A Unified Approach to Extremal Graphs for Different Indices

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Abstract: In this paper, we first introduce a linear program on graphical invariant of graph G. As a application, we attain the extremal graphs with lower bound on the first Zagreb index $M_1(G)$, the second Zagreb index $M_2(G)$, their multiplicative versions $\Pi_1^*(G)$, $\Pi_2(G)$ and atom-bond connectivity $ABC(G)$, respectively.
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1. Introduction

All graphs considered in this paper are finite, undirected and simple. Graph theoretical terms used but not defined can be found in Bollobás [1]. Let $G = (V, E)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The degree of $v \in V(G)$, denoted by $d_G(v)$, is the number of vertices in G adjacent to v. Let δ and Δ be the minimum and maximum degree of G, respectively. Let $\mathscr{G}(n, \delta, \Delta)$ be the class of graphs of order n with minimum degree δ and maximum degree Δ.

A graphical invariant is a function f on the class of all graphs such that $f(G_1) = f(G_2)$ whenever $G_1 \simeq G_2$. Many of these invariants of current interest in mathematical chemistry are defined in terms of vertex degrees of the molecular graph. For example, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined as follows:

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

Recently, M. Eliasi, A. Iranmanesha and I. Gutman [4], Todeschini et al. [14] introduced the multiplicative versions of the Zagreb indices, respectively, called *multiplicative Zagreb indices* by Gutman [9], namely:

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$$\Pi_1^*(G) = \prod_{uv \in E(G)} (d_G(u) + d_G(v)), \quad \Pi_2(G) = \prod_{uv \in E(G)} d_G(u) d_G(v).$$

In [5], Estrada et al. proposed an index, known as the atom-bond connectivity index ($ABC(G)$), is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) d_G(v)}}.$$

One of the major graph-theoretical problems in connection with these indices is the question which graphs from a given class maximize or minimize the index value. The Zagreb indices were well-studied during the past decades, see [2, 3, 10, 11, 13] for instance. For the multiplicative Zagreb indices, Gutman [9] determined that among all trees of order $n \geq 4$, the extremal trees with respect to $\Pi_2(G)$ are path P_n (with minimal $\Pi_2(G)$) and star S_n (with maximal $\Pi_2(G)$). J. Liu and Q. Zhang [12] gave some upper bounds for $\Pi_2(G)$ in terms of graph parameters including the order, size, the first Zagreb index and degree distance. In [4], it was determined that the path has minimal $\Pi_1^*(G)$. In [6], Furtula et al. showed that the star S_n is the unique tree with the maximal $ABC(G)$ index. In this paper, we will consider some lower bounds with respect to the above indices on graphs in $\mathscr{G}(n, \delta, \Delta)$.

For a graph $G \in \mathscr{G}(n, \delta, \Delta)$, let $x_{i,j}$ be the number of edges joining vertices of degrees i and j, n_i be the number of vertices of degree i , and $f(i,j)$ be a function on i, j. It is easy to see that the following relations hold.

$$(I) \begin{cases} 2x_{\delta,\delta} + x_{\delta,\delta+1} + x_{\delta,\delta+2} + \cdots + x_{\delta,\Delta} & = \delta n_\delta \\ x_{\delta,\delta+1} + 2x_{\delta+1,\delta+1} + x_{\delta+1,\delta+2} + \cdots + x_{\delta+1,\Delta} & = (\delta+1) n_{\delta+1} \\ x_{\delta,\delta+2} + x_{\delta+1,\delta+2} + 2x_{\delta+2,\delta+2} + \cdots + x_{\delta+2,\Delta} & = (\delta+2) n_{\delta+2} \\ \qquad \vdots & \\ x_{\delta,\Delta} + x_{\delta+1,\Delta} + x_{\delta+2,\Delta} + \cdots + 2x_{\Delta,\Delta} & = \Delta n_\Delta \\ n_\delta + n_{\delta+1} + n_{\delta+2} + \cdots + n_\Delta & = n \\ x_{i,j} \geq 0, \quad \delta \leq i \leq j \leq \Delta; \qquad n_i \geq 0, \quad \delta \leq i \leq \Delta & \end{cases}$$

From (I), we have

$$n_j = \frac{x_{\delta,j} + x_{\delta+1,j} + \cdots + x_{j-1,j} + 2x_{j,j} + x_{j,j+1} + \cdots + x_{j,\Delta}}{j}$$

for $\delta+1 \le j \le \Delta$. Further, we can obtain

$$n_\delta = n - \sum_{j=\delta+1}^{\Delta} \frac{x_{\delta,j}}{j} - \sum_{\delta+1\le i\le j\le\Delta} \left(\frac{1}{i}+\frac{1}{j}\right) x_{i,j} \tag{1.1}$$

$$x_{\delta,\delta} = \frac{\delta n}{2} - \frac{1}{2}\sum_{j=\delta+1}^{\Delta}\left(1+\frac{\delta}{j}\right)x_{\delta,j} - \frac{1}{2}\sum_{\delta+1\le i\le j\le\Delta}\left(\frac{\delta}{i}+\frac{\delta}{j}\right)x_{i,j} \tag{1.2}$$

For $G \in \mathscr{G}(n,\delta,\Delta)$, let $\psi = \sum_{uv\in E(G)} f(d_G(u), d_G(v))$. In order to find minimum value for ψ function, it suffices to consider the following problem:

$$\begin{aligned} &\min \psi, \\ &subject\ \ to\ \ (I). \end{aligned} \tag{1.3}$$

2. Some applications of (1.3)

Now we consider the generic approach of computing lower bounds of degree based topological indices presented here based on (1.3) in $\mathscr{G}(n,\delta,\Delta)$.

Theorem 2.1. *Let $G \in \mathscr{G}(n,\delta,\Delta)$, then $M_1 \ge \delta^2 n$. The equality is obtained by regular graphs of degree δ.*

Proof. Let $f(i,j) = i+j$, by (1.2) and (1.3), we have

$$M_1 = 2\delta x_{\delta,\delta} + \sum_{j=\delta+1}^{\Delta}(\delta+j)x_{\delta,j} + \sum_{\delta+1\le i\le j\le\Delta}(i+j)x_{i,j}$$

$$= \delta^2 n + \sum_{j=\delta+1}^{\Delta}\left(j-\frac{\delta^2}{j}\right)x_{\delta,j} + \sum_{\delta+1\le i\le j\le\Delta}\left(i+j-\frac{\delta^2}{i}-\frac{\delta^2}{j}\right)x_{i,j}$$

Note that

$$\begin{aligned} j-\frac{\delta^2}{j} &= \frac{j^2-\delta^2}{j} > 0, \\ i+j-\frac{\delta^2}{i}-\frac{\delta^2}{j} &= \frac{i^2-\delta^2}{i} + \frac{j^2\delta^2}{j} > 0. \end{aligned}$$

Then $M_1 \ge \delta^2 n$. The equality holds if we set $x_{ij} = 0$ for all $\delta \le i \le j \le \Delta$ except for $x_{\delta,\delta}$. □

Theorem 2.2. *Let $G \in \mathscr{G}(n,\delta,\Delta)$, then $M_2 \geq \frac{\delta^3 n}{2}$. The equality is obtained by regular graphs of degree δ.*

Proof. Let $f(i,j) = ij$, then

$$\begin{aligned} M_2 &= \sum_{\delta \leq i \leq j \leq \Delta} ij x_{i,j} = \delta^2 x_{\delta,\delta} + \sum_{j=\delta+1}^{\Delta} \delta j x_{\delta,j} + \sum_{\delta+1 \leq i \leq j \leq \Delta} ij x_{i,j} \\ &= \frac{\delta^3 n}{2} + \sum_{j=\delta+1}^{\Delta} \left(\delta j - \frac{\delta^2}{2} - \frac{\delta^3}{2j}\right) x_{\delta,j} + \sum_{\delta+1 \leq i \leq j \leq \Delta} \left(ij - \frac{\delta^3}{2i} - \frac{\delta^3}{2j}\right) x_{i,j} \end{aligned}$$

Note that

$$\begin{aligned} \delta j - \frac{\delta^2}{2} - \frac{\delta^3}{2j} &= \frac{\delta(j-\delta)}{2} + \frac{\delta(j^2-\delta^2)}{2j} > 0, \\ ij - \frac{\delta^3}{2i} - \frac{\delta^3}{2j} &= \frac{i^2 j - \delta^3}{2i} + \frac{ij^2 - \delta^3}{2j} > 0. \end{aligned}$$

So $M_2 \geq \frac{\delta^3 n}{2}$ and the equality holds if we set $x_{ij} = 0$ for all $\delta \leq i \leq j \leq \Delta$ except for $x_{\delta,\delta}$. □

Theorem 2.3. *Let $G \in \mathscr{G}(n,\delta,\Delta)$, then $\prod_1^*(G) \geq e^{\frac{n\delta \ln(2\delta)}{2}}$. The equality is obtained by regular graphs of degree δ.*

Proof. Let $B = \ln \Pi_1^*(G) = \sum_{\delta \leq i \leq j \leq \Delta} \ln(i+j) x_{i,j}$ and $f(i,j) = \ln(i+j)$, then we have

$$B = \ln(2\delta) x_{\delta,\delta} + \sum_{j=\delta+1}^{\Delta} \ln(\delta+j) x_{\delta,j} + \sum_{\delta+1 \leq i \leq j \leq \Delta} \ln(i+j) x_{i,j}$$

$$\sum_{\delta+1 \leq i \leq j \leq \Delta} \ln(i+j) x_{i,j}$$

$$\begin{aligned} = {} & \frac{n\delta \ln(2\delta)}{2} + \sum_{j=\delta+1}^{\Delta} \left[\ln(\delta+j) - \frac{\ln(2\delta)}{2} - \frac{\delta \ln(2\delta)}{2j}\right] x_{\delta,j} + \\ & \sum_{\delta+1 \leq i \leq j \leq \Delta} \left[\ln(i+j) - \frac{\delta \ln(2\delta)}{2i} - \frac{\delta \ln(2\delta)}{2j}\right] x_{i,j} \end{aligned}$$

Note that $\ln(\delta+j) - \frac{\ln(2\delta)}{2} - \frac{\delta \ln(2\delta)}{2j} = \frac{\ln(\delta+j) - \ln(2\delta)}{2} + \frac{j \ln(\delta+j) - \delta \ln(2\delta)}{2j} > 0$, and $\ln(i+j) - \frac{\delta \ln(2\delta)}{2i} - \frac{\delta \ln(2\delta)}{2j} = \frac{i \ln(i+j) - \delta \ln(2\delta)}{2i} + \frac{j \ln(i+j) - \delta \ln(2\delta)}{2j} > 0$. So $B \geq \frac{n\delta \ln(2\delta)}{2}$, then $\prod_1^*(G) \geq e^{\frac{n\delta \ln(2\delta)}{2}}$. The equality holds if we set $x_{ij} = 0$ for all $\delta \leq i \leq j \leq \Delta$ except for $x_{\delta,\delta}$. □

Theorem 2.4. *Let $G \in \mathscr{G}(n,\delta,\Delta)$, then $\prod_2 \geq e^{n\delta\ln\delta}$. The equality is obtained by regular graphs of degree δ.*

Proof. Let $A = \ln\prod_2 = \sum_{uv\in E(G)} \ln(d_G(u)d_G(v))$ and $f(i,j) = \ln i + \ln j$, then

$$\begin{aligned} A &= (\ln\delta + \ln\delta)x_{\delta,\delta} + \sum_{j=\delta+1}^{\Delta} (\ln\delta + \ln j)x_{\delta,j} + \sum_{\delta+1\leq i\leq j\leq\Delta} (\ln i + \ln j)x_{i,j} \\ &= n\delta\ln\delta + \sum_{j=\delta+1}^{\Delta}\left(\ln j - \frac{\delta\ln\delta}{j}\right)x_{\delta,j} + \\ &\quad \sum_{\delta+1\leq i\leq j\leq\Delta}\left(\ln i + \ln j - \frac{\delta\ln\delta}{i} - \frac{\delta\ln\delta}{j}\right)x_{i,j}. \end{aligned}$$

Note that

$$\begin{aligned} \ln j - \frac{\delta\ln\delta}{j} &= \frac{j\ln j - \delta\ln\delta}{j} > 0, \\ \ln i + \ln j - \frac{\delta\ln\delta}{i} - \frac{\delta\ln\delta}{j} &= \frac{i\ln i - \delta\ln\delta}{i} + \frac{j\ln j - \delta\ln\delta}{j} > 0. \end{aligned}$$

So $A \geq n\delta\ln\delta$ and $\prod_2 \geq e^{n\delta\ln\delta}$. The equality holds if we set $x_{ij} = 0$ for all $\delta \leq i \leq j \leq \Delta$ except for $x_{\delta,\delta}$. □

Theorem 2.5. *Let $G \in \mathscr{G}(n,\delta,\Delta)$, if $(2\delta-2)(2\Delta-2) > \Delta^2$, then $ABC(G) \geq \frac{\sqrt{2\delta-2}}{2}n$. The equality is obtained by regular graphs of degree δ.*

Proof. Let $f(i,j) = \sqrt{\frac{i+j-2}{ij}}$, then $ABC(G)$

$$\begin{aligned} &= \sqrt{\frac{2\delta-2}{\delta^2}}x_{\delta,\delta} + \sum_{j=\delta+1}^{\Delta}\sqrt{\frac{\delta+j-2}{\delta j}}x_{\delta,j} + \sum_{\delta+1\leq i\leq j\leq\Delta}\sqrt{\frac{i+j-2}{ij}}x_{i,j} \\ &= \frac{\sqrt{2\delta-2}}{2}n + \sum_{j=\delta+1}^{\Delta}\left[\sqrt{\frac{\delta+j-2}{\delta j}} - \frac{\sqrt{2\delta-2}}{2\delta} - \frac{\sqrt{2\delta-2}}{2j}\right]x_{\delta,j} + \\ &\quad \sum_{\delta+1\leq i\leq j\leq\Delta}\left[\sqrt{\frac{i+j-2}{ij}} - \frac{\sqrt{2\delta-2}}{2i} - \frac{\sqrt{2\delta-2}}{2j}\right]x_{i,j} \end{aligned}$$

Let $v(i,j) = \sqrt{\frac{i+j-2}{ij}} - \frac{\sqrt{2\delta-2}}{2i} - \frac{\sqrt{2\delta-2}}{2j}$, then $v(\delta,j) = \sqrt{\frac{\delta+j-2}{\delta j}} - \frac{\sqrt{2\delta-2}}{2\delta} -$

$\frac{\sqrt{2\delta-2}}{2j}$. Note that

$$\begin{aligned}\frac{\partial v(i,j)}{\partial i} &= \frac{1}{2i^2}\left(\sqrt{2\delta-2}+\frac{2\sqrt{i}}{\sqrt{j(i+j-2)}}-\frac{\sqrt{ij}}{\sqrt{i+j-2}}\right)\\ &> \frac{1}{2i^2}\left(\sqrt{2\delta-2}-\frac{\sqrt{ij}}{\sqrt{i+j-2}}\right)\end{aligned}$$

Let $g(i,j)=\sqrt{2\delta-2}-\frac{\sqrt{ij}}{\sqrt{i+j-2}}$, we have

$$\begin{aligned}\frac{\partial g(i,j)}{\partial i} &= -\frac{j(j-2)}{2(i+j-2)\sqrt{ij(i+j-2)}}<0\\ \frac{dg(\Delta,j)}{dj} &= -\frac{\Delta(\Delta-2)}{2(\Delta+j-2)\sqrt{\Delta j(\Delta+j-2)}}<0\end{aligned}$$

Then $g(i,j)>g(\Delta,j)>g(\Delta,\Delta)=\sqrt{2\delta-2}-\frac{\Delta}{\sqrt{2\Delta-2}}=\frac{\sqrt{(2\delta-2)(2\Delta-2)}-\Delta}{2\Delta-2}>0$ since $(2\delta-2)(2\Delta-2)>\Delta^2$. Hence $\frac{\partial v(i,j)}{\partial i}>0$. Then $v(i,j)>v(\delta,j)$. Note that $\frac{\partial v(\delta,j)}{\partial j}=\frac{1}{2j^2}\left(\sqrt{2\delta-2}+\frac{2-\delta}{\delta}\sqrt{\frac{\delta j}{\delta+j-2}}\right)$. Let $b(j)=\sqrt{2\delta-2}+\frac{2-\delta}{\delta}\sqrt{\frac{\delta j}{\delta+j-2}}$, then $\frac{db(j)}{dj}=-\frac{1}{2}\sqrt{\frac{\delta+j-2}{\delta j}}\cdot\frac{\delta(\delta-2)}{(\delta+j-2)^2}\leq 0$. So

$$\begin{aligned}b(j)\geq b(\Delta) &= \sqrt{2\delta-2}+\frac{2-\delta}{\delta}\sqrt{\frac{\delta\Delta}{\delta+\Delta-2}}>\sqrt{2\delta-2}-\sqrt{\frac{\delta\Delta}{\delta+\Delta-2}}\\ &\geq \frac{2(\delta-\frac{3}{2})^2-\frac{1}{2}}{\sqrt{\delta+\Delta-2}(\sqrt{(2\delta-2)(\delta+\Delta-2)}+\sqrt{\delta\Delta})}\geq 0.\end{aligned}$$

Then $\frac{\partial v(\delta,j)}{\partial j}>0$. Hence $v(i,j)>v(\delta,j)>v(\delta,\delta)=0$ and $ABC(G)\geq\frac{\sqrt{2\delta-2}}{2}n$. The equality holds if we set $x_{ij}=0$ for all $\delta\leq i\leq j\leq\Delta$ except for $x_{\delta,\delta}$. □

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