International J.Math. Combin. Vol.2(2017), 34-42

The First Zagreb Index, Vertex-Connectivity, Minimum Degree And Independent Number in Graphs

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Abstract: Let G be a simple, undirected and connected graph. Defined by $M_1(G)$ and $RMTI(G)$ the first Zagreb index and the reciprocal Schultz molecular topological index of G, respectively. In this paper, we determined the graphs with maximal M_1 among all graphs having prescribed vertex-connectivity and minimum degree, vertex-connectivity and bipartition, vertex-connectivity and vertex-independent number, respectively. As applications, all maximal elements with respect to $RMTI$ are also determined among the above mentioned graph families, respectively.

Key Words: Zagreb index, reciprocal molecular topological index, vertex connectivity, bipartite graph, independent number.

AMS(2010): 05C12.

§1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex v is the number of edges incident to v and denoted by $d(v)$. One of the most important topological indices is the well-known Zagreb indices introduced in [8, 10], the first and second Zagreb indices M_1 and M_2 of G, respectively, are defined as follows:

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

They reflect the extent of branching of the underlying molecular structure [8, 10, 20]. Their main properties were recently summarized in [1, 4, 6, 7, 9, 11, 12, 13, 15, 16, 23, 24, 25, 26].

Let G be a connected graph with n vertices. The distance matrix $\mathbf{D} = (D_{ij})_{n\times n}$ of G is an $n \times n$ matrix such that D_{ij} is the distance between vertices i and j in G [18]. The reciprocal distance matrix $\mathbf{R}$, also called the Harary matrix (see [14, 18]), is defined as an $n \times n$ matrix $R = (R_{ij})$ such that $R_{ij} = \frac{1}{D_{ij}}$ if $i \neq j$ and 0 otherwise. Let $R_i = \sum_{j=1}^{n} R_{ij}$. Then the

[1]Received October 12, 2016, Accepted May 14, 2017.

reciprocal molecular topological index $RMTI$ [20] of G is defined as

$$RMTI(G) = \sum_{i=1}^{n} R_i^2 + \sum_{i=1}^{n} d_i R_i.$$

Some formulations of reciprocal and constant-interval reciprocal Schultz-type topological indices, included RMTI, have been discussed in [20], and they were illustrated by the QSPR, which studied on physical constants of alkanes and cycloalkanes.

Recently, Zhou and Trinajstić [27] reported some properties of the reciprocal molecular topological index RMTI. They also derived the upper bounds for RMTI in terms of the number of vertices and the number of edges for various classes of graphs under some restricted conditions.

In this paper, we determined, respectively, the graphs with maximal value of M_1 among all graphs having prescribed graph invariants, such as, vertex-connectivity and minimum degree, vertex-connectivity and vertex-independent number. As applications, all maximum elements with respect to $RMTI(G)$ are also determined among the above mentioned graph families, respectively.

§2. Preliminaries

Denoted by $\delta(G)$ the minimum degree of G, and by $Diam(G)$ the diameter of a graph G, i.e., the maximum cardinality among all distance of any one pair of vertices in G. Let K_n be the complete graph with n vertices. Suppose that G_1 and G_2 are graphs with $V(G_1) \cap V(G_2) = \emptyset$. Denoted by $G_1 \cup G_2$ the new graph with vertex set $V(G_1 \cup G_2) = V(G_1) \cup V(G_2)$ and edge set $E(G_1 \cup G_2) = E(G_1) \cup E(G_2)$. The join of G_1 and G_2, denoted by $G_1 \vee G_2$, is the new graph with vertex set $V(G_1 \cup G_2) = V(G_1) \cup V(G_2)$ and edge set $E(G_1 \cup G_2) = E(G_1) \cup E(G_2) \cup \{xy | x \in V(G_1) \textit{ and } y \in V(G_2)\}$.

For $S, S' \subseteq V(G)$, the induced subgraph of S, denoted by $G[S]$, is the graph whose vertex set is S and edge set is composed of those edges with both ends in S. The induced subgraph of S and S', denoted by $G[S, S']$, is the graph whose vertex set is $S_1 \cup S_2$ and edge set is composed of those edges with one end in S and another end in S'.

The bipartite graph is the graph whose vertices can be divided into two disjoint sets U and V, such that every edge connects a vertex in U to one in V. Vertex sets U and V usually called the parts of the graph. A vertex cut of a connected graph G is a set of vertices whose removal renders G disconnected. The vertex-connectivity $\kappa(G)$ is the size of a minimal vertex cut. An independent set of G is a set of vertices in a graph G, no two of which are adjacent. A maximum independent set is an independent set of largest possible size for a given graph G. This size is called the independence number of G, and denoted by $\alpha(G)$.

For other notations and terminology not defined here, see [5].

By the definition of the first Zagreb index, the lemma follows immediately.

Lemma 2.1 *Let G be a simple graph with $u, v \in V(G)$ and $uv \notin E(G)$. Then*

$$M_1(G + uv) > M_1(G).$$

Lemma 2.2([27]) *Let G be a connected simple graph with n vertices and m edges. Then*

$$RMTI(G) \leq \frac{3}{2}M_1(G) + (n-1)m,$$

with equality holds if and if $Diam(G) \leq 2$.

§3. Graphs with Given Connectivity and Minimum Degree

Let n, k and δ be integers such that $n \geq \delta \geq k \geq 1$. Denoted by $\mathcal{G}(n,k,\delta)$ the set of n-vertex connected graphs with vertex-connectivity k and minimum degree δ, where $1 \leq k \leq \delta$ and $2 \leq \delta \leq n$.

Theorem 3.1 *If $G \in \mathcal{G}(n,k,\delta)$ with $k \leq \delta \leq n-1$. Then*

$$M_1(G) \leq n(n-1)^2 + (n-k)(k+\delta-2n+3)(k+\delta+1)$$

with equality holds if and only if $G = K_k \vee (K_{\delta-k+1} \bigcup K_{n-\delta-1})$.

Proof If $n = k+1$, then $k = \delta = n-1$, i.e., $\mathcal{G}(n,k,\delta) = \{K_{k+1}\}$. Suppose that $n \geq k+2$. Let G_{max} be graph in $\mathcal{G}(n,k,\delta)$ with maximal M_1- value in $\mathcal{G}(n,k,\delta)$, that is, $M_1(G) \leq M_1(G_{max})$ for all $G \in \mathcal{G}(n,k,\delta)$. Denoted by $S \subset V(G_{max})$ the vertex cut and $|S| = k$. We will prove the three claims as follows.

Claim 1. $G_{max} - S$ contain exactly two components.

Proof of Claim 1: Suppose by contrary that $G_{max} - S$ contain at least three components. Denoted two components of $G_{max} - S$ by C_1 and C_2. There exist vertices $u \in V(C_1), v \in V(C_2)$ such that $G_{max} + uv \in \mathcal{G}(n,k,\delta)$. By Lemma 2.1, $M_1(G_{max} + uv) > M_1(G_{max})$, which contradicts the choice of G_{max}. This completes the proof of Claim 1.

Therefore, we assume that $G_{max} - S$ contain exactly two connected components, denoted by C_1 and C_2. Denoted by $|V(C_1)| = n_1, |V(C_2)| = n_2$. Since $\delta \leq d(u) \leq n_1 - 1 + k$ and $\delta \leq d(v) \leq n_2 - 1 + k$ for $u \in V(C_1), v \in V(C_2)$, we have $n_1, n_2 \geq \delta - k + 1$.

Claim 2. $G_{max}[S \cup V(C_1)]$ and $G_{max}[S \cup V(C_2)]$ are cliques.

Proof of Claim 2: Without loss of generality, suppose by contrary that $G_{max}[S \bigcup V(C_1)]$ is not a clique. There are two cases as follows:

Case 1. There exists nonadjacent vertices $u, v \in S \bigcup V(C_1)$ such that $G_{max} + uv \in \mathcal{G}(n,k,\delta)$, then by Lemma 2.1, $M_1(G_{max} + uv) > M_1(G_{max})$, which contradicts the choice of G_{max}.

Case 2. Otherwise, adding a new edge to G_{max} will increase the minimum degree of G. From Eqn.(1) in the proof of Claim 3, we have

$$M_1(G_{max}) < M_1(K_s \vee (K_{n_1} \bigcup K_{n_2})) \leq M_1(K_k \vee (K_{\delta-k+1} \bigcup K_{n-\delta-1})),$$

which contradicts the choice of G_{max} since $K_k \vee (K_{\delta-k+1} \bigcup K_{n-\delta-1}) \in \mathcal{G}(n,k,\delta)$.

This complete the proof of Claim 2.

From Claim 2, we suppose that $G_{max} = K_k \vee (K_{n_1} \bigcup K_{n_2})$, where $n_1, n_2 \geq 1$ and $n_1 + n_2 = n - k$.

Claim 3. $n_1 = \delta - k + 1$ or $n_2 = \delta - k + 1$.

Proof of Claim 3: Consider the graph $K_k \vee (K_{n_1} \bigcup K_{n_2})$. Suppose by contrary that $n_1 \geq n_2 > \delta - k + 1$, by direct calculation, we have

$$\begin{aligned} & M_1(K_k \vee (K_{n_1+1} \bigcup K_{n_2-1})) > M_1(K_k \vee (K_{n_1} \bigcup K_{n_2})) \\ & = k(n-1)^2 + n_1(k+n_1-1)^2 + (n-k-n_1)(n-n_1-1)^2, \end{aligned} \tag{1}$$

which implies that $M_1(K_k \vee (K_{\delta-k+1} \bigcup K_{n-\delta-1})) > M_1(K_k \vee (K_{n_1} \bigcup K_{n_2}))$ if $n_1, n_2 > min\{\delta - k+1, n-\delta-1\}$. This complete the proof of Claim 3.

By combine above claims, we have $G_{max} = K_k \vee (K_{\delta-k+1} \bigcup K_{n-\delta-1})$. Then the result holds. □

Corollary 3.1 *Let $G \in \mathcal{G}(n,k,\delta)$ with m edges and $k \leq \delta \leq n-1$. Then*

$$RMTI(G) \leq \frac{3}{2}n(n-1)^2 + \frac{3}{2}n(n-k)(k+\delta-2n+3)(k+\delta+1) + (n-1)m$$

with equality if and only if $k = n-1$ and $G = K_{k+1}$.

§4. Bipartite Graphs with Given Connectivity

Let $\mathcal{B}(n,k)$ be the set of bipartite graphs with n vertices and $\kappa(G) = k$, and $B_{n,x}$ the graph obtained from $K_{x,n-x-1}$ by adding a new vertex v to k vertices of degree x of $K_{x,n-x-1}$.

Theorem 4.1 *Let $G \in \mathcal{B}(n,k)$ with $1 \leq k \leq n-1$. Then*

$$M_1(G) \leq max\{f(a), f(b)\},$$

with equality if and only if $G \in \{B_{n,a}, B_{n,b}\}$, where

$$\begin{aligned} f(x) &= nx(n-x) - x(2n+2k+1) + k(k-1), \\ a &= \left\lfloor \frac{(n-1)^2 - 2(k+1)}{2n} \right\rfloor \quad \text{and} \\ b &= \left\lceil \frac{(n-1)^2 - 2(k+1)}{2n} \right\rceil. \end{aligned}$$

Proof If $k = 1$, then $\mathcal{B}(n,k) = \{K_{1,n-1}\}$. Suppose that $1 < k \leq \frac{n}{2}$, let G_{max} be the graph with the maximal M_1- value in $\mathcal{B}(n,k)$, and S a $k-$vertex cut of G_{max}. Let A, B be vertex parts of $V(G_{max})$ such that $A \cup B = V(G_{max})$. Denoted by $S_A = S \cap A, S_B = S \cap B$. We will prove the four claims as follows.

Claim 1. $G_{max}[S]$ and $G_{max}[C \cup S]$ are complete bipartite graphs, where C is one of components in $G_{max} - S$.

Proof of Claim 1: Suppose by contrary that $G_{max}[S]$ or $G_{max}[C \cup S]$ is not a complete bipartite graph. There exist vertices $u, v \in V(G_{max})$ and $uv \notin E(G_{max})$ such that $G_{max} + uv \in \mathcal{B}(n,k)$. By Lemma 2.1, we have $M_1(G_{max} + uv) > M_1(G_{max})$, which contradicts the choice of G_{max}. This complete the proof of Claim 1.

Claim 2. If $S_A \neq \emptyset$ and $S_B \neq \emptyset$, then $G_{max} - S$ have exactly two components.

Proof of Claim 2: Suppose by contrary that $G_{max} - S$ contain at least three components. Let C_1 and C_2 be two components of $G_{max} - S$. Then there exist vertices $u \in V(C_1) \cap A$, $v \in V(C_2) \cap B$ such that $G_{max} + uv \in \mathcal{B}(n,k)$ and S is also a $k-$vertex cut of $G_{max} + uv$. By Lemma 2.1, $M_1(G_{max} + uv) > M_1(G_{max})$, which contradicts the choice of G_{max}. Thus Claim 2 holds.

Claim 3. $S_A = \emptyset$ or $S_B = \emptyset$.

Proof of Claim 3: Suppose by contrary that $S_A \neq \emptyset$ and $S_B \neq \emptyset$. From Claim 2, $G_{max} - S$ contain exactly two components, denoted by C_1, C_2. Let $u \in V(C_1) \cap A$ and $v \in V(C_2) \cap A$. Without loss of generality, we assume that $a = d(u) \geq d(v) = b > 0$ and $|N_{C_2}(v)| = c > 0$. Taking transformations on G_{max} as follows.

(1) Let $G_1 = G_{max} - \{wv : w \in N_{C_2}(v)\} + \{wu : w \in N_{C_2}(v)\}$. Then

$$M_1(G_1) - M_1(G_{max}) \quad = \quad (b+c)^2 + (a-c)^2 - (b^2 + a^2) = 2c(b - a + c) > 0,$$

(2) Consider the graph G_1. Using the definitions from G_{max}. Let $|S_B| = s$, and choose arbitrary vertices $v_1, v_2, \cdots, v_{k-s} \in B - S$. Let G_2 be the graph obtained from G_1 by adding more edges between $A - \{v\}$ and B as possible, and then adding edges $v_1v, v_2v, \cdots, v_{k-s}v$. It is obviously that $N_{G_2}(v)$ is the vertex cut of G_2 and $|N_{G_2}(v)| = k$, i.e., $G_2 \in \mathcal{B}(n,k)$. From 1) of Claim 3 and Lemma 2.1, we have

$$M_1(G_2) > M_1(G_{max}),$$

which contradicts the choice of G_{max}. Thus Claim 3 holds.

From Claim 3, without loss of generality, let $S \subset A$ be the $k-$vertex cut of G_{max}.

Claim 4. $G_{max} - S$ contains a isolated vertex.

Proof of Claim 4: From Claim 1, suppose by contrary that the components of $G_{max} - S$, denoted by C_1, C_2, are complete bipartite graphs. Let $V(C_1) = A_1 \cup B_1$ and $V(C_2) = A_2 \cup B_2$, where A_i, B_i are vertex parts of C_i, i.e., $A_i \subset A, B_i \subset B$, $i = 1, 2$.

Without loss of generality, suppose that $S \subset A$. Let $u \in B_1$. Let G^* be the graph obtained from G_{max} by deleting the edges connecting u and vertices in A_1, and adding more edges between $A - S$ and $B - \{u\}$ as possible, i.e., $G^* = G_{max} - \{xu : x \in A_1\} + \{xy : x \in A - S, y \in$

$B-\{u\}, xy \notin E(G_{max})\}$. Then S is also a $k-$vertex cut of G_2, and $G_2 \in \mathcal{B}(n,k)$. Similar to Claim 3(1), we have

$$M_1(G^*) - M_1(G_{max}) > 0,$$

which contradicts the choice of G_{max}. Thus $G_{max} = B_{n,x}$.

By calculation, we have

$$f(x) = M_1(B_{n,x}) = nx(n-x) - x(2n+2k+1) + k(k-1)$$

and $x = \frac{(n-1)^2-2(k+1)}{2n}$, and can obtains its maximal value by differentiating $f(x)$ on x. Since $k \le \frac{(n-1)^2-2(k+1)}{2n} \le n-2$, let

$$a = \left\lfloor \frac{(n-1)^2-2(k+1)}{2n} \right\rfloor \text{ and } b = \left\lceil \frac{(n-1)^2-2(k+1)}{2n} \right\rceil.$$

Then by Claim 4, we have $G_{max} \in \{B_{n,a}, B_{n,b}\}$. This completes the proof. □

Corollary 4.1 *Let $G \in \mathcal{B}(n,k)$ with m edges and $1 \le k \le n-1$. Then*

$$RMTI(G) \le \frac{3}{2}T + (n-1)m,$$

where

$$\begin{aligned} T &= max\{f(a), f(b)\}, \quad f(x) = nx(n-x) - x(2n+2k+1) + k(k-1), \\ a &= \left\lfloor \frac{(n-1)^2-2(k+1)}{2n} \right\rfloor \quad \textit{and} \\ b &= \left\lceil \frac{(n-1)^2-2(k+1)}{2n} \right\rceil. \end{aligned}$$

§5. Graphs with Given Connectivity and Independent Number

Let $\mathcal{D}(n,k,r)$ be the set of n-vertex graphs with $\kappa(G) = k$ and $\alpha(G) = r$.

Theorem 5.1 *Let $G \in \mathcal{D}(n,k,r)$ with $r \ge 1$ and $1 \le k \le n-1$. Then*

$$M_1(G) \le (r-1)(n-r)^2 + (n-r)(n-2)^2 + k^2 + k(2n-3),$$

with equalities hold if and only if $G = K_k \vee (K_1 \cup (K_{n-k-r} \vee (r-1)K_1))$.

Proof If $r=2$, then $M_1(G) \le M_1(K_k \vee (K_1 \cup K_{n-k-1}))$ from [11]. We assume that $2 \le r \le n-1$, let G_{max} be the graph with the maximal M_1- value in $\mathcal{D}(n,k,r)$. Denoted by S the $k-$vertex cut of G_{max}, and by D the maximum independent set of G_{max}. We will prove three claims as follows.

Claim 1. $G_{max}[C] = K_a \vee (c-a)K_1$, $G_{max}[S] = K_b \vee (k-b)K_1$ and $G_{max}[S \cup V(C)] = K_{a+b} \cup (k+c-a-b)K_1$, where C is one of components of $G_{max} - S$, $|V(C)| = c, |V(C) - D| = a$ and $|S - D| = b$.

Proof of Claim 1: By Lemma 2.1 and the definition of G_{max}, it clear that $G_{max} = G_{max}[S] \vee G_{max}[V(G) - S]$. Now suppose by contrary that $G_{max}[C] \neq K_a \vee (c-a)K_1$. There exist $u, v \in V(C) - D$ and $w \in V(C) \cap D$, such that $uv \notin E(G_{max})$ or $uw \notin E(G_{max})$. It is clear that $G_{max} + uv, G_{max} + uw \in \mathcal{D}(n,k,r)$. By Lemma 2.1, we have $M_1(G_{max} + uv) > M_1(G_{max})$ or $M_1(G_{max} + uw) > M_1(G_{max})$, which contradicts the choice of G_{max}. Similarly to S, we have $G_{max}[S] = K_b \vee (k-b)K_1$. Thus Claim 1 holds.

Claim 2. $G_{max} - S$ contain exactly two components.

Proof of Claim 2: Suppose by contrary that $G_{max} - S$ contain at least three components. Let C_1 and C_2 be two of components, and $u \in V(C_1) - D, v \in V(C_2) - D$. Then $G_{max} + uv \in \mathcal{D}(n,k,r)$. By Lemma 2.1, $M_1(G_{max} + uv) > M_1(G_{max})$, which contradicts the choice of G_{max}. Thus Claim 2 holds.

By Claim 2, $G_{max} - S = C_1 \cup C_2$, where C_1 and C_2 are components of $G_{max} - S$.

Claim 3. If $V(C_1) \geq V(C_2)$, then $|V(C_2)| = 1$.

Proof of Claim 3: Suppose by contrary that $|V(C_2)| \geq 2$. If $V(C_2) - D = \emptyset$, then $|V(C_2)| = 1$ since C_2 is a connected components. Suppose that $V(C_2) - D \neq \emptyset$, then $V(C_2) \bigcap D \neq \emptyset$. Otherwise, $V(C_2) \bigcap D = \emptyset$, choose $u \in V(C_2)$, and $D \bigcup \{u\}$ is a independent set, which contradicts the definition of D.

Using the definitions from G_{max} and constructing a new graph G^* as follows. Let $v \in V(C_2) \cap D$. Then

$$G^* = G_{max} - \{xv : x \in V(C_2) - D\} + \{xy : x \in V(C_2) - \{v\}, y \in V(C_1)\},$$

it is clear that S and D are also minimal vertex cut and maximal independent set of G^*, respectively. Thus $G^* \in \mathcal{D}(n,k,r)$.

Let $u \in V(G_{max}) - S - \{v\}$ and $w \in V(C_1) - D$. Then $d_{G^*}(u) > d_{G_{max}}(u)$ and

$$M_1(G^*) - M_1(G_{max}) > d_{G^*}(w)^2 + d_{G^*}(v)^2 - d_{G_{max}}(w)^2 - d_{G_{max}}(v)^2 > 0,$$

which contradicts the choice of G_{max}. Thus Claim 3 holds.

By combine above claims, we have

$$G_{max} \in \{G' : G' = (K_{n-r} \vee (r-1)K_1) \cup \{v\} \cup \{u_i v : u_i \in S, i = 1, 2, \cdots, k\},$$

where v is a isolated vertex of $G_{max} - S$. Let $|S \cap D| = a$. Then

$$\begin{aligned} M_1(G') &= a(n-r+1)^2 + (r-a-1)(n-r)^2 + (k-a)(n-1)^3 \\ &\quad + (n-r-k+a)(n-2)^2 + k^2 \\ &= (r-1)(n-r)^2 + (n-r)(n-2)^2 + k^2 + k(2n-3) - a(2r-4), \end{aligned}$$

and the point $a = 0$ attains the maximal value of $M_1(G)$. Therefore, $M_1(G_{max}) = (r-1)(n-r)^2 + (n-r)(n-2)^2 + k^2 + k(2n-3)$ and $G_{max} = K_k \vee (K_1 \cup (K_{n-k-1} \vee (r-1)K_1))$. This complete the proof. □

Corollary 5.1 *Let $G \in \mathcal{D}(n,k,r)$ with m edges, $r \geq 1$ and $1 \leq k \leq n-1$. Then*

$$RMTI(G) \leq \frac{3}{2}\left[(r-1)(n-r)^2 + (n-r)(n-2)^2 + k^2 + k(2n-3)\right] + (n-1)m.$$

Acknowledgement

This work was supported by NSF of Guangdong Province of China (2015A030313574,2014A030-310119, 2014B020004027), the Outstanding Young Teacher Training Program in Guangdong Universities (YQ2015155), the National Social Science Fund in China (15BTJ024) and the Scientific research innovation team Project of Huizhou University (HZUXl201523)

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