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Some Inequalities Between Degree– and Distance–Based Topological Indices of Graphs

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Abstract

The aim of this paper is to present some inequalities between degree distance and Gutman index with the Zagreb and reformulated Zagreb indices of graphs.

1 Introduction

Throughout this paper G is a finite, undirected and simple connected graphs with the vertex set $V(G)$ and edge set $E(G)$. The number of vertices and edges of G are called the order and size of G, respectively. Choose vertices u and v in $V(G)$. The degree of v, $deg_G(v)$, is the number of edges incident to v and $N[v, G]$ denotes the set of all vertices adjacent to v. The distance between u and v, denoted by $d_G(u, v)$ ($d(u, v)$ for short), is defined as the number of edges in a shortest path connecting them. We also use notations P_n for a path of order n, C_n for a cycle of size n and S_n to denote the star on n vertices.

Suppose $\mathcal{G}$ denotes the set of all non-isomorphic graphs and as usual $\mathbb{R}$ is the set of all real numbers. A **numerical graph invariant** is a function $\alpha : \mathcal{G} \longrightarrow \mathbb{R}$ such that $G \cong H$ implies that $\alpha(G) = \alpha(H)$. If α correlates a chemico-physical property of a class of molecules, then we use the word **topological index** for α. A topological index

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can be defined by degree of vertices is called a **degree-based topological index** and a topological index based on graph distances is said to be a **distance-based topological index**. It is well-known that distance-based topological indices can be used for characterizing molecular graphs, establishing relationships between structure and chemico-physical properties of molecules.

The degree distance of a graph is a degree analog of the well-known Wiener index. To define, we assume that G is a connected graph, $u \in V(G)$ and $D_G(u) = \sum_{v \in V(G)} d(u,v)$. Then this invariant can be defined as

$$D'(G) = \sum_{x \in V(G)} deg_G(x) D_G(x) = \frac{1}{2} \sum_{x,y \in V(G)} d(x,y)[deg(x) + deg(y)].$$

The degree distance invariant of graphs was first introduced by Dobrynin and Kochetova [4] and then by Gutman [10], who used a different name for this topological index and conjectured that the minimum degree distance of $n-$vertex graphs, $n \geq 2$, is $3n^2 - 7n + 4$ and the unique extremal graph is S_n. This conjecture was proved by Tomescu [20]. Tomescu also characterized connected unicyclic and bicyclic graphs in terms of the degree sequence and obtained minimal graphs in these classes with respect to the degree distance [22]. Ilić et al. [14] characterized $n-$vertex unicyclic graphs with girth k, having minimum and maximum degree distance, respectively. They also proved that the graph obtained from two triangles linked by a path, is the unique graph having the maximum degree distance among bicyclic graphs. Bucicovschi and Cioaba [2] determined the minimum degree distance of a connected graph of order n and size e. We refer the interested readers to consult papers [5, 6, 21] for more information on this topological index.

Gutman [10], introduced a topological index named the **modified Schultz index**. This invariant is now known as the Gutman index. The Gutman index of a graph G is defined as $Gut(G) = \sum_{\{u,v\} \subseteq V(G)} deg_G(u) deg_G(v) d_G(u,v)$. Chen and Liu [3] obtained bicyclic graphs with the smallest Gutman index and characterized the corresponding extremal graphs. Feng and Liu [9] proved that the graph formed from two triangles linked by a path has maximal Gutman index among all bicyclic graphs. Mazorodze et al. [18] obtained an asymptotically sharp upper bound for the Gutman index in terms of the minimum degree of the graph under consideration. Dankelmann et al. [7] gave an upper bound for Gutman index and Mukwembi [17] improved this bound.

The first and second Zagreb indices of a graph G [12] are denoted by $M_1(G)$ and

$M_2(G)$, respectively. These invariants can be defined as

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

A survey of properties of M_1 and M_2 are given in [11,19]. Khalifeh et al. [15] obtained this invariants under some graph operations and Habibi et al. [13], the first three maximum values of M_1 and the first two maximum values of M_2 on the class of $n-$vertex tetracyclic graphs with $n \geq 6$ vertices are computed. Borovičanin [1] et al., provided a survey of the most significant estimates about bounds for Zagreb indices, attempting to cover the existing literature up to the end of year 2016.

Miličević et al. [16], was introduced the first and second reformulated Zagreb indices as the edge counterpart of the first and second Zagreb indices, respectively. These are defined as $EM_1(G) = \sum_{e \in E(G)} deg_G(e)^2$ and $EM_2(G) = \sum_{e \sim f} deg_G(e)deg_G(f)$, where for $e = uv$, $deg_G(e) = deg_G(u) + deg_G(v) - 2$ denotes the degree of the edge e, and $e \sim f$ means that the edges e and f are incident. In addition Zhang and Zhang [23] introduced the general Zagreb index of G as $M_1^{(\alpha)}(G) = \sum_{u \in V(G)} deg_G(u)^\alpha$, where α is an arbitrary real number except from 0 and 1. Obviously $M_1^{(2)}(G) = M_1(G)$ and for $\alpha = 3$ one can obtain the forgotten index $F(G)$ [8].

The girth of a graph G, $g(G)$, is defined as the length of a shortest cycle contained in the graph G. If the graph G does not contain any cycles then its girth is defined to be infinite. The aim of this paper is to obtain some inequalities, relating degree distance and the first and second Zagreb indices of graphs.

2 Main Results

The diameter of a simple connected graph G, $diam(G)$, is the maximum distance between vertex pairs of G and for $x \in V(G)$, $d(G, x, k)$ denotes the number of vertices of G, say v, such that $d_G(x, v) = k$. Note that $d(G, x, k) = 0$, when $k > diam(G)$. In addition, it is clear that the, $d(G, x, 1) = deg_G(x)$. It is easy to see that $\sum_{k \geq 1} d(G, x, k) = |V(G) - 1|$. On the other hand, the degree distance of G can be expressed as $D'(G) = \sum_{x \in V(G)} d(x) \sum_{k \geq 1} kd(G, x, k)$.

Theorem 2.1 *Let G be a graph with n vertices, m edges and $g(G) > 4$. Then $D'(G) \geq 6nm - 6m - M_1(G) - 2M_2(G)$ with equality if and only if $diam(G) \leq 3$.*

Proof. By definition, we have

$$\begin{aligned} D'(G) &= \sum_{x\in V(G)} deg_G(x)\sum_{k\geq 1} kd(G,x,k) \\ &= \sum_{x\in V(G)} deg_G(x)\left[d(G,x,1)+2d(G,x,2)+\sum_{k\geq 3} kd(G,x,k)\right]. \end{aligned}$$

On the other hand, by this equality and our notations,

$$\begin{aligned} D'(G) &= \sum_{x\in V(G)} deg_G(x)\left[deg_G(x)+2\sum_{xu\in E(G)}(deg_G(u)-1)+\sum_{k\geq 3} kd(G,x,k)\right] \\ &\geq \sum_{x\in V(G)} deg_G(x)\left[deg_G(x)+2\sum_{xu\in E(G)}(deg_G(u)-1)+3\sum_{k\geq 3} d(G,x,k)\right] \\ &= \sum_{x\in V(G)} deg_G(x)\left[deg_G(x)+2\sum_{xu\in E(G)}(deg_G(u)-1)\right. \\ &+ \left. 3\left(n-1-deg_G(x)-\sum_{xu\in E(G)}(deg_G(u)-1)\right)\right] \\ &= \sum_{x\in V(G)} deg_G(x)\left[3n-3-2deg_G(x)-\sum_{xu\in E(G)}(deg_G(u)-1)\right] \\ &= \sum_{x\in V(G)} deg_G(x)\left[3n-3-2deg_G(x)+deg_G(x)-\sum_{xu\in E(G)} deg_G(u)\right] \\ &= 6nm-6m-M_1(G)-\sum_{x\in V(G)} deg_G(x)\sum_{xu\in E(G)} deg_G(u) \\ &= 6nm-6m-M_1(G)-2\sum_{xu\in E(G)} deg_G(x)deg_G(u) \\ &= 6nm-6m-M_1(G)-2M_2(G). \end{aligned}$$

It is clear that the equality holds if and only if $diam(G)\leq 3$. ■

As an example for the equality in Theorem 2.1 is a cycle of length five. Suppose $diam(G)\geq 3$ and define $\alpha=\max\{deg_G(v),deg_G(u)\mid d_G(u,v)=3\}$.

Theorem 2.2 *Let G be a graph with n vertices, m edges and $g(G)>6$. Then*

$$D'(G) \;\geq\; 8nm-2m(4+\alpha)+M_1(G)(2\alpha-1)-M_2(G)(2\alpha+4).$$

The equality holds if and only if $diam(G)\leq 4$ and

$$\{deg_G(v),deg_G(u)\mid d_G(u,v)=3\}=\{\alpha\}.$$

Proof. By definition and similar to the proof of Theorem 2.1,

$$\begin{aligned} D'(G) &= \sum_{x\in V(G)} deg_G(x)\sum_{k\geq 1} kd(G,x,k) \\ &= \sum_{x\in V(G)} deg_G(x)\left[d(G,x,1)+2d(G,x,2)+3d(G,x,3)+\sum_{k\geq 4} kd(G,x,k)\right]. \end{aligned}$$

On the other hand, by last equality and our notations,

$$\begin{aligned} &= \sum_{x\in V(G)} deg_G(x)\left[deg_G(x)+2\sum_{xu\in E(G)}(deg_G(u)-1)+3d(G,x,3)+\sum_{k\geq 4} kd(G,x,k)\right] \\ &\geq \sum_{x\in V(G)} deg_G(x)\left[deg_G(x)+2\sum_{xu\in E(G)}(deg_G(u)-1)+3d(G,x,3)+4\sum_{k\geq 4} d(G,x,k)\right] \\ &= \sum_{x\in V(G)} deg_G(x)\left[deg_G(x)+2\sum_{xu\in E(G)}(deg_G(u)-1)+3d(G,x,3)\right. \\ &+ \left. 4(n-1-deg_G(x)-\sum_{xu\in E(G)}(deg_G(u)-1)-d(G,x,3))\right] \\ &= \sum_{x\in V(G)} deg_G(x)\left[4n-4-3deg_G(x)-2\sum_{xu\in E(G)}(deg_G(u)-1)-d(G,x,3)\right] \\ &= \sum_{x\in V(G)} deg_G(x)\left[4n-4-3deg_G(x)+2deg_G(x)-2\sum_{xu\in E(G)} deg_G(u)-d(G,x,3)\right] \\ &= 8nm-8m-M_1(G)-2\sum_{x\in V(G)} deg_G(x)\sum_{xu\in E(G)} deg_G(u)-\sum_{x\in V(G)} deg_G(x)d(G,x,3) \\ &= 8nm-8m-M_1(G)-4\sum_{xu\in E(G)} deg_G(x)deg_G(u)-\sum_{x\in V(G)} deg_G(x)d(G,x,3) \\ &= 8nm-8m-M_1(G)-4M_2(G)-\sum_{x\in V(G)} deg_G(x)d(G,x,3) \\ &\geq 8nm-8m-M_1(G)-4M_2(G)-\alpha\sum_{x\in V(G)} d(G,x,3) \\ &= 8nm-8m-M_1(G)-4M_2(G)-2\alpha\sum_{uv\in E(G)}(deg_G(u)-1)(deg_G(v)-1) \\ &= 8nm-8m-M_1(G)-4M_2(G) \\ &- 2\alpha\sum_{uv\in E(G)}[deg_G(u)deg_G(v)-(deg_G(u)+deg_G(v))+1] \\ &= 8nm-8m-M_1(G)-4M_2(G)-2\alpha M_2(G)+2\alpha M_1(G)-2\alpha m \\ &= 8nm-2m(4+\alpha)+M_1(G)(2\alpha-1)-M_2(G)(2\alpha+4). \end{aligned}$$

It is clear that the equality holds if and only if $\{deg_G(v), deg_G(u) \mid d_G(u,v)=3\}=\{\alpha\}$ and $diam(G)\leq 4$. ■

As an example for the equality in Theorem 2.2 is the cycle of length seven. Define:

$$\beta = \beta(G) = \max\{deg_G(v) \mid v \textit{ is the middle point of a path of length 2}\}.$$

Theorem 2.3 *Let G be a graph with n vertices, m edges and $g(G) > 4$. Then $Gut(G) \geq M_2(G) + 2EM_2(G) - 2(\beta-2)EM_1(G) + \frac{(M_1(G))^3}{4m^2} - 5F(G) + 8M_1(G) - 8m$. The equality holds if and only if $diam(G) \leq 2$ and*

$$\{deg_G(v) \mid uvw \textit{ is a path of length two in } G\} = \{\beta\}.$$

Proof. By definition,

$$\begin{aligned}
Gut(G) &= \sum_{\{u,v\}\subseteq V(G)} deg_G(u)deg_G(v)d_G(u,v)\\
&= \sum_{uv\in E(G)} deg_G(u)deg_G(v) + 2\sum_{e\sim f, e=uv, f=vw} deg_G(u)deg_G(w)\\
&+ \sum_{\{u,v\}\subseteq V(G), deg_G(u,v)\geq 3} deg_G(u)deg_G(v)d_G(u,v)\\
&\geq \sum_{uv\in E(G)} deg_G(u)deg_G(v) + 2\sum_{e\sim f, e=uv, f=vw} deg_G(u)deg_G(w)\\
&= M_2(G) + 2\sum_{e\sim f, e=uv, f=vw} deg_G(u)deg_G(w)\\
&= M_2(G) + 2\sum_{e\sim f, e=uv, f=vw} \Big(deg_G(e) - (deg_G(v)-2)\Big)\Big(deg_G(f) - (deg_G(v)-2)\Big)
\end{aligned}$$

By expanding the terms under summation, we have

$$\begin{aligned}
Gut(G) &\geq M_2(G) + 2\sum_{e\sim f, e=uv, f=vw} deg_G(e)deg_G(f)\\
&- 2\sum_{e\sim f, e=uv, f=vw} (deg_G(v)-2)(deg_G(e)+deg_G(f))\\
&+ 2\sum_{e\sim f, e=uv, f=vw} (deg_G(v)-2)^2\\
&= M_2(G) + 2EM_2(G) - 2\sum_{e\sim f, e=uv, f=vw} (deg_G(v)-2)(deg_G(e)+deg_G(f))\\
&+ 2\sum_{v\in V(G)} \binom{deg_G(v)}{2}(deg_G(v)-2)^2,
\end{aligned}$$

and by simplifying last summations, we have

$$\begin{aligned}
Gut(G) &\geq M_2(G)+2EM_2(G)-2\sum_{e\sim f,e=uv,f=vw}(deg_G(v)-2)(deg_G(e)+deg_G(f))\\
&+\sum_{v\in V(G)}\left[deg_G^4(v)-5deg_G^3(v)+8deg_G^2(v)-4deg_G(v)\right]\\
&= M_2(G)+2EM_2(G)-2\sum_{e\sim f,e=uv,f=vw}(deg_G(v)-2)(deg_G(e)+deg_G(f))\\
&+ M_1^4(G)-5F(G)+8M_1(G)-8m\\
&\geq M_2(G)+2EM_2(G)-2(\beta-2)\sum_{e\sim f,e=uv,f=vw}(deg_G(e)+deg_G(f))\\
&+ M_1^4(G)-5F(G)+8M_1(G)-8m\\
&\geq M_2(G)+2EM_2(G)-2(\beta-2)EM_1(G)+M_1^{(4)}(G)-5F(G)+8M_1(G)-8m.
\end{aligned}$$

The result now follows from this fact that $M_1^{(4)}(G)\geq\frac{(M_1(G))^3}{4m^2}$. By our argument given above, one can easily seen that the equality holds if and only if $diam(G)\leq 2$ and $\{deg_G(v)\mid v\ \textit{is the middle point of a path of length 2}\}=\{\beta\}$. ■

Again the cycle graph of size five is an example for equality in Theorem 2.3.

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