G_1}(u) + 2t - 1)(d_{G_1}(u) - 1)) + t(d_{G_1}(u) + t - 1)^2 \\ &\geq t(d_{G_1}(u) + t - 1)^2 \\ &> 0. \end{split}$$

Transformation B: Let u and v be any two vertices of a simple connected graph G_1 such that there is a path of length $t \ge 1$, $P_t = u_0(= u), u_1, \ldots, u_{t-1}, u_t(= v)$ which connect the vertices u and v, see Figure 2. Here, we say that G_2 is obtained from G_1 by **transformation B** and write as $G_2 = G_1 - \{u_0u_1, u_1u_2, \ldots, u_{t-1}u_t\} + \{wu_1, wu_2, \ldots, wu_t\}$, where $w = u \circ v$.



Fig. 2. Representation of transformation B.

Lemma 2.2 If G_2 is obtained from G_1 using transformation B, then $EM_2(G_1) < EM_2(G_2)$.

Proof: Let $d_{G_1}(u) = a + 1$, and $d_{G_1}(v) = b + 1$, where $a \ge 1$, $b \ge 1$. Then the degree of edges $d_{G_1}(uu_1) = a + 1$, $d_{G_1}(vu_{t-1}) = b + 1$, and $d_{G_2}(wu_i) = (a + b + t - 1)$, for i = 1 to t. First we assume

that $t \geq 3$, then from the definition of $EM_2(G)$, we have

$$\begin{split} EM_{2}(G_{1}) &= \sum_{e_{i},e_{j} \in E(F_{1} \setminus \{u\})} d_{G_{1}}(e_{i})d_{G_{1}}(e_{j}) + \sum_{e_{i},e_{j} \in E(F_{2} \setminus \{v\})} d_{G_{1}}(e_{i})d_{G_{1}}(e_{j}) \\ &+ \sum_{x \in N_{F_{1}}(u)} \sum_{y \in N_{F_{1}}(x) \setminus \{u\}} d_{G_{1}}(ux)d_{G_{1}}(xy) + \sum_{x \in N_{F_{2}}(v)} \sum_{y \in N_{F_{2}}(x) \setminus \{v\}} d_{G_{1}}(vx)d_{G_{1}}(xy) \\ &+ \sum_{x,y \in N_{F_{1}}(u)} d_{G_{1}}(xu)d_{G_{1}}(uy) + \sum_{x,y \in N_{F_{2}}(v)} d_{G_{1}}(xv)d_{G_{1}}(vy) \\ &+ \sum_{x \in N_{F_{1}}(u)} d_{G_{1}}(xu)d_{G_{1}}(uu_{1}) + \sum_{x \in N_{F_{2}}(v)} d_{G_{1}}(xv)d_{G_{1}}(vu_{t-1}) \\ &+ 2d_{G_{1}}(uu_{1}) + 2d_{G_{1}}(u_{t-1}v) + 4(t-3). \end{split}$$

$$\begin{split} EM_{2}(G_{2}) &= \sum_{e_{i},e_{j}\in E(F_{1}\setminus\{w\})} d_{G_{1}}(e_{i})d_{G_{1}}(e_{j}) + \sum_{e_{i},e_{j}\in E(F_{2}\setminus\{w\})} d_{G_{1}}(e_{i})d_{G_{1}}(e_{j}) \\ &+ \sum_{x\in N_{F_{1}}(w)} \sum_{y\in N_{F_{1}}(x)\setminus\{w\}} d_{G_{2}}(wx)d_{G_{1}}(xy) + \sum_{x\in N_{F_{2}}(w)} \sum_{y\in N_{F_{2}}(x)\setminus\{w\}} d_{G_{2}}(wx)d_{G_{1}}(xy) \\ &+ \sum_{x,y\in N_{F_{1}}(w)} d_{G_{2}}(xw)d_{G_{2}}(wy) + \sum_{x,y\in N_{F_{2}}(w)} d_{G_{2}}(xw)d_{G_{2}}(wy) \\ &+ t\sum_{x\in N_{F_{1}}(w)} d_{G_{2}}(xw)(d_{G_{2}}(w) - 1) + t\sum_{x\in N_{F_{2}}(w)} d_{G_{2}}(xw)(d_{G_{2}}(w) - 1) \\ &+ \sum_{x\in N_{F_{1}}(w)} \sum_{y\in N_{F_{2}}(w)} d_{G_{2}}(xw)d_{G_{2}}(wy) + \frac{1}{2}t(t-1)(d_{G_{2}}(w) - 1)^{2}, \end{split}$$

since $d_{G_2}(w) = d_{G_1}(u) + d_{G_1}(v) + t - 2$, $N_{F_1}(w) = N_{F_1}(u)$ and $N_{F_2}(w) = N_{F_2}(v)$. Then

$$EM_{2}(G_{2}) - EM_{2}(G_{1}) > \sum_{x \in N_{F_{1}}(w)} \sum_{y \in N_{F_{2}}(w)} d_{G_{2}}(xw) d_{G_{2}}(wy) + \frac{1}{2}t(t-1)(d_{G_{2}}(w)-1)^{2}$$
$$- 2d_{G_{1}}(uu_{1}) - 2d_{G_{1}}(u_{t-1}v) - 4(t-3)$$
$$> (a+b+t-1)^{2} - 2(a+1) - 2(b+1) - 4(t-3)$$
$$\ge 2(a+1)(b+1)$$
$$> 0.$$

Similarly proof holds for the remaining values of t, that is, t = 1 or t = 2. We omit the proofs for brevity.

Transformation C: Suppose u and v are any two vertices of a simple connected graph G_0 . Let G_1 be the graph obtained from G_0 by adding pendant vertices $\{v_1, v_2, \ldots, v_t\}$, $\{u_1, u_2, \ldots, u_r\}$ at v and u respectively as shown in Figure 3. Now we have two possibilities for a transformation namely, $G_2 = G_1 - \{uu_1, uu_2, \ldots, uu_r\} + \{vu_1, vu_2, \ldots, vu_r\}$, and $G_3 = G_1 - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}$. Here, we say that G_2 and G_3 are obtained from G_1 by **transformation C.**

Lemma 2.3 If graphs G_2 and G_3 are obtained from graph G_1 by transformation C, then either $EM_2(G_1) < EM_2(G_2)$ or $EM_2(G_1) < EM_2(G_3)$.

Proof: Let $d_{G_0}(u) = p$, $d_{G_0}(v) = q$. Without loss of generality, we assume that $d_{G_0}(v) \le d_{G_0}(u)$, let p = q + a, where $a \ge 0$. Now, we prove this lemma by making conditions on the vertices u and v.



Fig. 3. Representation of transformation C.

Case 1: If vertex u and v are not adjacent. Then, we have two subcases. **Subcase 1.1:** If $N_{G_0}(u) \cap N_{G_0}(v) = \emptyset$, then from the definition of $EM_2(G)$, we have

$$\begin{split} EM_2(G_1) &= \sum_{e_i, e_j \in E(G_0 \setminus \{u, v\})} d_{G_1}(e_i) d_{G_1}(e_j) + \sum_{x \in N_{G_0}(u)} \sum_{y \in N_{G_0}(x) \setminus \{u\}} d_{G_1}(ux) d_{G_1}(xy) \\ &+ \sum_{x, y \in N_{G_0}(u)} d_{G_1}(xu) d_{G_1}(uy) + \sum_{x \in N_{G_0}(v)} \sum_{y \in N_{G_0}(x) \setminus \{v\}} d_{G_1}(vx) d_{G_1}(xy) \\ &+ \sum_{x, y \in N_{G_0}(v)} d_{G_1}(xv) d_{G_1}(vy) + r(q + a + r - 1) \sum_{x \in N_{G_0}(u)} d_{G_1}(xu) \\ &+ t(q + t - 1) \sum_{x \in N_{G_0}(v)} d_{G_1}(xv) + \frac{r(r - 1)}{2}(q + a + r - 1)^2 \\ &+ \frac{t(t - 1)}{2}(q + t - 1)^2, \end{split}$$

$$\begin{split} EM_2(G_2) &= \sum_{e_i, e_j \in E(G_0 \setminus \{u, v\})} d_{G_1}(e_i) d_{G_1}(e_j) + \sum_{x \in N_{G_0}(u)} \sum_{y \in N_{G_0}(x) \setminus \{u\}} (d_{G_1}(ux) - r) d_{G_1}(xy) \\ &+ \sum_{x, y \in N_{G_0}(u)} (d_{G_1}(xu) - r) (d_{G_1}(uy) - r) + \sum_{x \in N_{G_0}(v)} \sum_{y \in N_{G_0}(x) \setminus \{v\}} (d_{G_1}(vx) + r) d_{G_1}(xy) \\ &+ \sum_{x, y \in N_{G_0}(v)} (d_{G_1}(xv) + r) (d_{G_1}(vy) + r) + (r+t)(q+r+t-1) \sum_{x \in N_{G_0}(v)} (d_{G_1}(xv) + r) d_{G_1}(xy) \\ &+ \frac{(r+t)(r+t-1)}{2} (q+r+t-1)^2, \end{split}$$

and

$$\begin{split} EM_2(G_3) &= \sum_{e_i, e_j \in E(G_0 \setminus \{u, v\})} d_{G_1}(e_i) d_{G_1}(e_j) + \sum_{x \in N_{G_0}(u)} \sum_{y \in N_{G_0}(x) \setminus \{u\}} (d_{G_1}(ux) + t) d_{G_1}(xy) \\ &+ \sum_{x, y \in N_{G_0}(u)} (d_{G_1}(xu) + t) (d_{G_1}(uy) + t) + \sum_{x \in N_{G_0}(v)} \sum_{y \in N_{G_0}(x) \setminus \{v\}} (d_{G_1}(vx) - t) d_{G_1}(xy) \\ &+ \sum_{x, y \in N_{G_0}(v)} (d_{G_1}(xv) - t) (d_{G_1}(vy) - t) + \frac{(r+t)(r+t-1)}{2} (q+a+r+t-1)^2 \\ &+ (r+t)(q+a+r+t-1) \sum_{x \in N_{G_0}(u)} (d_{G_1}(xu) + t). \end{split}$$

Then,

$$\begin{split} EM_{2}(G_{2}) - EM_{2}(G_{1}) &= -r \sum_{x \in N_{G_{0}}(u)} \sum_{y \in N_{G_{0}}(x) \setminus \{u\}} d_{G_{1}}(xy) - r \sum_{x,y \in N_{G_{0}}(u)} (d_{G_{1}}(xu) + d_{G_{1}}(uy) - r) \\ &- r(q + r + a - 1) \sum_{x \in N_{G_{0}}(u)} d_{G_{1}}(xu) + r \sum_{x \in N_{G_{0}}(v)} \sum_{y \in N_{G_{0}}(x) \setminus \{v\}} d_{G_{1}}(xy) \\ &+ r \sum_{x,y \in N_{G_{0}}(v)} (d_{G_{1}}(xv) + d_{G_{1}}(vy) + r) + r(q + r + 2t - 1) \sum_{x \in N_{G_{0}}(v)} d_{G_{1}}(xv) \\ &+ qr(r + t)(q + r + t - 1) + rt(q + r + t - 1)^{2} + \frac{1}{2}rt(t - 1)(2q + r + 2t - 2) \\ &+ \frac{1}{2}r(r - 1)(t - a)(2q + 2r + t + a - 2), \end{split}$$
(1)

and

$$EM_{2}(G_{3}) - EM_{2}(G_{1}) = t \sum_{x \in N_{G_{0}}(u)} \sum_{y \in N_{G_{0}}(x) \setminus \{u\}} d_{G_{1}}(xy) + t \sum_{x,y \in N_{G_{0}}(u)} (d_{G_{1}}(xu) + d_{G_{1}}(uy) + t) + t(q + 2r + t + a - 1) \sum_{x \in N_{G_{0}}(u)} d_{G_{1}}(xu) - t \sum_{x \in N_{G_{0}}(v)} \sum_{y \in N_{G_{0}}(x) \setminus \{v\}} d_{G_{1}}(xy) - t \sum_{x,y \in N_{G_{0}}(v)} (d_{G_{1}}(xv) + d_{G_{1}}(vy) - t) - t(q + t - 1) \sum_{x \in N_{G_{0}}(v)} d_{G_{1}}(xv) + t(q + a)(r + t)(q + r + t + a - 1) + \frac{1}{2}rt(r - 1)(2q + 2r + t + 2a - 2) + rt(q + r + t + a - 1)^{2} + \frac{1}{2}t(t - 1)(r + a)(2q + r + 2t + a - 2).$$
(2)

Note that if either of the expressions (1) or (2) is greater than 0, then the lemma holds. Suppose $EM_2(G_2) - EM_2(G_1) \le 0$, then we will show that $EM_2(G_3) - EM_2(G_1)$ has to be greater than 0. We will now find a relation from Equation (1) by letting $EM_2(G_2) - EM_2(G_1) \le 0$ and use the same to prove our claim. That is, we get

$$\begin{aligned} q(r+t)(q+r+t-1) + t(q+r+t-1)^2 &+ \frac{1}{2}(r-1)(t-a)(2q+2r+t+a-2) \\ &+ \frac{1}{2}t(t-1)(2q+r+2t-2) \\ &\leq \sum_{x \in N_{G_0}(u)} \sum_{y \in N_{G_0}(x) \setminus \{u\}} d_{G_1}(xy) + \sum_{x,y \in N_{G_0}(u)} (d_{G_1}(xu) + d_{G_1}(uy) - r) \\ &+ (q+r+a-1) \sum_{x \in N_{G_0}(u)} d_{G_1}(xu) - \sum_{x \in N_{G_0}(v)} \sum_{y \in N_{G_0}(x) \setminus \{v\}} d_{G_1}(xy) \\ &- \sum_{x,y \in N_{G_0}(v)} (d_{G_1}(xv) + d_{G_1}(vy) + r) - (q+r+2t-1) \sum_{x \in N_{G_0}(v)} d_{G_1}(xv) \\ &\leq \sum_{x \in N_{G_0}(u)} \sum_{y \in N_{G_0}(x) \setminus \{u\}} d_{G_1}(xy) + \sum_{x,y \in N_{G_0}(u)} (d_{G_1}(xu) + d_{G_1}(uy) + t) \end{aligned}$$

$$+ (q + 2r + t + a - 1) \sum_{x \in N_{G_0}(u)} d_{G_1}(xu) - \sum_{x \in N_{G_0}(v)} \sum_{y \in N_{G_0}(x) \setminus \{v\}} d_{G_1}(xy) - \sum_{x,y \in N_{G_0}(v)} (d_{G_1}(xv) + d_{G_1}(vy) - t) - (q + t - 1) \sum_{x \in N_{G_0}(v)} d_{G_1}(xv).$$
(3)

Substituting for the first six terms of right hand side of equation (2) with the inequality (3), we have

$$\begin{split} & EM_2(G_3) - EM_2(G_1) \geq t\{q(r+t)(q+r+t-1) + \frac{1}{2}(r-1)(t-a)(2q+2r+t+a-2) \\ & + (q+a)(r+t)(q+r+t+a-1) + \frac{1}{2}t(t-1)(2q+r+2t-2) + t(q+r+t-1)^2 \\ & + \frac{1}{2}r(r-1)(2q+2r+t+2a-2) + \frac{1}{2}(t-1)(r+a)(2q+r+2t+a-2) \\ & + r(q+r+t+a-1)^2\} \\ & > 0, \text{ since } q \geq 2, \text{ and } r, t \geq 1. \end{split}$$

Subcase 1.2: If $N_{G_0}(u) \cap N_{G_0}(v) \neq \emptyset$, then from the definition of $EM_2(G)$, we have

$$EM_{2}(G_{1}) = \sum_{e_{i},e_{j}\in E(G_{0}\setminus\{u,v\})} d_{G_{1}}(e_{i})d_{G_{1}}(e_{j}) + \sum_{x\in N_{G_{0}}(u)\setminus N_{G_{0}}(v)} \sum_{y\in N_{G_{0}}(x)\setminus\{u\}} d_{G_{1}}(ux)d_{G_{1}}(xy)$$

$$+ \sum_{x,y\in N_{G_{0}}(u)} d_{G_{1}}(xu)d_{G_{1}}(uy) + \sum_{x,y\in N_{G_{0}}(v)} d_{G_{1}}(xv)d_{G_{1}}(vy) + r(q+a+r-1)\sum_{x\in N_{G_{0}}(u)} d_{G_{1}}(xu)$$

$$+ t(q+t-1)\sum_{x\in N_{G_{0}}(v)} d_{G_{1}}(xv) + \sum_{x\in N_{G_{0}}(v)\setminus N_{G_{0}}(u)} \sum_{y\in N_{G_{0}}(x)\setminus\{v\}} d_{G_{1}}(vx)d_{G_{1}}(xy)$$

$$+ \sum_{x\in N_{G_{0}}(u)\cap N_{G_{0}}(v)} d_{G_{1}}(ux)d_{G_{1}}(xv) + \frac{r(r-1)}{2}(q+a+r-1)^{2} + \frac{t(t-1)}{2}(q+t-1)^{2}, \quad (4)$$

$$EM_{2}(G_{2}) = \sum_{e_{i},e_{j}\in E(G_{0}\setminus\{u,v\})} d_{G_{1}}(e_{i})d_{G_{1}}(e_{j}) + \sum_{x\in N_{G_{0}}(u)\setminus N_{G_{0}}(v)} \sum_{y\in N_{G_{0}}(x)\setminus\{u\}} (d_{G_{1}}(ux) - r)d_{G_{1}}(xy) + \sum_{x,y\in N_{G_{0}}(v)} (d_{G_{1}}(xv) - r)(d_{G_{1}}(uy) - r) + \sum_{x,y\in N_{G_{0}}(v)} (d_{G_{1}}(xv) + r)(d_{G_{1}}(vy) + r) + \sum_{x\in N_{G_{0}}(v)\setminus N_{G_{0}}(u)} \sum_{y\in N_{G_{0}}(x)\setminus\{v\}} (d_{G_{1}}(vx) + r)d_{G_{1}}(xy) + \sum_{x\in N_{G_{0}}(u)\cap N_{G_{0}}(v)} (d_{G_{1}}(ux) - r)(d_{G_{1}}(xv) + r) + (r+t)(q+r+t-1)\sum_{x\in N_{G_{0}}(v)} (d_{G_{1}}(xv) + r) + \frac{(r+t)(r+t-1)}{2}(q+r+t-1)^{2},$$
(5)

and
$$EM_{2}(G_{3}) = \sum_{e_{i},e_{j}\in E(G_{0}\setminus\{u,v\})} d_{G_{1}}(e_{i})d_{G_{1}}(e_{j}) + \sum_{x\in N_{G_{0}}(u)\setminus N_{G_{0}}(v)} \sum_{y\in N_{G_{0}}(x)\setminus\{u\}} (d_{G_{1}}(ux) + t)d_{G_{1}}(xy) + \sum_{x,y\in N_{G_{0}}(u)} (d_{G_{1}}(xu) + t)(d_{G_{1}}(uy) + t) + (r+t)(q+a+r+t-1) \sum_{x\in N_{G_{0}}(u)} (d_{G_{1}}(xu) + t) + \sum_{x\in N_{G_{0}}(v)\setminus N_{G_{0}}(u)} \sum_{y\in N_{G_{0}}(v)\setminus\{v\}} (d_{G_{1}}(vx) - t)d_{G_{1}}(xy) + \sum_{x,y\in N_{G_{0}}(v)} (d_{G_{1}}(xv) - t)(d_{G_{1}}(vy) - t) + \sum_{x\in N_{G_{0}}(u)\cap N_{G_{0}}(v)} (d_{G_{1}}(ux) + t))(d_{G_{1}}(xv) - t) + \frac{(r+t)(r+t-1)}{2}(q+a+r+t-1)^{2}.$$
(6)

Then,

$$EM_{2}(G_{2}) - EM_{2}(G_{1}) = -r \sum_{x \in N_{G_{0}}(u) \setminus N_{G_{0}}(v)} \sum_{y \in N_{G_{0}}(x) \setminus \{u\}} d_{G_{1}}(xy)$$

$$-r \sum_{x,y \in N_{G_{0}}(u)} (d_{G_{1}}(xu) + d_{G_{1}}(uy) - r) + r \sum_{x,y \in N_{G_{0}}(v)} (d_{G_{1}}(xv) + d_{G_{1}}(vy) + r)$$

$$-r(q + r + a - 1) \sum_{x \in N_{G_{0}}(u)} d_{G_{1}}(xu) + r(q + r + 2t - 1) \sum_{x \in N_{G_{0}}(v)} d_{G_{1}}(xv)$$

$$+r \sum_{x \in N_{G_{0}}(v) \setminus N_{G_{0}}(u)} \sum_{y \in N_{G_{0}}(x) \setminus \{v\}} d_{G_{1}}(xy) - r \sum_{x \in N_{G_{0}}(u) \cap N_{G_{0}}(v)} [d_{G_{1}}(vx) - d_{G_{1}}(xu)]$$

$$+rt(q + r + t - 1)^{2} - r^{2}|N_{G_{0}}(u) \cap N_{G_{0}}(v)| + qr(r + t)(q + r + t - 1)$$

$$+ \frac{1}{2}r(r - 1)(t - a)(2q + 2r + t + a - 2)\frac{1}{2}rt(t - 1)(2q + r + 2t - 2).$$
(7)

$$EM_{2}(G_{3}) - EM_{2}(G_{1}) = t \sum_{x \in N_{G_{0}}(u) \setminus N_{G_{0}}(v)} \sum_{y \in N_{G_{0}}(x) \setminus \{u\}} d_{G_{1}}(xy)$$

$$+ t \sum_{x,y \in N_{G_{0}}(u)} (d_{G_{1}}(xu) + d_{G_{1}}(uy) + t) - t \sum_{x,y \in N_{G_{0}}(v)} (d_{G_{1}}(xv) + d_{G_{1}}(vy) - t)$$

$$+ t(q + 2r + t + a - 1) \sum_{x \in N_{G_{0}}(u)} d_{G_{1}}(xu) - t(q + t - 1) \sum_{x \in N_{G_{0}}(v)} d_{G_{1}}(xv)$$

$$- t \sum_{x \in N_{G_{0}}(v) \setminus N_{G_{0}}(u)} \sum_{y \in N_{G_{0}}(x) \setminus \{v\}} d_{G_{1}}(xy) + t \sum_{x \in N_{G_{0}}(u) \cap N_{G_{0}}(v)} [d_{G_{1}}(vx) - d_{G_{1}}(xu)]$$

$$- t^{2} |N_{G_{0}}(u) \cap N_{G_{0}}(v)| + t(q + a)(r + t)(q + r + t + a - 1) + rt(q + r + t + a - 1)^{2}$$

$$+ \frac{1}{2} rt(r - 1)(2q + 2r + t + 2a - 2) + \frac{1}{2} t(t - 1)(r + a)(2q + r + 2t + a - 2).$$
(8)

Again, if one of the expressions (7) and (8) is greater than 0, then the lemma holds. Suppose $EM_2(G_2) - EM_2(G_1) \leq 0$, then we will show that $EM_2(G_3) - EM_2(G_1)$ has to be greater than 0. Similar to Subcase 1.1, we will first obtain a relation from Equation (7) by letting $EM_2(G_2) - EM_2(G_1) \leq 0$. That is, we get

$$\begin{split} &q(r+t)(q+r+t-1)+t(q+r+t-1)^2+\frac{1}{2}(r-1)(t-a)(2q+2r+t+a-2) \\ &+\frac{1}{2}t(t-1)(2q+r+2t-2)-r|N_{G_0}(u)\cap N_{G_0}(v)| \\ &\leq \sum_{x\in N_{G_0}(u)\backslash N_{G_0}(v)}\sum_{y\in N_{G_0}(x)\backslash \{u\}}d_{G_1}(xy) +\sum_{x,y\in N_{G_0}(u)}(d_{G_1}(xu)+d_{G_1}(uy)-r) \\ &+(q+r+a-1)\sum_{x\in N_{G_0}(u)}d_{G_1}(xu) -\sum_{x\in N_{G_0}(v)\backslash N_{G_0}(u)}\sum_{y\in N_{G_0}(x)\backslash \{v\}}d_{G_1}(xy) \\ &-\sum_{x,y\in N_{G_0}(v)}(d_{G_1}(xv)+d_{G_1}(vy)+r)-(q+r+2t-1)\sum_{x\in N_{G_0}(v)}d_{G_1}(xv) \\ &+\sum_{x\in N_{G_0}(u)\cap N_{G_0}(v)}(d_{G_1}(vx)-d_{G_1}(xu)) \end{split}$$

$$\leq \sum_{x \in N_{G_{0}}(u) \setminus N_{G_{0}}(v)} \sum_{y \in N_{G_{0}}(x) \setminus \{u\}} d_{G_{1}}(xy) + \sum_{x,y \in N_{G_{0}}(u)} (d_{G_{1}}(xu) + d_{G_{1}}(uy) + t) + (q + 2r + t + a - 1) \sum_{x \in N_{G_{0}}(u)} d_{G_{1}}(xu) - \sum_{x \in N_{G_{0}}(v) \setminus N_{G_{0}}(u)} \sum_{y \in N_{G_{0}}(x) \setminus \{v\}} d_{G_{1}}(xy) - \sum_{x,y \in N_{G_{0}}(v)} [d_{G_{1}}(xv) + d_{G_{1}}(vy) - t] - (q + t - 1) \sum_{x \in N_{G_{0}}(v)} d_{G_{1}}(xv) + \sum_{x \in N_{G_{0}}(u) \cap N_{G_{0}}(v)} [d_{G_{1}}(vx) - d_{G_{1}}(xu)].$$
(9)

Substituting for the first seven terms of right hand side of Equation (8) by the inequality (9), we have

$$\begin{split} & EM_2(G_3) - EM_2(G_1) \geq t\{q(r+t)(q+r+t-1) + t(q+r+t-1)^2 \\ & + r(q+r+t+a-1)^2 + \frac{1}{2}(r-1)(t-a)(2q+2r+t+a-2) + \frac{1}{2}t(t-1)(2q+r+2t-2) \\ & + (q+a)(r+t)(q+r+t+a-1) + \frac{1}{2}r(r-1)(2q+2r+t+2a-2) \\ & + \frac{1}{2}(t-1)(r+a)(2q+r+2t+a-2) - (r+t)|N_{G_0}(u) \cap N_{G_0}(v)| \} \\ & > 0, \text{ since } |N_{G_0}(u) \cap N_{G_0}(v)| \leq q, \quad q \geq 2, \text{ and } r, t \geq 1. \end{split}$$

Case 2: If u and v are adjacent, then from the definition of $EM_2(G)$, we have

$$EM_{2}(G_{1}) = \sum_{e_{i},e_{j}\in E(G_{0}\setminus\{u,v\})} d_{G_{1}}(e_{i})d_{G_{1}}(e_{j}) + \sum_{x\in N_{G_{0}}(u)\setminus\{v,N_{G_{0}}(v)\}} \sum_{y\in N_{G_{0}}(x)\setminus\{u\}} d_{G_{1}}(ux)d_{G_{1}}(xy) + \sum_{x,y\in N_{G_{0}}(u)\setminus\{v\}} d_{G_{1}}(xu)d_{G_{1}}(uy) + \sum_{x\in N_{G_{0}}(v)\setminus\{u,N_{G_{0}}(u)\}} \sum_{y\in N_{G_{0}}(x)\setminus\{v\}} d_{G_{1}}(xu) + \sum_{x,y\in N_{G_{0}}(v)\setminus\{u\}} d_{G_{1}}(xv)d_{G_{1}}(vy) + r(q+a+r-1) \sum_{x\in N_{G_{0}}(u)\setminus\{v\}} d_{G_{1}}(xu) + t(q+t-1) \sum_{x\in N_{G_{0}}(v)\setminus\{u\}} d_{G_{1}}(xv) + \sum_{x\in N_{G_{0}}(u)\cap N_{G_{0}}(v)} d_{G_{1}}(ux)d_{G_{1}}(xv) + \sum_{x\in N_{G_{0}}(u)\setminus\{v\}} d_{G_{1}}(xu)d_{G_{1}}(uv) + \sum_{x\in N_{G_{0}}(v)\setminus\{u\}} d_{G_{1}}(xv)d_{G_{1}}(vu) + t(q+t-1)d_{G_{1}}(uv) + r(r+q+a-1)d_{G_{1}}(uv) + \frac{r(r-1)}{2}(q+a+r-1)^{2} + \frac{t(t-1)}{2}(q+t-1)^{2},$$

$$EM_{2}(G_{2}) = \sum d_{G_{1}}(e_{i})d_{G_{1}}(e_{j}) + \sum \sum (d_{G_{1}}(ux)-r)d_{G_{1}}(xy) d_{G_{1}}(xy) d_{G_{1}}(x$$

$$EM_{2}(G_{2}) = \sum_{e_{i},e_{j}\in E(G_{0}\setminus\{u,v\})} d_{G_{1}}(e_{i})d_{G_{1}}(e_{j}) + \sum_{x\in N_{G_{0}}(u)\setminus\{v,N_{G_{0}}(v)\}} \sum_{y\in N_{G_{0}}(x)\setminus\{u\}} (d_{G_{1}}(ux) - r)d_{G_{1}}(xy)$$

$$+ \sum_{x,y\in N_{G_{0}}(u)\setminus\{v\}} (d_{G_{1}}(xu) - r)(d_{G_{1}}(uy) - r) + \sum_{x\in N_{G_{0}}(v)\setminus\{u,N_{G_{0}}(u)\}} \sum_{y\in N_{G_{0}}(x)\setminus\{v\}} (d_{G_{1}}(vx) + r)d_{G_{1}}(xy)$$

$$+ \sum_{x,y\in N_{G_{0}}(v)\setminus\{u\}} (d_{G_{1}}(xu) - r)d_{G_{1}}(uv) + \sum_{x\in N_{G_{0}}(v)\setminus\{u\}} (d_{G_{1}}(xv) + r)d_{G_{1}}(uv)$$

$$+ \sum_{x\in N_{G_{0}}(u)\cap N_{G_{0}}(v)} (d_{G_{1}}(ux) - r)(d_{G_{1}}(xv) + r) + \frac{(r+t)((r+t-1))}{2}(q+r+t-1)^{2}$$

$$+ (r+t)(q+r+t-1)d_{G_{1}}(uv), \qquad (11)$$

and

$$\begin{split} EM_{2}(G_{3}) &= \sum_{e_{i}e_{j}\in E(G_{0}\backslash\{u,v\})} d_{G_{1}}(e_{i})d_{G_{1}}(e_{j}) + \sum_{x\in N_{G_{0}}(u)\backslash\{v,N_{G_{0}}(v)\}} \sum_{y\in N_{G_{0}}(v)\backslash\{u\}} (d_{G_{1}}(ux) + t)d_{G_{1}}(xy) \\ &+ \sum_{x,y\in N_{G_{0}}(v)\backslash\{v\}} (d_{G_{1}}(xu) + t)(d_{G_{1}}(uy) + t) + \sum_{x,y\in N_{G_{0}}(v)\backslash\{u\}} (d_{G_{1}}(xv) - t)(d_{G_{1}}(vy) - t) \\ &+ \sum_{x\in N_{G_{0}}(v)\backslash\{v\}} \sum_{y\in N_{G_{0}}(v)\backslash\{v\}} (d_{G_{1}}(vx) - t)d_{G_{1}}(xy) + \sum_{x\in N_{G_{0}}(v)\backslash\{v\}} (d_{G_{1}}(xu) + t)d_{G_{1}}(uv) \\ &+ (r+t)(q+a+r+t-1)\sum_{x\in N_{G_{0}}(v)\backslash\{v\}} (d_{G_{1}}(xv) - t) + \frac{(r+t)((r+t-1))}{2} (q+a+r+t-1)^{2} \\ &+ (r+t)(p+r+t-1)d_{G_{1}}(uv). \end{split}$$

$$\begin{aligned} &+ \sum_{x\in N_{G_{0}}(v)\backslash\{v\}} (d_{G_{1}}(xu) + d_{G_{1}}(uv) - t) + \frac{(r+t)((r+t-1))}{2} (q+a+r+t-1)^{2} \\ &+ (r+t)(p+r+t-1)d_{G_{1}}(uv). \end{aligned}$$

$$\begin{aligned} &+ \sum_{x\in N_{G_{0}}(v)\backslash\{v\}} [d_{G_{1}}(xu) + d_{G_{1}}(uy) - r] - r(q+r+a-1) \sum_{x\in N_{G_{0}}(v)\backslash\{v\}} d_{G_{1}}(xu) \\ &+ r\sum_{x\in N_{G_{0}}(v)\backslash\{v\}} [d_{G_{1}}(xu) + d_{G_{1}}(uy) - r] - r(q+r+a-1) \sum_{x\in N_{G_{0}}(v)\backslash\{v\}} d_{G_{1}}(xu) \\ &+ rt(q+r+t-1)^{2} + d_{G_{1}}(vy) + r) + r(q+r+2t-1) \sum_{x\in N_{G_{0}}(v)\backslash\{u\}} d_{G_{1}}(xv) \\ &+ rt(q+r+t-1)^{2} + d_{G_{1}}(vy) + r) + r(q+r+2t-1) \sum_{x\in N_{G_{0}}(v)\backslash\{u\}} d_{G_{1}}(xv) \\ &+ r(q-1)(r+t)(q+r+t-1) + \frac{r(r-1)}{2}(t-a)(2q+2r+t+a-1) \\ &+ \frac{rt(t-1)}{2}(2q+r+2t-2) \end{aligned}$$

and

$$\begin{split} & EM_{2}(G_{3}) - EM_{2}(G_{1}) = t \sum_{x \in N_{G_{0}}(u) \setminus \{v, N_{G_{0}}(v)\}} \sum_{y \in N_{G_{0}}(x) \setminus \{u\}} d_{G_{1}}(xy) \\ &+ t \sum_{x,y \in N_{G_{0}}(u) \setminus \{v\}} (d_{G_{1}}(xu) + d_{G_{1}}(uy) + t) + t(q + 2r + t + a - 1) \sum_{x \in N_{G_{0}}(u) \setminus \{v\}} d_{G_{1}}(xu) \\ &- t \sum_{x \in N_{G_{0}}(v) \setminus \{u, N_{G_{0}}(u)\}} \sum_{y \in N_{G_{0}}(x) \setminus \{v\}} d_{G_{1}}(xy) - t \sum_{x,y \in N_{G_{0}}(v) \setminus \{u\}} (d_{G_{1}}(xv) + d_{G_{1}}(vy) - t) \\ &- t(q + t - 1) \sum_{x \in N_{G_{0}}(v) \setminus \{u\}} d_{G_{1}}(xv) + t \sum_{x \in N_{G_{0}}(u) \cap N_{G_{0}}(v)} (d_{G_{1}}(vx) - d_{G_{1}}(xu)) \\ &- t^{2}|N_{G_{0}}(u) \cap N_{G_{0}}(v)| + 2t(r + a)d_{G_{1}}(uv) + t(q + a - 1)(r + t)(q + r + t + a - 1) \\ &+ rt(q + r + t + a - 1)^{2} + \frac{rt(r - 1)}{2}(2q + 2r + t + 2a - 2) \\ &+ \frac{t(t - 1)}{2}(r + a)(2q + r + 2t + a - 2). \end{split}$$

If either of the expressions in (13) or (14) is greater than 0, then the lemma holds. Suppose $EM_2(G_2) - EM_2(G_1) \leq 0$, then we will show that $EM_2(G_3) - EM_2(G_1)$ has to be greater than 0. Letting

 $EM_2(G_2) - EM_2(G_1) \le 0$ in Equation (13), we have

$$\begin{aligned} (q-1)(r+t)(q+r+t-1) &+ \frac{t(t-1)}{2}(2q+r+2t-2) + 2(t-a)d_{G_{1}}(uv) + t(q+r+t-1)^{2} \\ &+ \frac{1}{2}(r-1)(t-a)(2q+2r+t+a-1) - r|N_{G_{0}}(u) \cap N_{G_{0}}(v)| \\ &\leq \sum_{x \in N_{G_{0}}(u) \setminus \{v, N_{G_{0}}(v)\}} \sum_{y \in N_{G_{0}}(x) \setminus \{u\}} d_{G_{1}}(xy) + \sum_{x,y \in N_{G_{0}}(u) \setminus \{v\}} (d_{G_{1}}(xu) + d_{G_{1}}(uy) - r) \\ &+ (q+r+a-1) \sum_{x \in N_{G_{0}}(u) \setminus \{v\}} d_{G_{1}}(xu) - \sum_{x \in N_{G_{0}}(v) \setminus \{u, N_{G_{0}}(u)\}} \sum_{y \in N_{G_{0}}(v) \setminus \{u\}} d_{G_{1}}(xy) \\ &- \sum_{x,y \in N_{G_{0}}(v) \cap N_{G_{0}}(v)} (d_{G_{1}}(xv) + d_{G_{1}}(vy) + r) - (q+r+2t-1) \sum_{x \in N_{G_{0}}(v) \setminus \{u\}} d_{G_{1}}(xv) \\ &+ \sum_{x \in N_{G_{0}}(u) \cap N_{G_{0}}(v)} (d_{G_{1}}(vx) - d_{G_{1}}(xu)) \\ &\leq \sum_{x \in N_{G_{0}}(u) \setminus \{v, N_{G_{0}}(v)\}} \sum_{y \in N_{G_{0}}(u) \setminus \{v\}} d_{G_{1}}(xu) + \sum_{x,y \in N_{G_{0}}(v) \setminus \{u\}} (d_{G_{1}}(xv) + d_{G_{1}}(vy) + r) \\ &+ (q+2r+t+a-1) \sum_{x \in N_{G_{0}}(u) \setminus \{v\}} d_{G_{1}}(xu) - \sum_{x \in N_{G_{0}}(v) \setminus \{u, N_{G_{0}}(u)\}} \sum_{y \in N_{G_{0}}(x) \setminus \{v\}} d_{G_{1}}(xy) \\ &- \sum_{x,y \in N_{G_{0}}(v) \setminus \{u\}} (d_{G_{1}}(xv) + d_{G_{1}}(vy) - t) - (q+t-1) \sum_{x \in N_{G_{0}}(v) \setminus \{u\}} d_{G_{1}}(xv) \\ &+ \sum_{x \in N_{G_{0}}(v) \cap \{u\}} (d_{G_{1}}(vx) - d_{G_{1}}(xu)). \end{aligned}$$
(15)

Now, substituting for the first seven terms of right hand side of equation (14) by the inequality (15), we have

$$\begin{split} & EM_2(G_3) - EM_2(G_1) \geq t\{2(t-a)d_{G_1}(uv) + (q-1)(r+t)(q+r+t-1) \\ & + \frac{1}{2}(r-1)(t-a)(2q+2r+t+a-1) + \frac{t(t-1)}{2}(2q+r+2t-2) \\ & + (q+a-1)(r+t)(q+r+t+a-1) + 2(r+a)d_{G_1}(uv) + r(q+r+t+a-1)^2 \\ & + \frac{r(r-1)}{2}(2q+2r+t+2a-2) + \frac{(t-1)}{2}(r+a)(2q+r+2t+a-2) \\ & + t(q+r+t-1)^2 - (r+t)|N_{G_0}(u) \cap N_{G_0}(v)|\}. \end{split}$$

Since $|N_{G_0}(u) \cap N_{G_0}(v)| \le q$ and $d_{G_1}(uv) = (2q + r + t + a - 2)$, then above inequality can be written as

$$\begin{split} &EM_2(G_3) - EM_2(G_1) \geq t\{2(t+a)(2q+r+t+a-2) + (q-1)(r+t)(q+r+t-1) \\ &+ \frac{1}{2}(r-1)(t-a)(2q+2r+t+a-1) + \frac{t(t-1)}{2}(2q+r+2t-2) + r(q+r+t+a-1)^2 \\ &+ (q+a-1)(r+t)(q+r+t+a-1) + \frac{r(r-1)}{2}(2q+2r+t+2a-2) \\ &+ \frac{(t-1)}{2}(r+a)(2q+r+2t+a-2) + t(q+r+t-1)^2 - (r+t)q\} \\ &> 0, \ \text{since } q \geq 2, \text{ and } r, t \geq 1. \end{split}$$

Remark 2.1 If $G_0 = C_k$, where C_k is the cycle graph on k vertices, then in Lemma 2.3, vertices u and v have the same degree in graph G_0 .

Remark 2.2 If G_0 is a bicyclic graph which has no pendant vertex, see Figure 7. Then, in Lemma 2.3, possible degree of vertex u and v in graph G_0 are p = q or p = q + 1 or p = q + 2.

To estimate the upper bounds of $EM_2(G)$ for trees, unicyclic, and bicyclic graphs we will use the transformations **A**, **B** and **C**.

3. Three transformations which decrease the second reformulated Zagreb index

In this section, we make use of three more graph operations as defined in (Deng, 2007; Ji *et al.*, 2014) that are useful for finding the lower bounds of $EM_2(G)$.

Transformation D: Let G_0 be a non-trivial graph and u be any vertex of G_0 . Let G_1 be a graph obtained from G_0 by attaching at u two paths $P_1 = uu_1u_2 \ldots u_r$ of length r and $P_2 = uv_1v_2 \ldots v_t$ of length t. Let $G_2 = G_1 - \{uu_1\} + \{v_tu_1\}$; see Figure 4. Here G_2 is said to be obtained from G_1 by **transformation D**.



Fig. 4. Representation of transformation D

Lemma 3.1 Let G_2 be a graph obtained by Transformation D from G_1 as shown in Figure 4. Then, $EM_2(G_1) > EM_2(G_2)$.

Proof: Let $N_{G_0}(u)$ denote the neighborhood of the vertex of u in G_0 . Now, we prove this lemma by taking condition on path length r, t.

If $r, t \geq 3$ then by definition of $EM_2(G)$, we have

$$\begin{split} EM_2(G_1) - EM_2(G_2) &= \sum_{x \in N_{G_0}(u)} \sum_{y \in N_{G_0}(x) \setminus \{u\}} d_{G_1}(xy) + \sum_{x,y \in N_{G_0}(u)} (d_{G_1}(xu) + d_{G_1}(uy) - 1) \\ &+ \sum_{x \in N_{G_0}(u)} ((d_{G_1}(u) + 1)d_{G_1}(ux) + (d_{G_1}(u) - 1)) + d_{G_1}^2(u) + 2d_{G_1}(u) - 8 \\ &> 0, \text{ since } d_{G_1}(u) > 2. \end{split}$$

Similarly proof holds for the remaining values of r and t, that is, for $r = 2, t \ge 3$; $r = 1, t \ge 3$; r = 2, t = 2; r = 1, t = 2 and r = 1, t = 1. We omit the proofs for brevity.

Remark 3.1 Note that, we can convert any tree into a path graph by repeating transformation D.

Transformation E: Let G_0 be a non-trivial graph having vertices u and v. Let G_1 be a graph obtain from G_0 by adding two paths $\langle u, u_1, u_2, \ldots, u_r \rangle$ and $\langle v, v_1, v_2, \ldots, v_t \rangle$ at vertices u and v of length r and t, respectively. Let $G_2 := G_1 - \{uu_1\} + \{v_tu_1\}$. Here, G_2 is said to be obtained from G_1 by **transformation E**; see Figure 5.

Lemma 3.2 Let G_2 be the graph obtained from G_1 by using transformation E, then $EM_2(G_1) > EM_2(G_2)$.

Proof: We prove this lemma by making conditions on the path lengths r and t. First, we assume that $r \ge 3$ and $t \ge 3$. Now we have the following cases.



Fig. 5. Representation of transformation E.

Case 1: If vertex u and v are not adjacent, then we have two subcases. **Subcase 1.1:** If $N_{G_0}(u) \cap N_{G_0}(v) = \emptyset$, then from definition of $EM_2(G)$, we have

$$\begin{split} EM_2(G_1) - EM_2(G_2) &= \sum_{x \in N_{G_0}(u)} \sum_{y \in N_{G_0}(x) \setminus \{u\}} d_{G_1}(xy) + \sum_{x,y \in N_{G_0}(u)} (d_{G_1}(xu) + d_{G_1}(uy) - 1) \\ &+ \sum_{x \in N_{G_0}(u)} d_{G_1}(xu) d_{G_1}(uu_1) + 2d_{G_1}(uu_1) - 10 \\ &\geq d_{G_1}(xu) d_{G_1}(uu_1) + 2d_{G_1}(uu_1) - 10 \\ &> 0, \text{ since } d_{G_1}(xu) \geq 2, d_{G_1}(uu_1) \geq 3. \end{split}$$

Subcase 1.2: If $N_{G_0}(u) \cap N_{G_0}(v) \neq \emptyset$, then from definition of $EM_2(G)$, we have

$$\begin{split} EM_2(G_1) - EM_2(G_2) &= \sum_{x \in N_{G_0}(u) \setminus N_{G_0}(v)} \sum_{y \in N_{G_0}(x) \setminus \{u\}} d_{G_1}(xy) + \sum_{x,y \in N_{G_0}(u)} (d_{G_1}(xu) + d_{G_1}(uy) - 1) \\ &+ \sum_{x \in N_{G_0}(u)} d_{G_1}(xu) d_{G_1}(uu_1) + \sum_{x \in N_{G_0}(u) \cap N_{G_0}(v)} d_{G_1}(xv) + 2d_{G_1}(uu_1) - 10 \\ &\geq d_{G_1}(xu) d_{G_1}(uu_1) + 2d_{G_1}(uu_1) - 10 \\ &> 0, \text{ since } d_{G_1}(xu) \geq 2, d_{G_1}(uu_1) \geq 3. \end{split}$$

Case 2 If vertex u and v are adjacent then from definition of $EM_2(G)$, we have

$$\begin{split} & EM_2(G_1) - EM_2(G_2) = \sum_{x \in N_{G_0}(u) \setminus \{v, N_{G_0}(v)\}} \sum_{y \in N_{G_0}(x) \setminus \{u\}} d_{G_1}(xy) + \sum_{x \in N_{G_0}(u) \cap N_{G_0}(v)} d_{G_1}(xv) \\ & + \sum_{x, y \in N_{G_0}(u) \setminus \{v\}} (d_{G_1}(xu) + d_{G_1}(uy) - 1) + \sum_{x \in N_{G_0}(u) \setminus \{v\}} (d_{G_1}(xu) + d_{G_1}(uv) - 1) \\ & + \sum_{x \in N_{G_0}(v) \setminus \{u\}} d_{G_1}(xv) + d_{G_1}(vv_1) + 2d_{G_1}(uu_1) + d_{G_1}(uu_1)d_{G_1}(uv) - 10 \\ & \geq d_{G_1}(vv_1) + 2d_{G_1}(uu_1) + d_{G_1}(uu_1)d_{G_1}(uv) - 10 \\ & > 0, \text{ since } d_{G_1}(vv_1) \geq 3, \ d_{G_1}(uu_1) \geq 3 \text{ and } d_{G_1}(uv) \geq 3. \end{split}$$

Proof is complete for $r, t \geq 3$.

Similarly proof holds for the remaining values of r and t, that is, for (r, t) is one of the pairs (1, 2), (1, 3), (2, 2) and (2, 3). We omit the proofs for brevity.

Remark 3.2 By suitable and repeated application of transformations D and E to any unicyclic graph on n vertices and having girth k, we can obtain a (k, n - k)-tadpole graph. We denote a (k, n - k)-tadpole graph by C_n^k .

Note: A(p,q)-tadpole graph is a special type of unicyclic graph obtained by attaching a path graph on q vertices to a cycle graph on p (at least 3) vertices with a bridge.

Transformation F: Let G_0 be a graph containing a path of length at least 2, say $\langle u, x_1, v \rangle$. Let G_1 be the graph obtained from G_0 by attaching a path $\langle x_1, x_2, \ldots, x_k \rangle$, $(k \ge 1)$ at x_1 . Let $G_2 := G_1 - \{x_1v\} + \{x_kv\}$; see Figure 6. We say that G_2 is obtained from G_1 by **transformation F**.



Fig. 6. Representation of transformation F

Lemma 3.3 If G_2 is obtained from G_1 using transformation F, then $EM_2(G_1) > EM_2(G_2)$.

Proof: From the definition of $EM_2(G)$ and using the fact that $d_{G_2}(ux_1) = d_{G_1}(ux_1) - 1$, $d_{G_2}(x_kv) = d_{G_1}(x_1v) - 1$, we have

$$EM_2(G_1) - EM_2(G_2) \ge d_{G_1}(ux_1)d_{G_1}(x_1v) + 2d_{G_1}(ux_1) + 2d_{G_1}(x_1v) - 2d_{G_2}(ux_1) - 2d_{G_2}(x_kv)$$

= $d_{G_1}(ux_1)d_{G_1}(x_1v) + 4 > 0.$

Remark 3.3 Similarly, repeated application of the transformations D and E to a bicyclic graph will result in such a bicyclic graph where a path is attached to one of the graphs in Figure 7 and finally applying transformation F to the resultant graph will result in exactly one of the graphs in Figure 7.



Fig. 7. Bicyclic graphs which has no pendant vertices

4. Bounds of second reformulated Zagreb index

In this section, we compute the upper and lower bounds for trees, unicyclic, bicyclic and tricyclic graphs using the six transformations discussed in sections 2 and 3.

4.1 **Trees**

It is well known that the path graph is the only tree on 3 vertices and $EM_2(P_3) = 1$. For trees on at least 4 vertices we have the following theorem.

Theorem 4.1 If $T \neq \{P_n, S_n\}$ is a tree on $n \ge 4$ vertices, then $4n - 12 = EM_2(P_n) < EM_2(T) < EM_2(S_n) = \frac{1}{2}(n-1)(n-2)^3$.

Proof: Since any tree T can be transformed into a star S_n by using the transformations A and C, it follows immediately from Lemma 2.1 and Lemma 2.3, $EM_2(S_n) > EM_2(T)$.

Similarly, for the lower bound, we can see that the result follows directly from Lemma 3.1 and Remark

3.1.

By direct computation using the definition of the second reformulated Zagreb index, it follows that $EM_2(P_n) = 4n - 12$ and $EM_2(S_n) = \frac{1}{2}(n-1)(n-2)^3$ and hence the theorem holds.

From the above theorem, it is immediate that among the trees on n vertices, the path graph attains the least value and the star graph attains the greatest value for the second reformulated Zagreb index.

4.2 Unicyclic Graphs

Before finding the upper bounds for the unicyclic graph, let us fix some notation. Let U_n^k denotes the unicyclic graph obtained from the cycle C_k of girth k by attaching n - k pendent vertices to any one vertex on C_k . Let C_n^k denotes the tadpole graph with girth k, that is, the cycle of girth k is connected to a path P_{n-k} with a bridge.

Theorem 4.2 If G is a unicyclic graph on n vertices and girth k, then $EM_2(G) \leq EM_2(U_n^k)$. Equality holds if and only if $G \simeq U_n^k$

Proof: Proof follows from Lemma 2.1 and Lemma 2.3 as any unicyclic graph can be transformed into U_n^k by using transformations A and C.

Corollary 4.1 For fixed $n \ge 4$ and girth $4 \le k \le n$, $EM_2(U_n^k) \le EM_2(U_n^{k-1})$.

Proof: From the definition of $EM_2(G)$, we have upon simplification

$$EM_2(U_n^k) = \frac{1}{2}(n-k+1)^2[(n-k)^2 + 3(n-k+2)] + (4n-3)$$

Therefore,

$$EM_2(U_n^k) - EM_2(U_n^{k-1}) = -\frac{1}{2}(n-k)(n-k+1)(4n-4k+5) -6(n-k+2)(n-k+1) - 2(n-k+2) - 1 \le 0.$$

Hence the proof.

Theorem 4.3 U_n^3 is the unique graph with the largest $EM_2(G)$ among all the unicyclic graphs.

Proof: From Theorem 4.2 and Corollary 4.1, the result follows immediately. The value of $EM_2(U_n^3)$ can be directly computed and is given by $EM_2(U_n^3) = \frac{1}{2}(n-3)(n-4)(n-2)^2 + (n-1)(2n^2 - 9n + 15)$.

Theorem 4.4 Let G be a unicyclic graph on n vertices. If $G \neq \{C_n, C_n^k\}$, then $EM_2(G) > EM_2(C_n^k) > EM_2(C_n)$, where C_n^k is a tadpole graph.

Proof: From Remark 3.2, Lemma 3.1, Lemma 3.2, and Lemma 3.3, the result follows immediately and we have $EM_2(G) > EM_2(C_n^k) > EM_2(C_n)$.

Theorem 4.5 The value of
$$EM_2(C_n) = 4n$$
 and $EM_2(C_n^k) = \begin{cases} 4n+17, & n=k+1; \\ 4n+22, & n=k+2; \\ 4n+23, & n \ge k+3 \end{cases}$

Proof: Proof follows by direct computation.

4.3 Bicyclic Graphs

Before proving the bounds of bicyclic graph, we define some notations. Let $\mathbb{B}(n, n + 1)$ be the set of bicyclic graphs of n vertices and n + 1 edges. Any bicyclic graph belong to any one of the following collection of bicyclic graphs.

- Let B¹_n(p,q) ⊂ B(n, n + 1) be the set of bicyclic graphs on n vertices, where p + q − 1 ≤ n, is such that if G ∈ B¹_n(p,q), then two cycles C_p and C_q are attached by a common vertex in G. Let D¹_n(p,q) ⊂ B¹_n(p,q) be the set of graphs having exactly n = p + q − 1 vertices, that is, if G ∈ D¹_n(p,q), then G has no any pendant vertex, see Figure 7(a).
- 2. Let $\mathbb{B}_n^2(p,q,l) \subset \mathbb{B}(n,n+1)$ be the set of bicyclic graphs on n vertices, where $p+q+l \leq n+1$, is such that if $G \in \mathbb{B}_n^2(p,q,l)$, then the two cycles C_p and C_q are connected by a path of length $l \geq 1$ in G. Let $D_n^2(p,q,l) \subset \mathbb{B}_n^2(p,q,l)$ be the set of graphs having exactly n+1 = p+q+lvertices, that is, if $G \in D_n^2(p,q,l)$, then G has no pendant vertex, see Figure 7(b).
- Let B³_n(p,q,l) ⊂ B(n, n + 1) be the set of bicyclic graphs on n vertices, where p + q l ≤ n + 1, is such that if G ∈ B³_n(p,q,l), then the two cycles C_p and C_q have a common path of length l ≥ 1 in G. Let D³_n(p,q,l) ⊂ B³_n(p,q,l) be the set of graphs having exactly n + 1 = p + q l vertices, that is, if G ∈ D³_n(p,q,l), then G has no pendant vertex, see Figure 7(c).

Theorem 4.6 F_n^3 is the unique graph which has the largest value of $EM_2(G)$ among all bicyclic graph.

Proof:Let $G \in \mathbb{B}(n, n + 1)$ be a bicyclic graph. G lies in one of the classes of bicyclic graphs $\mathbb{B}_n^1(p, q)$, $\mathbb{B}_n^2(p, q, l)$, $\mathbb{B}_n^3(p, q, l)$.

Suppose $G \in \mathbb{B}_n^1(p,q)$ or $G \in \mathbb{B}_n^2(p,q,l)$: By repeated and suitable application of the operations A, B and C on graph G, G is transformed into one of the graphs of the form F_n^1 or F_n^2 as shown in Figure 8(a) or 8(b), respectively. Hence by Lemma 2.1, Lemma 2.2 and Lemma 2.3, we have $EM_2(G) \leq EM_2(F_n^1)$ or $EM_2(G) \leq EM_2(F_n^2)$, respectively.



Fig. 8. Some bicyclic graphs which are using in upper bounds

Similarly, if $G \in \mathbb{B}_n^3(p,q)$ and upon repeated application of the transformations A, B and C suitably we can convert the graph G into one of the graphs of the form F_n^3 or F_n^4 as shown in Figure 8(c), 8(d), respectively. Hence by Lemma 2.1, Lemma 2.2 and Lemma 2.3, we have $EM_2(G) \leq EM_2(F_n^3)$ or $EM_2(G) \leq EM_2(F_n^4)$.

As a resultant, we only need to compare the values of EM_2 for graphs in F_n^1, F_n^2, F_n^3 and F_n^4 . By direct computation, we obtain the following.

$$EM_{2}(F_{n}^{1}) = \frac{1}{2} \{n^{4} - 7n^{3} + 26n^{2} - 36n + 36\}, \quad EM_{2}(F_{n}^{2}) = \frac{1}{2} \{n^{4} - 15n^{3} + 92n^{2} - 240n + 406\}$$
$$EM_{2}(F_{n}^{3}) = \frac{1}{2} \{n^{4} - 7n^{3} + 26n^{2} - 28n + 56\}, \quad EM_{2}(F_{n}^{4}) = \frac{1}{2} \{n^{4} - 11n^{3} + 53n^{2} - 101n + 172\}$$

Thus, by comparing the above values, we get

$$EM_2(G) \le \frac{1}{2} \{ n^4 - 7n^3 + 26n^2 - 28n + 56 \} = EM_2(F_n^3)$$

Theorem 4.7 If G is a bicyclic graph on $n \ge 8$ vertices, then $EM_2(G) \ge 4n + 58$. Equality holds if and only if either $G \in D_n^2(p,q,l)$ for $l \ge 3$ or $G \in D_n^3(p,q,l)$ for $p \ge 6, q \ge 6, l \ge 3$.

Proof: From our observation in Remark 3.3, it is immediate that any bicyclic graph G on n vertices can be transformed into a graph in one of the classes $D_n^1(p,q)$, $D_n^2(p,q,l)$, or $D_n^3(p,q,l)$ on n vertices using repeated application of transformations D, E and F. Hence by Lemmas 3.2 and Lemma 3.3, the smallest value of $EM_2(G)$ is attained by the graphs in one of the above classes.

As a resultant, we only need to compare the value of EM_2 for graphs in each of the class $D_n^1(p,q)$, $D_n^2(p,q,l)$, and $D_n^3(p,q,l)$. As the computations are straight forward, we present the values directly.

For a graph $H \in D_n^1(p,q)$, $EM_2(H) = 4n + 108$, $n \ge 5$.

For $H \in D_n^2(p,q,l)$, the cycles C_p and C_q are connected by a path of length $l \ge 1$. By direct caluclation, we have $EM_2(H) = 4n + 66$, $n \ge 6$ and $H \in D_n^2(p,q,1)$. $EM_2(H) = 4n + 59$, $n \ge 7$ and $H \in D_n^2(p,q,2)$. $EM_2(H) = 4n + 58$, $n \ge 8$ and $H \in D_n^2(p,q,l)$ for $l \ge 3$.

For $H \in D_n^3(p,q,l)$, recall in H, the cycles C_p and C_q have a common path of length $l \ge 1$.

- 1. If n = 4 or (p = 3, q = 3 and l = 1), then $EM_2(D_4^3(3, 3, 1)) = 84$.
- 2. If $H \in D_n^3(p, 3, 1)$ for $n \ge 5$, and $p \ge 4$, then $EM_2(H) = 4n + 67$.
- 3. If $H \in D_n^3(p, q, 1)$ for $n \ge 6, p \ge 4$, and $q \ge 4$, then $EM_2(H) = 4n + 66$.
- 4. If n = 5 or (p = 4, q = 4 and l = 2), then $EM_2(D_3(4, 4, 2)) = 81$.
- 5. If $H \in D_n^3(p, 4, 2)$ for $n \ge 6$ and $p \ge 5$, then $EM_2(H) = 4n + 60$.
- 6. If $H \in D_n^3(p, q, 2)$ for $n \ge 7$, $p \ge 5$ and $q \ge 5$, then $EM_2(H) = 4n + 59$.
- 7. If $H \in D_n^3(p,q,l)$ for $n \ge 8, p \ge 6, q \ge 6$ and $l \ge 3$, then $EM_2(H) = 4n + 58$.

Thus, from the above values we get the desired results.

4.4 Tricyclic Graphs

Before proving the bounds of tricyclic graphs, we will fix some notations that will be used in our proof. Let \mathbb{X}^n be the set of tricyclic graphs of n vertices. We define two interesting sub collections of tricyclic graphs that are required.

- 1. Let $\mathbb{X}_0^n \subset \mathbb{X}^n$ be the set of tricyclic graphs of n vertices such that if $G \in \mathbb{X}_0^n$, then G has no pendent vertices. There are 15 possible collections of graphs in \mathbb{X}_0^n , whose representation is given in Figure 10.
- 2. Let $\mathbb{X}_1^n \subset \mathbb{X}_0^n$ be the set of tricyclic graphs such that if $G \in \mathbb{X}_1^n$, then G has maximum vertex degree three and any two vertices of degree three are connected by a path of length atleast two in G. Representation of graphs in \mathbb{X}_1^n is given in Figure 11.

Theorem 4.8 Let $G \in \mathbb{X}^n$ be a tricyclic graph of vertex n. Then

$$EM_2(G) \le \frac{1}{2}(n^4 - 7n^3 + 30n^2 - 20n + 176),$$

where the equality holds if and only if $G \simeq \gamma_5^n$ or $G \simeq \gamma_6^n$, as in Figure 9.



Fig. 9. Tricyclic graphs which attains the upper bounds

Proof: If, we are repeating transformations A, B and C, then, the tricyclic graph G can be converted into one of the six graphs shown in Figure 9. Then, from Lemma 2.1, Lemma 2.2 and Lemma 2.3, we have $EM_2(G) \leq EM_2(\gamma_i^n), i = 1, ..., 6$. Hence, as before, we only need to compare the value of $EM_2(\gamma_i^n)$, i = 1, ..., 6. By direct computation we have

$$EM_{2}(\gamma_{1}^{n}) = \frac{1}{2}(n^{4} - 7n^{3} + 30n^{2} - 28n + 118), \quad EM_{2}(\gamma_{2}^{n}) = \frac{1}{2}(n^{4} - 7n^{3} + 30n^{2} - 36n + 82)$$
$$EM_{2}(\gamma_{3}^{n}) = \frac{1}{2}(n^{4} - 7n^{3} + 30n^{2} - 44n + 62), \quad EM_{2}(\gamma_{4}^{n}) = \frac{1}{2}(n^{4} - 23n^{3} + 210n^{2} - 844n + 1682)$$
$$EM_{2}(\gamma_{5}^{n}) = \frac{1}{2}(n^{4} - 7n^{3} + 30n^{2} - 20n + 176), \quad EM_{2}(\gamma_{6}^{n}) = \frac{1}{2}(n^{4} - 7n^{3} + 30n^{2} - 20n + 176).$$

Thus, by comparing the above expressions, we get

$$EM_2(G) \le \frac{1}{2}(n^4 - 7n^3 + 30n^2 - 20n + 176).$$

Hence we see that G attains the upper bound when G is isomorphic to a graph in γ_5^n or γ_6^n .

Theorem 4.9 Let $G \in \mathbb{X}^n$ be a tricyclic graph of vertex n. Then $EM_2(G) \ge 4n + 116$. Equality holds if and only if $G \in \mathbb{X}_1^n$.

Proof: By repeated application of the operations D, E and F to the tricyclic graph G, we can transform the graph G into one of the 15 tricyclic graphs as shown in Figure 10. From Lemma 3.1, Lemma 3.2, and Lemma 3.3, we have $EM_2(G) \ge EM_2(\alpha_i^n)$, where $\alpha_i^n \in \mathbb{X}_0^n$, for $1 \le i \le 15$. Among the graphs in \mathbb{X}_0^n , we observe that the five collection of graphs in \mathbb{X}_1^n attain the lowest value of EM_2 . By direct computation, we get

$$EM_2(\alpha_i) \ge EM_2(\beta_i^n) = 4n + 116$$

where $\beta_j^n \in \mathbb{X}_1^n \subset \mathbb{X}_0^n$, $j = 1, \dots, 5$.

5. Conclusion

In this paper, we have computed the bounds of the second reformulated Zagreb index, $EM_2(G)$, using six different graph transformations. In this process, we also identify the extremal graphs which attain that bound for trees, unicyclic, bicyclic and tricyclic graphs. Our focus here was to study the graphs with cyclomatic number at most 3. In the future, we would like to extend this study to any graphs particularly planar graphs.



Fig. 10. Representation of tricyclic graphs in \mathbb{X}_0^n which has no pendant vertices.



Fig. 11. Tricyclic graphs in \mathbb{X}_1^n

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