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Relation between Degree Distance and Gutman Index of Graphs

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Abstract

Let $G = (V, E)$ be a simple connected graph with n vertices and m edges. The degree distance of a graph G is

$$D'(G) = \sum_{\{v_i, v_j\} \subseteq V(G)} (d_G(v_i) + d_G(v_j))\, d_G(v_i, v_j).$$

where $d_G(v_i, v_j)$ is the shortest distance between vertices v_i and v_j, and $d_G(v_i)$ is the degree of the vertex v_i in G. The Gutman index (also known as Schultz index of the second kind) of a graph G is defined as

$$\mathrm{Gut}(G) = \sum_{\{v_i, v_j\} \subseteq V(G)} d_G(v_i)\, d_G(v_j)\, d_G(v_i, v_j).$$

We obtain some lower and upper bounds on $D'(G)$ and $\mathrm{Gut}(G)$ of a graph G in terms of n, m, Δ and δ and characterize the extremal graphs. Moreover, we present some relations between $D'(G)$ and $\mathrm{Gut}(G)$ of graph G.

1 Introduction

Throughout this paper, let $G = (V, E)$ be a simple connected graph with vertex set $V = V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. For $v_i \in V(G)$, the degree of a vertex v_i, written by $d_G(v_i)$ (or d_i), is the number of edges incident with v_i. The maximum and minimum degree of a graph G is denoted by Δ and δ, respectively. Let μ_i be the average degree of the adjacent vertices of vertex v_i in G. For a graph G, the distance $d_G(v_i, v_j)$ (or d_{ij}) between vertices v_i and v_j is defined as the length of the shortest path between them. The sum of distances between a vertex v_i of G and all other vertices is denoted by $D_G(v_i)$ (or D_i), that is,

$$D_G(v_i) = \sum_{v_j \in V(G)} d_G(v_i, v_j).$$

The degree distance of a vertex $v_i \in V(G)$ is defined by $D'_G(v_i) = d_G(v_i)\, D_G(v_i)$, where $d_G(v_i)$ is the degree of the vertex v_i.

Topological indices and graph invariants based on the distances between the vertices of a graph are widely used in theoretical chemistry to establish relations between the structure and the properties of molecules. They provide correlations with physical, chemical and thermodynamic parameters of chemical compounds [11–13, 23, 27].

The Wiener index is a well-known topological index which equals the sum of distances between all pairs of vertices of a molecular graph [21]. The Wiener index is denoted by $W(G)$ and is defined as

$$W(G) = \sum_{\{v_i, v_j\} \subseteq V(G)} d_G(v_i, v_j) = \frac{1}{2} \sum_{v_i \in V(G)} D_G(v_i)\,. \tag{1}$$

This molecular structure descriptor is one of the most used topological indices, well correlated with many physical and chemical properties of a variety of classes of chemical compounds. For details, see the survey paper [14]. Dobrynin and Kotchetova [15] and Gutman [20] introduced a new graph invariant that is more sensative than the wiener index. The degree distance of G is

$$D'(G) = \sum_{v_i \in V(G)} D'_G(v_i) = \sum_{v_i \in V(G)} d_G(v_i)\, D_G(v_i) = \sum_{\{v_i, v_j\} \subseteq V(G)} (d_G(v_i) + d_G(v_j))\, d_G(v_i, v_j). \tag{2}$$

The degree distance of graphs is well studied in the literature. The main properties of degree distance $D'(G)$ were summarized in [1, 3, 22, 24–26].

The Gutman index (also known as Schultz index of the second kind) of a graph G is defined as

$$\mathrm{Gut}(G) = \sum_{\{v_i, v_j\} \subseteq V(G)} d_G(v_i)\, d_G(v_j)\, d_G(v_i, v_j).$$

The Gutman index of graphs attracts attention just recently. Some properties of Gutman index can be found in [2,3,19].

Define the inverse degree of a graph G with no isolated vertices as

$$ID(G) = \sum_{v_i \in V(G)} \frac{1}{d_G(v_i)}\,,$$

where $d_G(v_i)$ is the degree of the vertex $v_i \in V(G)$. The inverse degree first attracted attention through conjectures of the computer program Graffiti [18]. It has been studied by several authors, see for example [4,17].

The first and second Zagreb indices, $M_1(G)$ and $M_2(G)$, of a graph G are among the oldest and the most studied graph invariants in mathematical chemistry. They are defined as:

$$M_1(G) = \sum_{v_i \in V(G)} d_G(v_i)^2 \qquad \text{and} \qquad M_2(G) = \sum_{v_i v_j \in E(G)} d_G(v_i)\, d_G(v_j)\,.$$

For more details on these indices see the recent papers [5,7–10] and the references therein.

The paper is organized as follows. In section 2, we present some upper and lower bounds on $D'(G)$ and $\mathrm{Gut}(G)$ of a graph G and characterize the extremal graphs. In section 3, we obtain some relations between $D'(G)$ and $\mathrm{Gut}(G)$ of graph G.

2 Bounds on the degree distance of graphs

In this section we present some upper and lower bounds on $D'(G)$ and $\mathrm{Gut}(G)$ of a graph G and characterize the extremal graphs.

Theorem 2.1. *Let G be a connected graph with n vertices, m edges, minimum degree δ and maximum degree Δ. Then*

$$4(n-1)m - M_1(G) + 2\delta\Big(W(G) + m - n(n-1)\Big) \le D^{'}(G) \le 4(n-1)m - M_1(G) + 2\Delta\Big(W(G) + m - n(n-1)\Big), \tag{3}$$

where $W(G)$ is the Wiener index of graph G. Moreover, both the equalities hold in (3) *if and only if $G \cong K_n$ or G is a graph of diameter 2 or G is a regular graph of diameter greater than or equal to 3.*

Proof: We have

$$\begin{aligned}
D^{'}(G) &= \sum_{v_i\in V(G)} d_i D_i = \sum_{v_i\in V(G)} d_i \sum_{v_j\in V(G)} d_{ij} = \sum_{\{v_i,\,v_j\}\subseteq V(G)} (d_i+d_j)\, d_{ij} \\
&= \sum_{v_i\,v_j\in E(G)} (d_i+d_j) + \sum_{\substack{\{v_i,\,v_j\}\subseteq V(G)\\ d_{ij}\geq 2}} 2(d_i+d_j) + \sum_{\substack{\{v_i,\,v_j\}\subseteq V(G)\\ d_{ij}\geq 2}} (d_i+d_j)\,(d_{ij}-2) \\
&= \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n}\Big[d_i(n-d_i-1) + (2m-d_i-d_i\mu_i)\Big] + \sum_{\substack{1\leq i<j\leq n\\ d_{ij}\geq 2}} (d_i+d_j)\,(d_{ij}-2) \\
&\qquad\qquad \text{as} \quad d_i\mu_i = \sum_{v_j:\, v_iv_j\in E(G)} d_j \\
&\leq 4(n-1)m - M_1(G) + 2\Delta \sum_{\substack{1\leq i<j\leq n\\ d_{ij}\geq 2}} (d_{ij}-2) \quad \text{as } M_1(G) = \sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} d_i\mu_i \ (4) \\
&= 4(n-1)m - M_1(G) + 2\Delta\Big(\sum_{\substack{1\leq i<j\leq n\\ d_{ij}\geq 2}} d_{ij} - 2\sum_{\substack{1\leq i<j\leq n\\ d_{ij}\geq 2}} 1\Big) \\
&= 4(n-1)m - M_1(G) + 2\Delta\Big(W(G) + m - n(n-1)\Big) \quad \text{by (1).}
\end{aligned}$$

Now suppose that the right equality holds in (3). Then the equality holds in (4). From equality in (4), we get $d_i = \Delta$ for all $v_i \in V(G)$ when G has diameter 3 or more. Thus $G \cong K_n$ or G is a graph of diameter 2 or G is a regular graph of diameter greater than or equal to 3.

Conversely, one can see easily that the equality holds in (3) for complete graph K_n or graph of diameter 2 or regular graph of diameter greater than or equal to 3.

Similarly, we can prove that

$$D^{'}(G) \geq 4(n-1)m - M_1(G) + 2\delta\Big(W + m - n(n-1)\Big)$$

with equality holding if and only if $G \cong K_n$ or G is a graph of diameter 2 or G is a regular graph of diameter greater than or equal to 3. ■

In a similar manner as Theorem 2.1, we can prove the following result for Gutman index:

Theorem 2.2. *Let G be a connected graph with n vertices, m edges, minimum degree δ and maximum degree Δ. Then*

$$4m^2 - M_1(G) - M_2(G) + \delta^2 \Big(W(G) + m - n(n-1)\Big) \leq Gut(G) \leq 4m^2 - M_1(G)$$
$$-M_2(G) + \Delta^2 \Big(W(G) + m - n(n-1)\Big),$$

where $W(G)$ is the Wiener index of graph G. Moreover, both the equalities hold if and only if $G \cong K_n$ or G is a graph of diameter 2 or G is a regular graph of diameter greater than or equal to 3.

3 Relation between degree distance and Gutman index of graphs

In this section we give some relations between degree distance and Gutman index of graphs. For this we need the following result:

Lemma 3.1. [16] *If $\overline{a} = (a_1, a_2, \ldots, a_N)$, $\overline{b} = (b_1, b_2, \ldots, b_N)$ are sequences of real numbers and $\overline{c} = (c_1, c_2, \ldots, c_N)$, $\overline{e} = (e_1, e_2, \ldots, e_N)$ are nonnegative sequences, then*

$$\sum_{i=1}^{N} e_i \sum_{i=1}^{N} c_i\, a_i^2 + \sum_{i=1}^{N} c_i \sum_{i=1}^{N} e_i\, b_i^2 \geq 2 \sum_{i=1}^{N} c_i\, a_i \sum_{i=1}^{N} e_i\, b_i\,. \qquad (5)$$

If c_i and e_i $(i = 1, 2, \ldots, N)$ are positive, then the equality holds in (5) if and only if $\overline{a} = \overline{b} = \overline{k}$, where $\overline{k} = (k, k, \ldots, k)$ is a constant sequence.

Theorem 3.2. *Let G be a connected graph of order n with m edges and diameter d. Then*

$$2\, D'(G)\, Gut(G) \leq \left(\frac{(n-1)\,\Delta\,\delta}{\Delta+\delta} + \frac{(n-1)\,(n-2)}{2}\,\frac{\Delta}{2} + (n-1)\, ID(G)\right)$$
$$\times \left(2\, m\, d^2\, M_1(G) - (d^2-1)\Big[2m - (n-1)\Delta\Big]\, M_1(G) - (d^2\,\Delta - \Delta + 1)\,\delta\, M_1(G)\right), \qquad (6)$$

where Δ and δ are the maximum degree and minimum degree, respectively. Moreover, the equality holds in (6) if and only if $G \cong K_3$.

Proof: Suppose that each i in Lemma 3.1 corresponds to a vertex pair (v_i, v_j) such that $N = \frac{n(n-1)}{2}$. Setting $c_i = e_i = d_i\, d_j\, (d_i + d_j)\, d_{ij}^2$ and each a_i is replaced by $\frac{1}{d_i\, d_j\, d_{ij}}$ and b_i is replaced by $\frac{1}{(d_i+d_j)\, d_{ij}}$, then from (5), we get

$$\sum_{i<j} d_i\, d_j\, (d_i + d_j)\, d_{ij}^2 \sum_{i<j} \left(\frac{d_i\, d_j}{d_i + d_j} + \frac{d_i + d_j}{d_i\, d_j}\right) \geq 2 \sum_{i<j} d_i\, d_j\, d_{ij} \sum_{i<j} (d_i + d_j)\, d_{ij}\,. \qquad (7)$$

Since

$$\sum_{i=1}^{n} d_i = 2m \quad \text{and} \quad \sum_{i=1}^{n} d_i^2 = M_1(G),$$

we have

$$\begin{aligned}
\sum_{i<j} d_i\, d_j\, (d_i + d_j) &= \sum_{i<j} (d_i^2\, d_j + d_i\, d_j^2) \\
&= \sum_{i=1}^{n} d_i^2\, (2m - d_i) \\
&= 2m\, M_1(G) - \sum_{i=1}^{n} d_i^3\,.
\end{aligned}$$

and

$$\begin{aligned}
\sum_{v_i v_j \in E(G)} d_i\, d_j\, (d_i + d_j) &= \sum_{v_i v_j \in E(G)} d_i^2\, d_j + \sum_{v_i v_j \in E(G)} d_i\, d_j^2 \\
&= \sum_{i=1}^{n} d_i^3\, \mu_i \\
&\geq \sum_{i=1}^{n} d_i^2\, [2m - d_i - (n - d_i - 1)\Delta] \\
&\qquad \text{as} \;\; d_i\, \mu_i \geq 2m - d_i - (n - d_i - 1)\Delta \\
&= \Big[2m - (n-1)\,\Delta\Big]\, M_1(G) + (\Delta - 1) \sum_{i=1}^{n} d_i^3\,.
\end{aligned}$$

Using the above results, we get

$$\begin{aligned}
\sum_{i<j} d_i\, d_j\, (d_i + d_j)\, d_{ij}^2 &= \sum_{v_i v_j \in E(G)} d_i\, d_j\, (d_i + d_j) + \sum_{i<j,\, d_{ij} \geq 2} d_i\, d_j\, (d_i + d_j)\, d_{ij}^2 \\
&\leq \sum_{v_i v_j \in E(G)} d_i\, d_j\, (d_i + d_j) + d^2 \sum_{i<j,\, d_{ij} \geq 2} d_i\, d_j\, (d_i + d_j) \\
&= d^2 \sum_{i<j} d_i\, d_j\, (d_i + d_j) - (d^2 - 1) \sum_{v_i v_j \in E(G)} d_i\, d_j\, (d_i + d_j) \\
&\leq 2\, m\, d^2\, M_1(G) - (d^2 - 1)\Big[2m - (n-1)\Delta\Big]\, M_1(G) \\
&\qquad - (d^2\,\Delta - \Delta + 1) \sum_{i=1}^{n} d_i^3 \qquad (8) \\
&\leq 2\, m\, d^2\, M_1(G) - (d^2 - 1)\Big[2m - (n-1)\Delta\Big]\, M_1(G)
\end{aligned}$$

$$- (d^2\,\Delta - \Delta + 1)\,\delta\, M_1(G)\,. \qquad (9)$$

Since

$$\frac{2}{\Delta} \le \frac{1}{d_i} + \frac{1}{d_j} \le \frac{2}{\delta},$$

we have

$$\frac{d_i\,d_j}{d_i + d_j} \le \frac{\Delta}{2}\,.$$

Again since

$$\frac{1}{d_i} + \frac{1}{\delta} \ge \frac{1}{\Delta} + \frac{1}{\delta},$$

we have

$$\frac{d_i\,\delta}{d_i + \delta} \le \frac{\Delta\,\delta}{\Delta + \delta}\,.$$

Suppose that v_n is the minimum degree vertex of degree δ. Using the above results, we have

$$\begin{aligned} \sum_{i<j} \frac{d_i\,d_j}{d_i + d_j} &= \sum_{i=1}^{n-1} \frac{d_i\,\delta}{d_i + \delta} + \sum_{i<j<n} \frac{d_i\,d_j}{d_i + d_j} \\ &\le \frac{(n-1)\,\Delta\,\delta}{\Delta + \delta} + \left(\frac{n\,(n-1)}{2} - (n-1)\right)\frac{\Delta}{2} \\ &= \frac{(n-1)\,\Delta\,\delta}{\Delta + \delta} + \frac{(n-1)\,(n-2)}{2}\,\frac{\Delta}{2}\,. \end{aligned} \qquad (10)$$

and

$$\sum_{i<j} \frac{d_i + d_j}{d_i\,d_j} = \sum_{i<j}\left(\frac{1}{d_i} + \frac{1}{d_j}\right) = \sum_{i=1}^{n} \frac{n-1}{d_i} = (n-1)\,ID(G). \qquad (11)$$

From the above two results, we get

$$\sum_{i<j}\left(\frac{d_i\,d_j}{d_i + d_j} + \frac{d_i + d_j}{d_i\,d_j}\right) \le \frac{(n-1)\,\Delta\,\delta}{\Delta + \delta} + \frac{(n-1)\,(n-2)}{2}\,\frac{\Delta}{2} + (n-1)\,ID(G)\,. \qquad (12)$$

Using the above result with (9) in (7), we get the required result in (6). First part of the proof is done.

Now suppose that equality holds in (6). From equality in (7), by Lemma 3.1, we get

$$\frac{1}{d_i\,d_j\,d_{ij}} = \frac{1}{d_i\,d_k\,d_{ik}} = \frac{1}{(d_i + d_j)\,d_{ij}} = \frac{1}{(d_i + d_k)\,d_{ik}} \quad \text{for any} \quad v_i,\, v_j,\, v_k \in V(G)\,.$$

From the above,

$$d_i + d_j = d_i\,d_j, \quad \text{that is,} \;\; d_i = d_j = 2 \;\; \text{for any} \quad v_i,\, v_j \in V(G).$$

Again from the above, we get $d_{ij} = d_{ik}$ for any $v_i,\, v_j,\, v_k \in V(G)$. Thus we have $d = 1$. Hence $G \cong K_3$.

Conversely, one can see easily that the equality holds in (6) for K_3. ■

Corollary 3.3. *Let G be a connected graph of order n with m edges and diameter d. Then*

$$2\,D'(G)\,Gut(G) \le \left(\frac{(n-1)\,\Delta\,\delta}{\Delta+\delta} + \frac{(n-1)\,(n-2)}{2}\,\frac{\Delta}{2} + (n-1)\,ID(G)\right)$$

$$\times\left(2\,m\,d^2\,M_1(G) - (d^2-1)\Big[2m-(n-1)\Delta\Big]\,M_1(G)\right.$$

$$\left. -(d^2\,\Delta-\Delta+1)\left(\delta\,M_1(G)-(\delta-1)p\right)\right), \tag{13}$$

where Δ, δ and p are the maximum degree, minimum degree and the number of pendant vertices in G. Moreover, the equality holds in (13) *if and only if $G \cong K_3$.*

Proof: Since p is the number of pendant vertices in G, we have

$$\sum_{i=1}^{n} d_i^3 = p + \sum_{v_i\in V(G),\,d_i\neq 1} d_i^3 \ge p + \delta \sum_{v_i\in V(G),\,d_i\neq 1} d_i^2 = p + \delta\,(M_1(G)-p).$$

Using this result in (8), we get the required result in (13). Moreover, the equality holds in (13) if and only if $G \cong K_3$. ■

Lemma 3.4. (Radon's inequality) *For real numbers $p > 0$, $x_1,\, x_2, \ldots,\, x_r \ge 0$, $a_1,\, a_2, \ldots,\, a_r > 0$, the following inequality holds:*

$$\sum_{k=1}^{r} \frac{x_k^{p+1}}{a_k^p} \ge \frac{\left(\sum\limits_{k=1}^{r} x_k\right)^{p+1}}{\left(\sum\limits_{k=1}^{r} a_k\right)^{p}}.$$

We now give another relation between degree distance and Gutman index of graphs.

Theorem 3.5. *Let G be a connected graph of order n with m edges and maximum degree Δ, minimum degree δ. Then*

$$\Delta\,\delta\,D'(G)^2 \le (\Delta+\delta)^2\,Gut(G)\,W(G) \tag{14}$$

with equality holding if and only if G is a regular graph.

Proof: Suppose that each k in Lemma 3.4 corresponds to a vertex pair (v_i, v_j) with $r = \frac{n(n-1)}{2}$ and $p = 1$. Setting each x_k is replaced by $(d_i + d_j)\, d_{ij}$ and a_k is replaced by $d_i\, d_j\, d_{ij}$, then from Lemma 3.4, we get

$$\frac{\left(\sum\limits_{i<j} (d_i + d_j)\, d_{ij}\right)^2}{\sum\limits_{i<j} d_i\, d_j\, d_{ij}} \leq \sum_{i<j} \frac{(d_i + d_j)^2}{d_i\, d_j}\, d_{ij}\,,$$

that is,

$$\frac{D'(G)^2}{Gut(G)} \leq \sum_{i<j} \left(\sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}}\right)^2 d_{ij}\,.$$

In [6], it has been shown that

$$\left(\sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}}\right)^2 \leq \frac{(\Delta + \delta)^2}{\Delta\, \delta}\,.$$

Moreover, the equality holds if and only if G is a regular graph or G is a bipartite semiregular graph.

From the above two results, we obtain

$$\frac{D'(G)^2}{Gut(G)} \leq \frac{(\Delta + \delta)^2}{\Delta\, \delta} \sum_{i<j} d_{ij} \leq \frac{(\Delta + \delta)^2}{\Delta\, \delta}\, W(G)\,.$$

Moreover, the equality holds if and only if G is a regular graph. ■

Theorem 3.6. *Let G be a connected graph of order n with m edges and the number of pendant vertices p. Then*

$$\begin{aligned} Gut(G) \;\; &\leq \;\; D'(G) + \frac{(2m-n)(2m-n+1)(n-p-1)}{2} + m - (n-p-2)\, M_2(G) \\ &\qquad + \frac{(n-p-3)}{2}\, M_1(G) - W(G) \qquad (15) \end{aligned}$$

with equality holding if and only if the distance between any two non-pendant vertices in G is at most 2.

Proof: We have

$$\begin{aligned} \sum_{v_iv_j \in E(G)} (d_i - 1)(d_j - 1) \;\; &= \;\; \sum_{v_iv_j \in E(G)} d_i\, d_j - \sum_{v_iv_j \in E(G)} (d_i + d_j) + \sum_{v_iv_j \in E(G)} 1 \\ &= \;\; M_2(G) - M_1(G) + m. \end{aligned}$$

and

$$\begin{aligned}
\sum_{i<j}(d_i-1)(d_j-1) &= \sum_{i<j,\, d_i,\, d_j\geq 2}(d_i-1)(d_j-1)\\
&= \sum_{i<j,\, d_i,\, d_j\geq 2} d_i\, d_j - \sum_{i<j,\, d_i,\, d_j\geq 2}(d_i+d_j) + \sum_{i<j,\, d_i,\, d_j\geq 2} 1\\
&= \frac{1}{2}\sum_{v_i\in V(G),\, d_i\geq 2} d_i(2m-d_i-p) - \frac{1}{2}\sum_{v_i\in V(G),\, d_i\geq 2}\Big[(n-p-1)\, d_i\\
&\qquad + 2m-d_i-p\Big] + \frac{(n-p)(n-p-1)}{2}\\
&= \frac{1}{2}(2m-p)^2 - \frac{1}{2}(M_1(G)-p) - (n-p-1)(2m-p)\\
&\qquad + \frac{(n-p)(n-p-1)}{2}\\
&= \frac{1}{2}\Big[(2m-n)(2m-n+1)+2m-M_1(G)\Big].
\end{aligned}$$

Using the above two results, we get

$$\begin{aligned}
Gut(G)-D'(G)+W(G) &= \sum_{i<j}(d_i\, d_j - d_i - d_j + 1)\, d_{ij}\\
&= \sum_{v_iv_j\in E(G)}(d_i-1)(d_j-1) + \sum_{\substack{i<j,\, d_{ij}\geq 2\\ d_i,\, d_j\geq 2}}(d_i-1)(d_j-1)\, d_{ij}\\
&\leq \sum_{v_iv_j\in E(G)}(d_i-1)(d_j-1) + (n-p-1)\\
&\qquad \times \sum_{\substack{i<j,\, d_{ij}\geq 2\\ d_i,\, d_j\geq 2}}(d_i-1)(d_j-1) \qquad (16)\\
&= (n-p-1)\sum_{i<j}(d_i-1)(d_j-1) - (n-p-2)\\
&\qquad \times \sum_{v_iv_j\in E(G)}(d_i-1)(d_j-1)\\
&= \frac{(2m-n)(2m-n+1)(n-p-1)}{2} + m - (n-p-2)\, M_2(G)\\
&\qquad + \frac{(n-p-3)}{2}\, M_1(G) - W(G).
\end{aligned}$$

First part of the proof is done.

Moreover, the equality holds in (15) if and only if the equality holds in (16), that is, if and only if $d_{ij} = 2$ for any v_i, $v_j \in V(G)$, $v_iv_j \notin E(G)$ with d_i, $d_j \geq 2$. Hence the equality holds in (15) if and only if the distance between any two non-pendant vertices in G is at most 2. ■

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