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Zagreb Indices of Trees, Unicyclic and Bicyclic Graphs With Given (Total) Domination

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ABSTRACT Let $G = (V, E)$ be a (molecular) graph. For a family of graphs G, the first Zagreb index M_1 and the second Zagreb index M_2 have already studied. In particular, it has been presented, the first Zagreb index M_1 and the second Zagreb index M_2 of trees T in terms of domination parameter. In this paper, we present upper bounds on Zagreb indices of unicyclic and bicyclic graphs with a given domination number and also find upper bounds on the Zagreb indices of trees, unicyclic, and bicyclic graphs with a given total domination number.

INDEX TERMS Domination, total domination, Zagreb indices, tree, unicyclic, bicyclic graph.

I. INTRODUCTION

Throughout this paper, all graphs are assumed to be simple connected, undirected with $n \geq 1$ vertices and m edges. Let $G = (V, E)$ be a graph with the vertex set $V = V(G)$ and the edge set $E = E(G)$. By the neighborhood of a vertex v of G, we mean the set $N_G(v) = N(v) = \{u \in V \ : uv \in E\}$. The closed neighborhood of vertex v is $N_G[v] = N(v) \cup \{v\}$. For $S \subseteq V$, the neighborhood of S is $N(S) = \bigcup_{v \in S} N(v)$ and the closed neighborhood of S is $N[S] = N(S) \cup S$.

A topological index for a graph is a numerical quantity which is invariant under automorphisms of the graph. The simplest topological indices are the number of vertices and edges of the graph. The first Zagreb index M_1 and the second Zagreb index M_2 of G are defined as:

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

where $d_G(v) = deg(v)$ is the degree of vertex $v \in G$.

Zagreb indices, first is appeared in the topological formula for the total π-electron of conjugated molecules that has been derived in 1972 [10]. These indices have been used as a branching indices. Later the Zagreb indices found applications in Quantitative Structure-Activity Relationships (QSAR) and Quantitative Structure-Property Relationships (QSPR) were studied [7], [13], [16], [17]. This theory is developed well (for example see [9], [13]).

The main properties of M_1 and M_2 were summarized in [3], [5], [13], [19]. In particular, Deng [6] gave a unified approach to determine extremal values of Zagreb indices for trees, unicyclic and bicyclic graphs.

A subset $D \subseteq V(G)$ is a *dominating set* of G if every vertex of $V(G) - D$ has a neighbor in D. The *domination number* of G, denoted by $\gamma(G)$, is the minimum cardinality of a dominating set of G.

A subset $D \subseteq V(G)$ is a *total dominating set*, abbreviated TDS, of G if every vertex of G has a neighbor in D. The *total domination number* of G, denoted by $\gamma_t(G)$ and introduced by Cockayne *et al.* [4].

Domination in graphs has been an extensively researched branch of graph theory [14]. Graph theory is one of the most flourishing branches of modern mathematics and computer applications. The last 30 years have witnessed spectacular growth of graph theory due to its wide applications to discrete optimization, combinatorial and classical algebraic problems [15]. It has a very wide range of applications to many fields like engineering, physical, social and biological sciences; linguistics etc. The theory of domination has been the nucleus of research activity in graph theory in recent n-times. This is largely due to a variety of new parameters that can be developed from the basic definition of domination [11]. The graph G is said to be unicyclic (bicyclic) graph

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respectively if it has only one cycle (exactly two cycles) and denoted by U_n (B_n).

The interested readers can see sharp upper bounds for first and second Zagreb indices of bicyclic graphs with a given perfect matching [8], [12] and with a given clique number in [18]. The relation between various topological indices and domination number of a graph G is in the focus of interest of the researchers for quite many years and this topic is vital nowadays as well [1], [7]. This paper is continuation of these investigations. We discuss on upper bounds of Zagreb indices of unicyclic and bicyclic graphs with a given domination number, we also determine the unique tree whose first and second Zagreb indices attains maximum among the trees with a given domination number. As a consequence, we obtain the upper bound on Zagreb indices of trees, unicycles and bicycles with a given total domination number.

II. ZAGREB INDICES OF UNICYLIC AND BICYCLIC GRAPHS WITH A GIVEN DOMINATION

Before continuing our discussion of techniques and formulas for calculating the upper bound of first and second Zagreb indices of unicyclic and bicyclic graphs with given domination number recall some definitions and properties that we need for proof of theorem. In [2], authors introduced some notations and calculated on extremal Zagreb indices of trees with given domination number as follow:

Let $T_{n,\gamma}$ be the tree obtained from the star $K_{1,n-\gamma}$ by attaching a pendant edge to its $\gamma - 1$ pendent vertices. If $\Delta = n - \gamma$ in a tree T of order n and domination number γ, then $T \cong T_{n,\gamma}$, i.e. T be a $T_{n,\gamma}$ fo given n and γ. The first and second Zagreb indices of a tree $T_{n,\gamma}$ can easily be calculated as

$$M_1(T_{n,\gamma}) = (n-\gamma)(n-\gamma+1) + 4(\gamma-1), \tag{1}$$

and

$$M_2(T_{n,\gamma}) = 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1) \tag{2}$$

Theorem 1 ([2], Theorem 2.1): Let T be a tree with domination number γ. Then

$$M_1(T) \le (n-\gamma)(n-\gamma+1) + 4(\gamma-1).$$

The equality holds if and only if $T \cong T_{n,\gamma}$.

Theorem 2 ([2], Theorem 2.2): Let T be a tree with domination number γ. Then

$$M_2(T) \le 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1).$$

The equality holds if and only if $T \cong T_{n,\gamma}$.

The following lemma has straightforward proof and we leave it.

Lemma 1: Let G be a graph and D be a minimum dominating set with $|D| = \gamma(G)$. If e is an edge of G, then $\gamma(G-e) \in \{\gamma(G), \gamma(G)+1\}$.

Proof: Let D be a $\gamma(G)$-set and $e = \{u, v\}$ be any edge of G. It is clear that $\gamma(G-e) \ge \gamma(G)$. If $\{u, v\} \cap D = \{u, v\}$ or $\{u, v\} \cap D = \emptyset$, then D is a dominating set of $G-e$. If $u \in D$ and $v \notin D$ ($u \notin D$ and $v \in D$), then $D \cup \{v\}$ ($D \cup \{u\}$) is dominating set of $G-e$. Therefore $\gamma(G-e) \in \{|D|, |D|+1\} = \{\gamma(G), \gamma(G)+1\}$. □

Now we obtain upper bound for Zagreb indices of unicyclic and bicyclic graphs with given domination number and maximum degree of graph G (denoted by Δ).

Theorem 3: Let U_n be an unicyclic graph with n vertices and domination number γ. Then

$$M_1(U_n) \le (n-\gamma)(n-\gamma+1) + 4(\gamma+\Delta) - 6.$$

The bound is sharp.

Proof: Let C be the cycle in U_n. We consider an arbitrary edge $e = uv$ from C and put $T = U_n - e$. Then using Lemma 1, we have

$$\begin{aligned} M_1(U_n) &= M_1(T) + (d(u))^2 - (d(u)-1)^2 \\ &\quad + (d(v))^2 - (d(v)-1)^2 \\ &= M_1(T) + 2(d(u)+d(v)-1) \\ &\le (n-\gamma(T))(n-\gamma(T)+1) + 4(\gamma(T)-1) \\ &\quad + 2(2\Delta-1) \\ &\le (n-\gamma(T))(n-\gamma(T)+1) + 4(\gamma(T)+\Delta) - 6. \end{aligned}$$

Now there exist two cases.

If $\gamma(T) = \gamma(U_n) = \gamma$, then it is obviously $M_1(U_n) \le (n-\gamma)(n-\gamma+1) + 4(\gamma+\Delta) - 6$.

If $\gamma(T) = \gamma(U_n) + 1$, and we replace $\gamma(T)$ with $\gamma(U_n) + 1 = \gamma + 1$ in above equation, then we will have $M_1(U_n) \le (n-\gamma-1)(n-\gamma-1+1) + 4(\gamma+1-1) + 2(2\Delta-1) = (n-\gamma)(n-\gamma+1) - 2(n-\gamma) + 4\gamma + 2(2\Delta-1)$.

Since U_n has at least three vertices, then $n-\gamma \ge 2$ and $-2(n-\gamma) \le -4$. Therefore $M_1(U_n) \le (n-\gamma)(n-\gamma+1) + 4(\gamma+\Delta) - 6$.

For sharpness, if U_n is a cycle C_3, corona of cycle C_3, or the cycle C_4, then it is obvious the equality holds. □

By similar discussion and using the same notation as in the proof of Theorem 3, we can calculate upper bound for second Zagreb index for unicyclic graphs.

Theorem 4: Let U_n be an unicyclic graph with n vertices and domination number γ. Then

$$\begin{aligned} M_2(U_n) &\le 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1) \\ &\quad + 3\Delta^2 - 2\Delta. \end{aligned}$$

The bound is sharp.

Proof: Let C be the cycle in U_n. We consider an arbitrary edge $e = uv$ from C and put $T = U_n - e$. Then using Lemma 1, we have

$$\begin{aligned} M_2(U_n) &= M_2(T) + d(u)d(v) + \sum_{z\in N(u), z\neq v} d(z) \\ &\quad + \sum_{z\in N(v), z\neq u} d(z) \\ &\le 2(n-\gamma(T)+1)(\gamma(T)-1) \\ &\quad + (n-\gamma(T))(n-2\gamma(T)+1) \\ &\quad + \Delta^2 + 2\Delta(\Delta-1). \end{aligned}$$

Now there exist two cases.

If $\gamma(T) = \gamma(U_n) = \gamma$, then it is obviously $M_2(U_n) \leq 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1) + 3\Delta^2 - 2\Delta$.

If $\gamma(T) = \gamma(U_n) + 1 = \gamma + 1$, we replace $\gamma(T)$ with $\gamma(U_n)+1 = \gamma+1$ in above equation we will have $M_2(U_n) \leq 2(n-\gamma-1+1)(\gamma+1-1) + (n-\gamma-1)(n-2\gamma-2+1) + 3\Delta^2 - 2\Delta = 2(n-\gamma+1)(\gamma-1) + (n-\gamma-1)(n-2\gamma+1) + 3\Delta^2 - 2\Delta + (2n-4\gamma+2) - 2(n-\gamma) - (n-2\gamma-1) = 2(n-\gamma+1)(\gamma-1)+(n-\gamma)(n-2\gamma+1)+3\Delta^2-2\Delta+3-n \leq 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1) + 3\Delta^2 - 2\Delta$.

For sharpness, if U_n is a cycle C_3, or the cycle C_4, then it is obvious the equality holds. □

As we have already seen, there are sharp bounds for above results. But we may pose the problem.

Problem: Do there exist any necessary and sufficient conditions such that the equalities in Theorems 3 and 4 hold?

Now we focus on bicyclic graphs B_n and investigate the first and second Zagreb indices of B_n. First we study the first Zagreb index.

Theorem 5: Let B_n be a bicyclic graph with n vertices and domination number γ. Then

$$M_1(B_n) \leq (n-\gamma)(n-\gamma+1) + 4(\gamma+2\Delta) - 8.$$

Proof: Let C_r and C_s be two cycles of B_n. Suppose that D is a dominating set of B_n with $|D| = \gamma$. Let $e = uv$ and $e' = xy$ be two edges of B_n, $T = (B_n - e) - e'$ be a tree, such that e and e' are edges of C_r and C_s, respectively. Then $\gamma(T) \in \{\gamma, \gamma+1, \gamma+2\}$ by 1 and therefor:

$$\begin{aligned} M_1(B_n) &\leq M_1(T) + 4(\Delta^2 - (\Delta-1)^2) \\ &\leq (n-\gamma(T))(n-\gamma(T)+1) \\ &\quad + 4(\gamma(T)-1) + 4(2\Delta-1) \\ &= (n-\gamma(T))(n-\gamma(T)+1) \\ &\quad + 4(\gamma(T)+2\Delta) - 8. \end{aligned}$$

Now there are three cases:

If $\gamma(T) = \gamma$, then it is easy to see that $M_1(B_n) \leq (n-\gamma)(n-\gamma+1) + 4(\gamma+2\Delta) - 8$.

If $\gamma(T) = \gamma+1$, then $M_1(B_n) \leq (n-\gamma-1)(n-\gamma-1+1) + 4(\gamma+1+2\Delta) - 8 = (n-\gamma)(n-\gamma+1) + 4(\gamma+2\Delta) - 8 - 2(n-\gamma) + 4$. Since $n-\gamma \geq 2$ hence $M_1(B_n) \leq (n-\gamma)(n-\gamma+1) + 4(\gamma+2\Delta) - 8$.

If $\gamma(T) = \gamma+2$, then $M_1(B_n) \leq (n-\gamma-2)(n-\gamma-2+1)+4(\gamma+2+2\Delta)-8 = (n-\gamma)(n-\gamma+1)+4(\gamma+2\Delta)-8-(n-\gamma-2)-3(n-\gamma)+8$. Since $-(n-\gamma-2)-3(n-\gamma)+8 = -4(n-\gamma)+10$ and for $n \geq 4$ it can be $n-\gamma \geq 3$ hence $M_1(B_n) \leq (n-\gamma)(n-\gamma+1) + 4(\gamma+2\Delta) - 8$. □

Similarly, we can obtain the upper bound and equality condition for second Zagreb index of bicyclic graphs.

Theorem 6: Let B_n be a bicyclic graph with n vertices and domination number γ. Then

$$\begin{aligned} M_2(B_n) \leq\ & 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1) \\ & + 6\Delta^2 - 4\Delta. \end{aligned}$$

Proof: Let $e = uv$ and $e' = xy$ be two edges of bicyclic graph B_n with cycles C and C'. Let $T = (B_n - e) - e'$.

$$\begin{aligned} M_2(B_n) &= M_2(T) + d(u)d(v) + d(x)d(y) \\ &\quad + \sum_{z \in N(u), z \neq u} d(z) + \sum_{z \in N(v), z \neq v} d(z) \\ &\quad + \sum_{z \in N(x), z \neq x} d(z) + \sum_{z \in N(y), z \neq y} d(z) \\ &\leq 2(n-\gamma(T)+1)(\gamma(T)-1) \\ &\quad + (n-\gamma(T))(n-2\gamma(T)+1) \\ &\quad + 6\Delta^2 - 4\Delta. \end{aligned}$$

Like previous results there are three cases.

If $\gamma(T) = \gamma(B_n) = \gamma$, then it is clear.

If $\gamma(T) = \gamma+1$, then $M_2(B_n) \leq 2(n-\gamma-1+1)(\gamma+1-1) + (n-\gamma-1)(n-2\gamma-2+1) + 6\Delta^2 - 4\Delta = 2(n-\gamma+1)(\gamma-1) - 2\gamma + 2(n-\gamma+1) + (n-\gamma)(n-2\gamma+1) - (n-2\gamma-1) - 2(n-\gamma) + 6\Delta^2 - 4\Delta = 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1) + 6\Delta^2 - 4\Delta + 3 - n \leq 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1) + 6\Delta^2 - 4\Delta$.

If $\gamma(T) = \gamma+2$, then $M_2(B_n) \leq 2(n-\gamma-2+1)(\gamma+2-1) + (n-\gamma-2)(n-2\gamma-4+1) + 6\Delta^2 - 4\Delta = 2(n-\gamma-1)(\gamma+1) + (n-\gamma-2)(n-2\gamma-3) + 6\Delta^2 - 4\Delta = 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1) + 4(n-\gamma+1) - 4(\gamma+1) - 4(n-\gamma) - 2(n-2\gamma-3) + 6\Delta^2 - 4\Delta = 2(n-\gamma+1)(\gamma-1)+(n-\gamma)(n-2\gamma+1)+6\Delta^2-4\Delta+6-2n \leq 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1) + 6\Delta^2 - 4\Delta$. □

As we have already seen, we didn't show the sharp bounds for Theorems 5 and 6.

Problem: Are the bounds of Theorems 5 and 6 sharp?

III. ZAGREB INDICES OF TREES, UNICYCLIC AND BICYCLIC GRAPHS WITH GIVEN TOTAL DOMINATION

In this section we compute upper bound for Zagreb indices of trees, unicyclic and bicyclic graphs with given total domination number.

Theorem 7: Let T be a tree with total domination number γ_t. Then

$$M_1(T) \leq (n-\gamma_t+1)(n-\gamma_t+2) + 4(\gamma_t-2)$$

This bound is sharp.

Proof: Let $v_1, v_2, \ldots, v_{d+1}$ be a longest path in T, where d is a diameter of T. Also D be a dominating set of T, where $|D| = \gamma$. Clearly v_1 and v_{d+1} are pendent vertices.

By the definition of total domination number, it is obvious that $\Delta \leq n - \gamma_t + 1$. We prove the theorem by induction on n. If $n = 2$, then $T = K_2$ and inequality holds. Now assume that the theorem holds for a positive integer $n-1$, and prove that the statement remains true when n is replaced by $n+1$. We note that $\gamma_t(T) - 1 \leq \gamma_t(T - v_1) \leq \gamma_t(T)$. By induction hypothesis, we have two cases.

Let $\gamma_t(T - v_1) = \gamma_t(T) = \gamma_t$. Then

$$\begin{aligned} M_1(T) &= M_1(T - v_1) + 2d(v_2) \\ &\leq (n-\gamma_t)(n-\gamma_t+1) + 4(\gamma_t-2) + 2d(v_2) \end{aligned}$$

$$= (n-\gamma_t+1)(n-\gamma_t+2)+4(\gamma_t-2) + 2[d(v_2)-(n-\gamma_t+1)]$$

Since $d(v_2) \leq n-\gamma_t+1$, therefore:

$$M_1(T) \leq (n-\gamma_t+1)(n-\gamma_t+2)+4(\gamma_t-2)$$

Suppose next that $\gamma_t(T-v_1)=\gamma_t(T)-1$. By definition of domination number , it must be $d(v_2)=2$. By the induction, we have:

$$\begin{aligned} M_1(T) &= M_1(T-v_1)+2d(v_2) \\ &\leq (n-\gamma_t)(n-\gamma_t+1)+4(\gamma_t-2)+2d(v_2) \\ &= (n-\gamma_t+1)(n-\gamma_t+2)+4(\gamma_t-2) \\ &\quad +2d(v_2)-4 \\ &= (n-\gamma_t+1)(n-\gamma_t+2)+4(\gamma_t-2) \end{aligned}$$

For sharpness, let T be the star graph $K_{1,n}$. Then $\gamma_t(K_{1,n})=2$ and $M_1(K_{1,n})=n+n^2$. In the other side $(n+1-\gamma_t+1)(n+1-\gamma_t+2)+4(\gamma_t-2)=n(n+1)=M_1(K_{1,n})$ □

Theorem 8: Let T be a tree with total domination number γ_t. Then

$$M_2(T) \leq 2(n-\gamma_t+2)(\gamma_t-2)+(n-\gamma_t+1)(n-2\gamma_t+3).$$

This bound is sharp.

Proof: We prove the theorem by induction on n. It can be easily verified that the statement of the theorem holds for $n \leq 5$. Without loss of generality we assume $n \geq 6$. Let the result holds for a positive integer $n-1$, and show that the statements remains true when n is replaced by $n+1$. Let $P_{d+1}: v_1, v_2, \ldots, v_{d+1}$ be a longest path in T (d is a diameter of T) and let D be a minimum total dominating set of T. Then $|D|=\gamma_t$ and both vertices v_1 and v_{d+1} are pendent.

By the definition of total domination number, it is obvious that $\Delta \leq n-\gamma_t+1$. If v_1 is not in total dominating set clearly $\gamma_t(T-v_1) \leq \gamma_t(T)$. It is well known that every support vertex is in any total dominating set. Thus if v_1 is in a total dominating set, then v_2 is in total dominating set too. Now let $\gamma_t(T-v_1)=\gamma_t(T)$.

$$\begin{aligned} M_2(T) &= M_2(T-v_1)+d(v_2)+\sum_{v_1\neq v\in N(v_2)} d(v) \\ &= M_2(T-v_1)+\sum_{v\in V(T)} d(v)-d(v_2) \\ &\quad -\sum_{uv_2\notin E(T)} d(u)+d(v_2)-1 \\ &\leq 2(n-\gamma_t+1)(\gamma_t-2)+(n-\gamma_t)(n-2\gamma_t+2) \\ &\quad +2(n-1)-d(v_2)-(n-1-d(v_2)) \\ &\quad +d(v_2)-1 \\ &\leq 2(n-\gamma_t+1)(\gamma_t-2) \\ &\quad +(n-\gamma_t)(n-2\gamma_t+2)+n-1+d(v_2)-1 \\ &\leq 2(n-\gamma_t+1)(\gamma_t-2)+(n-\gamma_t)(n-2\gamma_t+2) \\ &\quad +(n-1)+(n-\gamma_t+1)-1 \\ &= 2(n-\gamma_t+2)(\gamma_t-2) \\ &\quad +(n-\gamma_t+1)(n-2\gamma_t+3)+(n-1) \\ &\quad +(n-\gamma_t)-2(\gamma_t-2)-(n-\gamma_t) \\ &\quad -(n-2\gamma_t+2)-1 \\ &\leq 2(n-\gamma_t+2)(\gamma_t-2) \\ &\quad +(n-\gamma_t+1)(n-2\gamma_t+3). \end{aligned}$$

Now next that $\gamma_t(T-v_1)=\gamma_t(T)-1$. By the induction hypothesis, we have:

$$\begin{aligned} M_2(T) &= M_2(T-v_1)+d(v_3)+d(v_2) \\ &\leq 2(n-\gamma_t+2)(\gamma_t-3) \\ &\quad +(n-\gamma_t+1)(n-2\gamma_t+4)+d(v_3)+2 \\ &\leq 2(n-\gamma_t+2)(\gamma_t-2) \\ &\quad +(n-\gamma_t+1)(n-2\gamma_t+3) \\ &\quad -2(n-\gamma_t+2)+(n-\gamma_t+1) \\ &\quad +(n-\gamma_t+1)+2 \\ &= 2(n-\gamma_t+2)(\gamma_t-2) \\ &\quad +(n-\gamma_t+1)(n-2\gamma_t+3). \end{aligned}$$

For sharpness, let T be the star graph $K_{1,n}$. Then $\gamma_t(K_{1,n})=2$ and $M_2(K_{1,n})=n^2$. In the other side $2(n+1-\gamma_t+2)(\gamma_t-2)+(n+1-\gamma_t+1)(n+1-2\gamma_t+3)=n^2$. Therefore the result holds. □

Problem: Do there exist any necessary and sufficient conditions such that the equalities in Theorems 7 and 8 hold?

We also pose the following Lemma which use in proof the two next theorems.

Lemma 2: Let G be a graph and D be a total dominating set with $|D|=\gamma_t$. Then for any edge e in G, if $G-e$ does not have isolated vertex, then $\gamma_t(G-e) \in \{\gamma_t, \gamma_t+1, \gamma_t+2\}$.

Proof: 1) It is well known that $\gamma_t(G-x) \leq \gamma_t$ for any vertex x. Let y be a vertex such that $\gamma_t(G-y) \leq \gamma_t-2$. Now let u be an adjacent vertex of y. Since u is adjacent to a vertex in a $\gamma_t(G-y)$-set, then G is totaly dominated by $\gamma_t(G-x)$-set union with $\{u\}$, a contradiction.

2) It is well known that $\gamma_t(G-e) \geq \gamma_t$. Let $e=uv$ be an edge such that $\gamma_t(G-e) \geq \gamma_t+3$. Then $\gamma_t(G-e)$-set union with $\{u, v\}$ is a total dominating set for G with size $|D|-1$, a contradiction. □

Theorem 9: Let U_n be an unicyclic graph with total domination number γ_t. Then

(i) $M_1(U_n) \leq (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t+4\Delta-10$.

(ii) $M_2(U_n) \leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)+3\Delta^2-6\Delta-4$.

Moreover, these bounds are sharp,

Proof: Let $e=uv$ be an edge of the cycle of U_n so that $T=U_n-e$ be a tree.

(i) Then there exist three cases.

Let $\gamma_t(U_n-e)=\gamma_t(U_n)=\gamma_t$. Then

$$\begin{aligned} M_1(U_n) &= M_1(T)+d^2(u)-(d(u)-1)^2 \\ &\quad +d^2(v)-(d(v)-1)^2 \\ &\leq (n-\gamma_t(T)+1)(n-\gamma_t(T)+2) \\ &\quad +4(\gamma_t(T)-2)+2(d(u)+d(v)-1) \end{aligned}$$

$$
\begin{aligned}
&= (n-\gamma_t+1)(n-\gamma_t+2)+4(\gamma_t-2)\\
&\quad +2(d(u)+d(v)-1)\\
&\leq (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t-8\\
&\quad +2(2\Delta-1)\\
&= (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t+4\Delta-10.
\end{aligned}
$$

Let $\gamma_t(U_n-e)=\gamma_t(U_n)+1=\gamma_t+1$. Then

$$
\begin{aligned}
M_1(U_n) &= M_1(T)+d^2(u)-(d(u)-1)^2\\
&\quad +d^2(v)-(d(v)-1)^2\\
&\leq (n-\gamma_t(T)+1)(n-\gamma_t(T)+2)\\
&\quad +4(\gamma_t(T)-2)+2(d(u)+d(v)-1)\\
&= (n-\gamma_t)(n-\gamma_t+1)+4(\gamma_t-1)\\
&\quad +2(d(u)+d(v)-1)\\
&\leq (n-\gamma_t+1)(n-\gamma_t+2)-2(n-\gamma_t+1)\\
&\quad +4(\gamma_t-1)+2(2\Delta-1)\\
&\leq (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t-4-4\\
&\quad +2(2\Delta-1)(\textit{in this case } n\geq 6)\\
&= (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t+4\Delta-10.
\end{aligned}
$$

Let $\gamma_t(U_n-e)=\gamma_t(U_n)+2=\gamma_t+2$. Then

$$
\begin{aligned}
M_1(U_n) &= M_1(T)+d^2(u)-(d(u)-1)^2\\
&\quad +d^2(v)-(d(v)-1)^2\\
&\leq (n-\gamma_t(T)+1)(n-\gamma_t(T)+2)\\
&\quad +4(\gamma_t(T)-2)+2(d(u)+d(v)-1)\\
&= (n-\gamma_t-1)(n-\gamma_t)+4(\gamma_t)\\
&\quad +2(d(u)+d(v)-1)\\
&\leq (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t\\
&\quad -2(n-\gamma_t+1)\\
&\quad -2(n-\gamma_t)+2(2\Delta-1)\\
&\leq (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t-6-4\\
&\quad +2(2\Delta-1)(\textit{in this case } n\geq 8)\\
&\leq (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t+4\Delta-10.
\end{aligned}
$$

(ii) For $M_2(U_n)$, there exist three cases too.

Let $T=U_n-e$ where $e=uv$ is an edge of the cycle and $\gamma_t(U_n-e)=\gamma_t(U_n)=\gamma_t$.

Then

$$
\begin{aligned}
M_2(U_n) &= M_2(T)+d(u)d(v)+\sum_{z\in N(v),z\neq u} d(z)\\
&\quad +\sum_{z\in N(u),z\neq v} d(z)\\
&\leq 2(n-\gamma_t(T)+2)(\gamma_t(T)-2)\\
&\quad +(n-\gamma_t(T)+1)(n-2\gamma_t(T)+3)\\
&\quad +\Delta^2+2\Delta(\Delta-1)\\
&= 2(n-\gamma_t+2)(\gamma_t-2)\\
&\quad +(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad +\Delta^2+2\Delta(\Delta-1)\\
&= 2\gamma_t(n-\gamma_t+2)-4(n-\gamma_t+2)\\
&\quad +(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad +\Delta^2+2\Delta(\Delta-1)\\
&= 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad -4(n-\gamma_t+1)-4+\Delta^2+2\Delta(\Delta-1)\\
&\leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad -4\Delta-4+\Delta^2+2\Delta(\Delta-1)\\
&= 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad +3\Delta^2-6\Delta-4.
\end{aligned}
$$

Let $\gamma_t(U_n-e)=\gamma_t(U_n)+1=\gamma_t+1$. Then

$$
\begin{aligned}
M_2(U_n) &= M_2(T)+d(u)d(v)+\sum_{x\in N(v),x\neq u} d(x)\\
&\quad +\sum_{y\in N(u),y\neq v} d(y)\\
&= 2(n-\gamma_t(T)+2)(\gamma_t(T)-2)\\
&\quad +(n-\gamma_t(T)+1)(n-2\gamma_t(T)+3)\\
&\quad +\Delta^2+2\Delta(\Delta-1)\\
&= 2(n-\gamma_t+1)(\gamma_t-1)+(n-\gamma_t)(n-2\gamma_t+1)\\
&\quad +\Delta^2+2\Delta(\Delta-1)\\
&\leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad -4(n-\gamma_t+1)-(n+1)+\Delta^2+2\Delta(\Delta-1)\\
&\leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad -4\Delta-(n+1)+\Delta^2+2\Delta(\Delta-1)\\
&\leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad +3\Delta^2-6\Delta-(n+1)\\
&\leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad +3\Delta^2-6\Delta-4.
\end{aligned}
$$

Let $\gamma_t(U_n-e)=\gamma_t(U_n)+2=\gamma_t+2$. Then

$$
\begin{aligned}
M_2(U_n) &= M_2(T)+d(u)d(v)\\
&\quad +\sum_{z\ inN(v),z\neq u} d(z)+\sum_{z\in N(u),z\neq v} d(z)\\
&= 2(n-\gamma_t(T)+2)(\gamma_t(T)-2)\\
&\quad +(n-\gamma_t(T)+1)(n-2\gamma_t(T)+3)\\
&\quad +\Delta^2+2\Delta(\Delta-1)\\
&\leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad -2\gamma_t-2(n-\gamma_t-1)-4(n-\gamma_t-1)\\
&\quad +\Delta^2+2\Delta(\Delta-1)\\
&= 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad -2(n-\gamma_t-1)\\
&\quad -4(n-\gamma_t+1)+\Delta^2+2\Delta(\Delta-1)\\
&\leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad +3\Delta^2-6\Delta-2(n-\gamma_t-1)\\
&\leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\
&\quad +3\Delta^2-6\Delta-4(\textit{since } n-\gamma_t-1\geq 2).
\end{aligned}
$$

For sharpness of these two cases, if U_n is the cycle C_3, then the equalities for both (i) and (ii) hold. □

Theorem 10: Let B_n be a bicyclic graph with total domination number γ_t. Then

(i) $M_1(B_n) \leq (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t+6\Delta-12$, and this bound is sharp.

(ii) $M_2(B_n) \leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)+6\Delta^2-4\Delta$.

Proof: Let $e \in B_n$ be an edge. Then by Lemma 2 $\gamma_t(B_n-e) \in \{\gamma_t(B_n), \gamma_t(B_n)+1, \gamma_t(B_n)+2\}$.

Let $U_n = B_n - e$, where $e = uv$ be an edge of one of the cycles C_r of B_n. Then $M_1(B_n) = M_1(U_n)+2d(u)+2d(v)-2$. Now there exist three cases:

Let $\gamma_t(B_n-e) = \gamma_t(B_n) = \gamma_t$. Then by Theorem 9

$$\begin{aligned}M_1(B_n) &\leq M_1(U_n)+2(2\Delta-1))\\ &\leq (n-\gamma_t(U_n)+1)(n-\gamma_t(U_n)+2)\\ &\quad+4\gamma_t(U_n)+2\Delta-10+2(2\Delta-1)\\ &= (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t+6\Delta-12.\end{aligned}$$

Let $\gamma_t(B_n-e) = \gamma_t(B_n)+1 = \gamma_t+1$. Then by Theorem 9

$$\begin{aligned}M_1(B_n) &\leq M_1(U_n)+2(2\Delta-1))\\ &\leq (n-\gamma_t(U_n)+1)(n-\gamma_t(U_n)+2)\\ &\quad+4\gamma_t(U_n)+2\Delta-10+2(2\Delta-1)\\ &\leq (n-\gamma_t)(n-\gamma_t+1)+4(\gamma_t+1)\\ &\quad+2\Delta-10+2(2\Delta-1)\\ &= (n-\gamma_t+1)(n-\gamma_t+2)-4(n-\gamma_t+1)\\ &\quad+4\gamma_t+4+6\Delta-12\\ &\leq (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t\\ &\quad-2\Delta+4+6\Delta-12\\ &= (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t+6\Delta-12.\end{aligned}$$

Let $\gamma_t(B_n-e) = \gamma_t(B_n)+2 = \gamma_t+2$. Then by Theorem 9

$$\begin{aligned}M_1(B_n) &\leq M_1(U_n)+2(2\Delta-1))\\ &\leq (n-\gamma_t(U_n)+1)(n-\gamma_t(U_n)+2)\\ &\quad+4\gamma_t(U_n)+6\Delta-12\\ &\leq (n-\gamma_t-1)(n-\gamma_t)+4(\gamma_t+2)\\ &\quad+6\Delta-12\\ &= (n-\gamma_t+1)(n-\gamma_t+2)-2(n-\gamma_t-1)\\ &\quad-2(n-\gamma_t)+4\gamma_t+8+6\Delta-12\\ &\leq (n-\gamma_t+1)(n-\gamma_t+2)4\gamma_t\\ &\quad-2\Delta-4+8+6\Delta-12\\ &\leq (n-\gamma_t+1)(n-\gamma_t+2)+4\gamma_t+6\Delta-12.\end{aligned}$$

For sharpness, if B_n is the complete graph K_4 dropping an edge K_4-e, then the equality holds.

(ii) For $M_2(B_n)$, there exist three cases too.

Let $U_n = B_n - e$ where $e = uv$ is an edge of the cycle and $\gamma_t(B_n-e) = \gamma_t(B_n) = \gamma_t$. Then

$$\begin{aligned}M_2(B_n) &= M_2(U_n)+d(u)d(v)+\sum_{z\in N(u),z\neq u} d(z)\\ &\quad+\sum_{z\in N(v),z\neq v} d(z)\\ &\leq 2\gamma_t(U_n)(n-\gamma_t(U_n)+2)\\ &\quad+(n-\gamma_t(U_n)+1)(n-2\gamma_t(U_n)+3)\\ &\quad+3\Delta^2-2\Delta+\Delta^2+2\Delta(\Delta-1)\\ &\leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\ &\quad+6\Delta^2-4\Delta.\end{aligned}$$

Let $\gamma_t(U_n) = \gamma_t(B_n-e) = \gamma_t(B_n)+1 = \gamma_t+1$. Then

$$\begin{aligned}M_2(B_n) &= M_2(U_n)+d(u)d(v)+\sum_{z\in N(u),z\neq u} d(z)\\ &\quad+\sum_{z\in N(v),z\neq v} d(z)\\ &\leq 2\gamma_t(U_n)(n-\gamma_t(U_n)+2)\\ &\quad+(n-\gamma_t(U_n)+1)(n-2\gamma_t(U_n)+3)\\ &\quad+3\Delta^2-2\Delta+\Delta^2+2\Delta(\Delta-1)\\ &\leq 2(\gamma_t+1)(n-\gamma_t+1)+(n-\gamma_t)(n-2\gamma_t+1)\\ &\quad+6\Delta^2-4\Delta\\ &= 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\ &\quad-2\gamma_t-(n-2\gamma_t+1)+6\Delta^2-4\Delta\\ &\leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)\\ &\quad+6\Delta^2-4\Delta.\end{aligned}$$

Let $\gamma_t(U_n) = \gamma_t(B_n-e) = \gamma_t(B_n)+2 = \gamma_t+2$. Then it is easy to see that

$M_2(B_n) \leq 2\gamma_t(n-\gamma_t+2)+(n-\gamma_t+1)(n-2\gamma_t+3)+6\Delta^2-4\Delta$. □

Problem: Is the bounds of Theorem 10 (ii) sharp?

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