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Nordhaus–Gaddum relations for proximity and remoteness in graphs

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ABSTRACT

The transmission of a vertex in a connected graph is the sum of all distances from that vertex to the others. It is said to be normalized if divided by $n - 1$, where n denotes the order of the graph. The proximity of a graph is the minimum normalized transmission, while the remoteness is the maximum normalized transmission. In this paper, we give Nordhaus–Gaddum-type inequalities for proximity and remoteness in graphs. The extremal graphs are also characterized for each case.

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1. Introduction

In this paper, $G = (V, E)$ denotes a simple connected graph, with vertex set V and edge set E, on $n = |V|$ vertices and $m = |E|$ edges. The degree of a vertex $v \in V$ is denoted by $d_G(v)$, or $d(v)$ when no confusion is possible. The minimum, average and maximum degrees are denoted by δ, $\overline{d}$ and Δ, respectively. The distance between two vertices u and v in G, denoted by $d(u, v)$, is the length of a shortest path between u and v. The average distance between all pairs of vertices in G is denoted by $\bar{l}$. The eccentricity $e(v)$ of a vertex v in G is the largest distance from v to another vertex of G. The minimum eccentricity in G, denoted by r, is the radius of G. The maximum eccentricity of G, denoted by D, is the diameter of G. The average eccentricity of G is denoted by ecc. That is,

$$r = \min_{v \in V} e(v), \qquad D = \max_{v \in V} e(v) \quad \text{and} \quad ecc = \frac{1}{n} \sum_{v \in V} e(v).$$

It is trivial that $r \leq ecc \leq D$ and $\bar{l} \leq ecc$. The transmission $t(v)$ of a vertex v is the sum of the distances from v to all other vertices in G. It is said to be normalized, and then denoted $\tilde{t}(v)$, when divided by $n - 1$. The proximity π and remoteness ρ [1,2] of G are, respectively, the minimum and the maximum normalized transmission in G. That is,

$$\pi = \min_{v \in V} \tilde{t}(v) \quad \text{and} \quad \rho = \max_{v \in V} \tilde{t}(v).$$

Note that, by definition,

$$\pi \leq r \leq ecc \leq D, \qquad \pi \leq \bar{l} \leq \rho \leq D \quad \text{and} \quad \bar{l} = \frac{1}{n} \sum_{v \in V} \tilde{t}(v).$$

Thus normalizing $t(v)$ helps in comparing graph invariants. Sharp bounds, proved in [3], on the proximity and the remoteness of a graph G on n vertices are

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$$1 \le \pi \le \begin{cases} \dfrac{n+1}{4} & \text{if } n \text{ is odd,} \\ \dfrac{n}{4} + \dfrac{n}{4(n-1)} & \text{if } n \text{ is even} \end{cases} \quad \text{and} \quad 1 \le \rho \le \frac{n}{2}.$$

The lower bound on π is reached if and only if G contains a dominating vertex, i.e. $\Delta = n-1$; the upper bound on π is attained if and only if G is either the cycle C_n or the path P_n; the lower bound on ρ is reached if and only if G is the complete graph K_n; the upper bound on ρ is attained if and only if G is the path P_n.

Let G be a graph and $\overline{G}$ its complement. If I is an invariant of G, we denote by $\bar{I}$ the same invariant but in $\overline{G}$. Nordhaus–Gaddum relations for the graph invariant I are inequalities of the following form:

$$L_1(n) \le I + \bar{I} \le U_1(n) \quad \text{and} \quad L_2(n) \le I \cdot \bar{I} \le U_2(n),$$

where $L_1(n)$ and $L_2(n)$ are lower bounding functions of the order n, and $U_1(n)$ and $U_2(n)$ upper bounding functions of the order n. Note that sometimes, in addition to the order n, other graph invariants are used in the bounds. These types of relation are named after Nordhaus and Gaddum [4], who were the first authors to give such relations, namely

$$2\sqrt{n} \le \chi + \overline{\chi} \le n+1 \quad \text{and} \quad n \le \chi \cdot \overline{\chi} \le \left(\frac{n+1}{2}\right)^2, \tag{1}$$

where χ is the chromatic number of a graph. Finck [5] characterized the extremal graphs for the inequalities in (1). Since then many graph theorists have been interested in finding such relations for various graph invariants. See [6] for a review of early results of Nordhaus–Gaddum type. A variety of more recent papers devoted to such results can be found in the graph theory literature, e.g. [7–14].

In order to get conjectures on the bounds in the Nordhaus–Gaddum-type inequalities for proximity and remoteness of a graph and its complement, we used the AutoGraphiX 2 (AGX 2, for short) system [15–18]. This "discovery system" is described, together with its results, in a series of papers under the common title "Variable Neighborhood Search for Extremal Graphs"; see [16] for references. It is based on the following observation: a large variety of problems in extremal graph theory can be viewed as parametric combinatorial optimization ones defined on the family of all graphs (or some restriction thereof) and solved by a generic heuristic. The parameter is usually the order n of the graphs considered (sometimes the order n and the size m or another graph invariant). The heuristic fits in the Variable Neighborhood Search metaheuristic framework [17,19,20]. Presumably extremal graphs are found by performing a series of local changes (removal, addition or rotation of an edge, etc.) until a local optimum is reached, then applying increasingly large perturbations, followed by new descents; if a graph better than the incumbent one is found, the search is recentered there. After the parametric family of extremal graphs has been found, relationships between graph invariants may be deduced from them using various data mining techniques [18]. These include (i) a numerical method based on Principal Component Analysis which yields a basis of affine relations between the graph invariants considered; (ii) a geometric method which uses a gift-wrapping algorithm to find the convex hull of extremal graphs viewed as points in the invariants space; facets of this convex hull give inequality relations; (iii) an algebraic method which recognizes families of graphs then exploits a database of formulae giving expressions of invariants as functions of n on these families; substitution then leads to linear or nonlinear conjectures.

2. Proximity

In this section, we prove results of Nordhaus–Gaddum type for proximity in a graph and its complement. First, we prove the lower and upper bounds, and characterize the associated extremal graphs, on the sum $\pi + \overline{\pi}$.

Theorem 1. *For any connected graph G on $n \ge 5$ vertices for which $\overline{G}$ is connected,*

$$\frac{2n}{n-1} \le \pi + \overline{\pi} \le \begin{cases} \dfrac{n+1}{4} + \dfrac{n+1}{n-1} & \text{if } n \text{ is odd,} \\ \dfrac{n}{4} + \dfrac{n}{4(n-1)} + \dfrac{n+1}{n-1} & \text{if } n \text{ is even.} \end{cases}$$

The lower bound is attained if and only if $\Delta(G) = \Delta(\overline{G}) = n-2$. The upper bound is attained if and only if either G or $\overline{G}$ is the cycle C_n.

Proof.

Lower bound: Note that, if G is a connected graph such that $\overline{G}$ is also connected, then $\Delta \le n-2$. So

$$\pi \ge \frac{\Delta + 2(n-\Delta-1)}{n-1} = \frac{2n-\Delta-2}{n-1} \ge \frac{(n-2)+2}{n-1} = \frac{n}{n-1}. \tag{2}$$

Thus, the lower bound follows. Moreover, equality in (2) holds if and only if $\Delta = n-2$. Then, the lower bound is attained if and only if $\Delta = n-2$ and $\overline{\Delta} = n-2$ (or equivalently $\Delta = n-2$ and $\delta = 1$).

Upper bound: Assume, without loss of generality, that $r \geq \overline{r}$. Since G and $\overline{G}$ are connected, we have $r, \overline{r} \geq 2$. Thus, we consider two cases according to the values of r.

Case 1. $r \geq 3$. Let v be a vertex in G. Let $v' \in V$ such that $d_G(v, v') = e_G(v) \geq r$. For any vertex $w \in V \setminus \{v, v'\}$, $wv \notin E$ or $wv' \notin E$. Indeed, $wv \in E$ and $wv' \in E$ would imply $d_G(v, v') \leq d_G(v, w) + d_G(w, v') = 2$, which contradicts the choice of v'. Thus, $e_{\overline{G}}(v) = 2$ and then $\overline{r} = 2$. Therefore,

$$t_{\overline{G}}(v) = d_{\overline{G}}(v) + 2\left(n - 1 - d_{\overline{G}}(v)\right) = 2(n-1) - d_{\overline{G}}(v) = n - 1 + d_G(v).$$

Thus

$$\overline{\pi} = 1 + \frac{\delta}{n-1}.$$

Case 1.1. $\delta \leq 2$. We have

$$\begin{aligned}
\pi + \overline{\pi} &\leq \begin{cases} \dfrac{n+1}{4} + 1 + \dfrac{\delta}{n-1} & \text{if } n \text{ is odd,} \\ \dfrac{n}{4} + \dfrac{n}{4(n-1)} + 1 + \dfrac{\delta}{n-1} & \text{if } n \text{ is even} \end{cases} \\
&\leq \begin{cases} \dfrac{n+1}{4} + 1 + \dfrac{2}{n-1} & \text{if } n \text{ is odd,} \\ \dfrac{n}{4} + \dfrac{n}{4(n-1)} + 1 + \dfrac{2}{n-1} & \text{if } n \text{ is even} \end{cases}
\end{aligned}$$

with equality if and only if G is the cycle C_n.

Case 1.2. $\delta = 3$. Let u be a central vertex in G, i.e., $e_G(v) = r$. Let S_i denote the set of vertices $u \in V$ such that $d(v, u) = i$. In [21], Erdös et al. proved that a graph G with radius r contains an induced path of length at least $2r - 1$. From the proof of that result, it is easy to see that S_i contains at least two vertices, for $i = 2, \ldots r - 1$. Also, since $\delta = 3$, $|S_1| \geq 3$. Then

$$\begin{aligned}
t(v) &= \sum_{i=1}^{r} i|S_i| \\
&\leq 3 + 2\sum_{i=2}^{r-1} i + (n - 2r) \cdot r = 1 + 2\sum_{i=1}^{r-1} i + nr - 2r^2 \\
&= (n-1) \cdot r - r^2 + 1.
\end{aligned}$$

This bound, as a function of r, is increasing (using calculus, for example). On the other hand, Erdös et al. [22] proved that the radius r of a connected graph with minimum degree δ is at most $3(n-3)/(2\delta+2) + 5$. In our case, $\delta = 3$, so $r \leq 3(n-3)/8 + 5 = (3n+31)/8$. Therefore

$$t(v) \leq (n-1)\left(\frac{3n+31}{8}\right) - \left(\frac{3n+31}{8}\right)^2 + 1 = \frac{15n^2 + 38n - 1145}{64}.$$

Thus

$$\pi \leq \tilde{t}(v) \leq \frac{15n+53}{64} - \frac{273}{16(n-1)}.$$

Now, applying to the sum $\pi + \overline{\pi}$, we have

$$\begin{aligned}
\pi + \overline{\pi} &\leq \frac{15n+53}{64} - \frac{273}{16(n-1)} + 1 + \frac{3}{n-1} \\
&= \frac{15n+117}{64} - \frac{225}{16(n-1)} \\
&< \begin{cases} \dfrac{n+1}{4} + \dfrac{n+1}{n-1} & \text{if } n \text{ is odd,} \\ \dfrac{n}{4} + \dfrac{n}{4(n-1)} + \dfrac{n+1}{n-1} & \text{if } n \text{ is even} \end{cases}
\end{aligned}$$

for all $n \geq 5$.

Case 1.3. $\delta \geq 4$. It is proved in [23] that $\overline{l} \leq (n-1)/\delta$. So, as $\pi \leq \overline{l}$,

$$\pi + \overline{\pi} \leq \frac{n-1}{\delta} + 1 + \frac{\delta}{n-1}.$$

This bound, considered as a function of δ, is decreasing for $4 \le \delta \le n-1$, and therefore it reaches its maximum for $\delta = 4$. Thus

$$\pi + \overline{\pi} \le \frac{n-1}{4} + 1 + \frac{4}{n-1} < \begin{cases} \frac{n+1}{4} + 1 + \frac{2}{n-1} & \text{if } n \text{ is odd,} \\ \frac{n}{4} + \frac{n}{4(n-1)} + 1 + \frac{2}{n-1} & \text{if } n \text{ is even,} \end{cases}$$

for all $n \ge 6$. Note that, since G and $\overline{G}$ are connected, and $\delta \ge 4$, the number of vertices is at least 7.

Case 2. $r = 2$. Let u_1 (resp. u_2) be a central vertex in G (resp. $\overline{G}$). We have

$$\pi \le \tilde{t}_G(u_1) = 2 - \frac{d_1}{n-1} \quad \text{and} \quad \overline{\pi} \le \tilde{t}_{\overline{G}}(u_2) = 1 + \frac{d_2}{n-1},$$

where d_1 and d_2 are, respectively, the degrees of u_1 and u_2 in G. Thus

$$\pi + \overline{\pi} \le 2 - \frac{d_1}{n-1} + 1 + \frac{d_2}{n-1} = 3 + \frac{d_2 - d_1}{n-1}.$$

Note that a center in a graph cannot be a pending vertex. So $2 \le d_1, d_2 \le n-3$, and therefore $d_2 - d_1 \le n-5$ with equality if and only if $d_1 = 2$ and $d_2 = n-3$.

Case 2.1. $d_1 = 2$ and $d_2 = n-3$.

$$\begin{aligned} \pi + \overline{\pi} &\le \tilde{t}_G(u_2) + \tilde{t}_{\overline{G}}(u_1) = \frac{n-3+2\times 2}{n-1} + \frac{n-3+2\times 2}{n-1} \\ &= \frac{2n+2}{n-1} = 2 + \frac{4}{n-1} < \begin{cases} \frac{n+1}{4} + \frac{n+1}{n-1} & \text{if } n \text{ is odd,} \\ \frac{n}{4} + \frac{n}{4(n-1)} + \frac{n+1}{n-1} & \text{if } n \text{ is even,} \end{cases} \end{aligned}$$

for all $n \ge 6$.

If $n = 5$, then each of G and $\overline{G}$ contains a vertex of degree 3. Each of these two vertices has a normalized transmission of at most $5/4$. So $\pi + \overline{\pi} \le 5/2$, which is less than the desired bound.

Case 2.2. $d_2 - d_1 \le n-6$. We have

$$\pi + \overline{\pi} \le 3 + \frac{n-6}{n-1} = 4 - \frac{5}{n-1} < \begin{cases} \frac{n+1}{4} + \frac{n+1}{n-1} & \text{if } n \text{ is odd,} \\ \frac{n}{4} + \frac{n}{4(n-1)} + \frac{n+1}{n-1} & \text{if } n \text{ is even,} \end{cases}$$

for all $n \ge 5$. This completes the proof. □

Now, we turn to the bounds on the product $\pi \cdot \overline{\pi}$.

Theorem 2. *For any connected graph G on $n \ge 5$ vertices for which $\overline{G}$ is connected,*

$$\frac{n^2}{(n-1)^2} \le \pi \cdot \overline{\pi} \le \begin{cases} \frac{(n+1)^2}{4(n-1)} & \text{if } n \text{ is odd,} \\ \frac{n(n+1)}{4(n-1)} + \frac{n(n+1)}{4(n-1)^2} & \text{if } n \text{ is even.} \end{cases}$$

The lower bound is attained if and only if $\Delta(G) = \Delta(\overline{G}) = n-2$. The upper bound is attained if and only if either G or $\overline{G}$ is the cycle C_n.

The proof is similar to that of Theorem 1, and is omitted here.

3. Remoteness

In the following theorem, we state and prove the lower and upper bounds on the sum $\rho + \overline{\rho}$. The extremal graphs are also characterized.

Recall that a *comet* $Co_{n,\Delta}$ is obtained from a star $S_{\Delta+1}$ by appending a path $P_{n-\Delta-1}$ to one of its pending vertices. Moreover, a *path-complete* graph $PK_{n,m}$ on n vertices and m edges is the graph obtained from a path P_k, $k \ge 1$, and a clique K_{n-k} by adding at least one edge between one endpoint of the path and the vertices of K_{n-k}, where $(n-k)(n-k-1)/2 + k \le m \le (n-k+1)(n-k)/2 + k - 1$. One can verify that there is exactly one path-complete graph $PK_{n,m}$ for all n and m such that $1 \le n-1 \le m \le n(n-1)/2$.

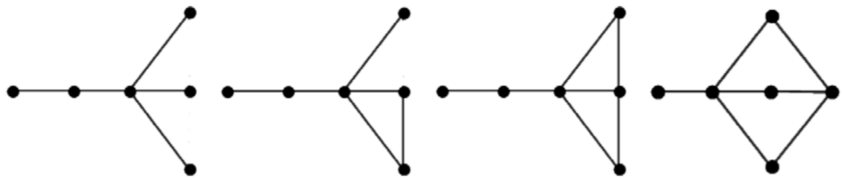

Fig. 1. Graphs with $D = 3$ that maximize $\rho + \overline{\rho}$ for $n = 6$.

Theorem 3. *For any connected graph G on $n \geq 6$ vertices for which $\overline{G}$ is connected,*

$$3 \leq \rho + \overline{\rho} \leq \frac{n+2}{2} + \frac{2}{n-1}.$$

The lower bound is attained if and only if $n \geq 8$, G is regular and $D = \overline{D} = 2$. The upper bound is attained if and only if G or $\overline{G}$ is the path P_n, the comet $Co_{n,3}$ or the path-complete graph $PK_{n,n}$ when $n \geq 7$, and if and only if G or $\overline{G}$ is the path P_6, the comet $Co_{6,3}$, the path-complete graph $PK_{6,6}$ or one of the graphs in Fig. 1.

Proof.

Lower bound: For a vertex v in a connected graph G,

$$\tilde{t}(v) \geq \frac{d(v) + 2(n - d(v) - 1)}{n-1} = 2 - \frac{d(v)}{n-1}.$$

So

$$\rho \geq 2 - \frac{\delta}{n-1},$$

with equality if and only if the diameter of G is 2.

Applying this to both G and $\overline{G}$,

$$\rho + \overline{\rho} \geq 4 - \frac{\delta + \overline{\delta}}{n-1} = 3 + \frac{\Delta - \delta}{n-1} \geq 3.$$

Thus the lower bound follows. Moreover, it is attained if and only if G is regular and $D = \overline{D} = 2$. Note that such pair of graphs does not exist if $n = 6$ or $n = 7$. Indeed, a connected regular graph G on six vertices, for which $\overline{G}$ is connected, is the cycle C_6 or its complement. In this case we have $\rho + \overline{\rho} = 3.2$. Also, a connected regular graph on seven vertices, for which $\overline{G}$ is connected, is the cycle C_7 or its complement. In this case we have $\rho + \overline{\rho} = 10/3$.

Upper bound: According to the fact that if the diameter of G is at least 4, then the diameter of $\overline{G}$ is 2, and assuming, without loss of generality, that $D \geq \overline{D}$, we will consider three cases. (i) $\overline{D} = 2$ and $D \geq 3$. In this case,

$$\overline{\rho} = \frac{\overline{\delta} + 2(n - \overline{\delta} - 1)}{n-1} = 2 - \frac{\overline{\delta}}{n-1} = 1 + \frac{\Delta}{n-1},$$

where $\overline{\delta}$ denotes the minimum degree in $\overline{G}$ and Δ denotes the maximum degree in G. In addition, for a connected graph with diameter D, it is easy to see that the remoteness ρ is bounded as follows:

$$\rho \leq \frac{1 + 2 + \cdots + (D-1) + D \cdot (n-D)}{n-1} = \frac{(2n-1)D - D^2}{2(n-1)}.$$

Now, using the inequality $\Delta \leq n - D + 1$ for connected graphs, we get

$$\begin{aligned} \rho + \overline{\rho} &\leq \frac{(2n-1)D - D^2}{2(n-1)} + 1 + \frac{\Delta}{n-1} \\ &\leq \frac{(2n-1)D - D^2}{2(n-1)} + 1 + \frac{n-D+1}{n-1} \\ &= \frac{(2n-3)D - D^2}{2(n-1)} + 2 + \frac{2}{n-1}. \end{aligned}$$

It is easy to see that the last expression is maximum if and only if $D = n-1$ or $D = n-2$. Therefore, replacing D by $n-2$ or $n-1$,

$$\rho + \overline{\rho} \leq \frac{n+2}{2} + \frac{2}{n-1}$$

with equality if and only if $D = n - 1$ or $D = n - 2$. If $D = n - 1$, the corresponding graph is the path P_n. If $D = n - 2$ and under the condition that ρ is maximum, the corresponding graphs are the comet $Co_{n,3}$ and the path-complete graph $PK_{n,n}$.

(ii) $\overline{D} = 2$ and $D = 2$. In this case we have

$$\rho + \overline{\rho} = 2 - \frac{\delta}{n-1} + 2 - \frac{\overline{\delta}}{n-1} = 3 - \frac{\delta}{n-1} + \frac{\Delta}{n-1} = 3 + \frac{\Delta - \delta}{n-1}.$$

Note that, if $D = \overline{D} = 2$, then $\Delta \le n - 2$ and $\delta \ge 2$. Thus

$$\rho + \overline{\rho} \le 3 + \frac{n-4}{n-1} < \frac{n+2}{2} + \frac{2}{n-1}$$

for all $n \ge 6$.

(iii) $\overline{D} = D = 3$. In this case, we have

$$\rho \le \frac{1 + 2 + 3(n-3)}{n-1} = \frac{3n-6}{n-1} \quad \text{and} \quad \overline{\rho} \le \frac{3n-6}{n-1}. \tag{3}$$

First, assume that both inequalities in (3) are strict, so

$$\rho + \overline{\rho} \le 2 \cdot \frac{1 + 4 + 3(n-4)}{n-1} = 6 - \frac{8}{n-1} \le \frac{n+2}{2} + \frac{2}{n-1}$$

for all $n \ge 6$. The inequality being strict whenever $n \ge 7$.

Now assume that one of the inequalities in (3) is an equality, without loss of generality, say

$$\rho = \frac{1 + 2 + 3(n-3)}{n-1} = \frac{3n-6}{n-1}.$$

In this case, G must contain a vertex (of maximum transmission) v_1 of degree 1, its unique neighbor v_2 of degree 2, a unique vertex v_3 at distance 2 from v_1, and $n-3$ vertices $u_1, u_2, \ldots u_{n-3}$ at distance 3 from v_1, such that $u_i v_j \notin E$ for $i = 1, \ldots n-3$ and $j = 1, 2$. Under these conditions, we have in $\overline{G}$,

$$\tilde{t}_{\overline{G}}(v_1) = \frac{(n-2) + 2}{n-1} = 1 + \frac{1}{n-1},$$
$$\tilde{t}_{\overline{G}}(v_2) = \frac{(n-3) + 2 + 3}{n-1} = 1 + \frac{3}{n-1},$$
$$\tilde{t}_{\overline{G}}(v_3) = \frac{1 + 2(n-3) + 3}{n-1} = 2,$$
$$\tilde{t}_{\overline{G}}(u_i) \le \frac{2 + 2(n-3)}{n-1} = 2 - \frac{2}{n-1}, \quad \text{for } i = 1, \ldots n-3.$$

Therefore, $\overline{\rho} = 2$ for all $n \ge 6$. Thus

$$\rho + \overline{\rho} = \frac{3n-6}{n-1} + 2 = 5 - \frac{3}{n-1} \le \frac{n+2}{2} + \frac{2}{n-1}$$

with equality if and only if $n = 6$.

The extremal graphs for $n = 6$ are P_6, $Co_{6,3}$ and $PK_{6,6}$ in the case (i) (as shown above). In addition, it is easy to see that the bound is reached (for $n = 6$) for all the graphs given in Fig. 1, and using the graph-generating system Nauty (available at http://cs.anu.edu.au/~bdm/nauty/), one can easily check that those graphs and their complements are the only ones for which the bound is reached. □

The following lemma will be used in the proof of the next theorem.

Lemma 4. *The function $f(t) = t^3 - (4n-1)t^2 + (4n^2 - 2n)t$, for $1 \le t \le n-1$, where n is an integer, is maximum for $t^* = \left(4n - 1 - \sqrt{4n^2 - 2n + 1}\right)/3$. Moreover, if t is assumed to be integer, then the function reaches its maximum for $t^* = 2n/3$ if $n = 0 \pmod 3$, for $t^* = 2(n-1)/3$ and for $t^* = (2n+1)/3$ if $n = 1 \pmod 3$, and for $t^* = (2n-1)/3$ if $n = 2 \pmod 3$.*

Proof. It is easy to check that $f(t)$ is maximum for

$$t^* = \frac{4n - 1 - \sqrt{4n^2 - 2n + 1}}{3}.$$

Moreover, we have $(2n-1)/3 < t^* < 2n/3$. So, assuming that t^* is an integer, we get

$$\frac{2n-3}{3} \le t^* \le \frac{2n}{3} \quad \text{if } n = 0 \pmod 3,$$
$$\frac{2n-2}{3} \le t^* \le \frac{2n+1}{3} \quad \text{if } n = 1 \pmod 3,$$
$$\frac{2n-1}{3} \le t^* \le \frac{2n+2}{3} \quad \text{if } n = 2 \pmod 3.$$

Substitutions show that the maximum value of $f(t)$ is

$$f\left(\frac{2n}{3}\right) = \frac{(32n+40)(n-1)^2+48(n-1)+8}{27} \quad \text{if } n = 0 \pmod 3,$$
$$f\left(\frac{2n-2}{3}\right) = f\left(\frac{2n+1}{3}\right) = \frac{(32n+40)(n-1)^2+36(n-1)}{27} \quad \text{if } n = 1 \pmod 3,$$
$$f\left(\frac{2n-1}{3}\right) = \frac{(32n+40)(n-1)^2+48(n-1)+10}{27} \quad \text{if } n = 2 \pmod 3.$$

This completes the proof. □

In the following theorem, we prove the upper bound on the product $\rho \cdot \overline{\rho}$. Moreover, we show that the bound is sharp for every value $n \ge 7$.

Theorem 5. *For any connected graph G on $n \ge 7$ vertices for which $\overline{G}$ is connected,*

$$\rho \cdot \overline{\rho} \le \begin{cases} \frac{16n+20}{27} + \frac{8}{9(n-1)} + \frac{4}{27(n-1)^2} & \textit{if } n = 0 \pmod 3, \\ \frac{16n+20}{27} + \frac{2}{3(n-1)} & \textit{if } n = 1 \pmod 3, \\ \frac{16n+20}{27} + \frac{8}{9(n-1)} + \frac{5}{27(n-1)^2} & \textit{if } n = 2 \pmod 3. \end{cases}$$

The upper bound is the best possible, as shown by the comets $Co_{n,\lceil \frac{n}{3} \rceil + 1}$, and $Co_{n,\lceil \frac{n}{3} \rceil}$ if $n = 1 \pmod 3$.

Proof. We proceed as in the case of the upper bound in Theorem 3 and consider three cases according to the values of D and $\overline{D}$.

Case $\overline{D} = 2$ and $D \ge 3$. We have

$$\rho \cdot \overline{\rho} \le \left(2 - \frac{D-2}{n-1}\right) \cdot \left(\frac{D \cdot (2n-D-1)}{2(n-1)}\right) = \frac{(4n^2-2n) \cdot D - (4n-1) \cdot D^2 + D^3}{2(n-1)^2}.$$

Using Lemma 4, we have

$$\rho \cdot \overline{\rho} \le \begin{cases} \frac{16n+20}{27} + \frac{8}{9(n-1)} + \frac{4}{27(n-1)^2} & \text{if } n = 0 \pmod 3, \\ \frac{16n+20}{27} + \frac{2}{3(n-1)} & \text{if } n = 1 \pmod 3, \\ \frac{16n+20}{27} + \frac{8}{9(n-1)} + \frac{5}{27(n-1)^2} & \text{if } n = 2 \pmod 3. \end{cases}$$

with equality if and only if $D = 2n/3$ for $n = 0 \pmod 3$, $D = 2(n-1)/3$ or $D = (2n+1)/3$ for $n = 1 \pmod 3$, and $D = (2n-1)/3$ for $n = 2 \pmod 3$. In each of these cases, the bound is attained as shown by the comets $Co_{n,\lceil \frac{n}{3} \rceil + 1}$, and also $Co_{n,\lceil \frac{n}{3} \rceil}$ if $n = 1 \pmod 3$.

Case $D = \overline{D} = 2$. In this case we have

$$\rho \cdot \overline{\rho} \le \left(2 - \frac{\delta}{n-1}\right) \cdot \left(1 + \frac{\Delta}{n-1}\right) = 2 + \frac{2\Delta}{n-1} - \frac{\delta}{n-1} - \frac{\delta\Delta}{(n-1)^2}$$
$$< 2 + \frac{2\Delta - \delta}{n-1} \le 2 + \frac{2(n-2)-2}{n-1} \le 4 - \frac{4}{n-1} < \frac{16n+20}{27}$$

for all $n \ge 7$.

Table 1
Upper bounds on $\rho \cdot \overline{\rho}$ for possible values of n_1, n_2, n_3.

(n_1, n_2, n_3)	$(1, 1, 4)$	$(1, 2, 3)$	$(1, 3, 2)$	$(1, 4, 1)$	$(2, 1, 3)$
Upper bound on $\rho \cdot \overline{\rho}$	5	$4 + \frac{2}{3}$	$4 + \frac{25}{36}$	5	$4 + \frac{25}{36}$
(n_1, n_2, n_3)	$(2, 2, 2)$	$(2, 3, 1)$	$(3, 1, 2)$	$(3, 2, 1)$	$(4, 1, 1)$
Upper bound on $\rho \cdot \overline{\rho}$	$4 + \frac{1}{3}$	$4 + \frac{5}{18}$	$4 + \frac{5}{18}$	$3 + \frac{8}{9}$	$3 + \frac{3}{4}$

Case $D = \overline{D} = 3$. Let $v, v' \in V$ such that $\rho = \tilde{t}_G(v)$ and $\overline{\rho} = \tilde{t}_{\overline{G}}(v')$. If $e_G(v) = 2$ (similarly $e_{\overline{G}}(v') = 2$), then

$$\rho \cdot \overline{\rho} \le 2\left(\frac{1+2+3(n-3)}{n-1}\right) = 2\left(3 - \frac{3}{n-1}\right) = 6 - \frac{6}{n-1} < \frac{16n+20}{27}$$

for all $n \ge 8$. If $n = 7$, the bound is reached and the corresponding value is 5.

If $e_G(v) = e_{\overline{G}}(v') = 3$ (necessarily $v \ne v'$), let n_i be the number of vertices at distance i from v in G. Note that $n_1 + n_2 + n_3 = n - 1$. Thus

$$\rho = \frac{n_1 + 2n_2 + 3n_3}{n-1} = 1 + \frac{n_2 + 2n_3}{n-1}; \tag{4}$$

$$\overline{\rho} \le \begin{cases} \dfrac{n_3 + 2n_1 + 3n_2}{n-1} = 1 + \dfrac{n_1 + 2n_2}{n-1} & \text{if } d_G(v, v') = 1, \\ \dfrac{1 + 2(n_2 + n_3 - 1) + 3n_1}{n-1} = 2 + \dfrac{n_1 - 1}{n-1} & \text{if } d_G(v, v') = 2. \end{cases} \tag{5}$$

Note that $d_G(v, v') \le 2$. Indeed, $d_G(v, v') = 3$ would imply $e_{\overline{G}}(v') = 2 \ne 3$. Now, we consider two subcases according to the value of $d_G(v, v')$.

If $d_G(v, v') = 1$, then

$$\begin{aligned} \rho \cdot \overline{\rho} &\le \left(1 + \frac{n_2 + 2n_3}{n-1}\right) \cdot \left(1 + \frac{n_1 + 2n_2}{n-1}\right) \\ &= 1 + \frac{n_1 + 3n_2 + 2n_3}{n-1} + \frac{(n_2 + 2n_3)(n_1 + 2n_2)}{(n-1)^2} \\ &= 3 + \frac{n_2 - n_1}{n-1} + \frac{(n - 1 + n_3 - n_1)(n - 1 + n_2 - n_3)}{(n-1)^2} \\ &= 4 + \frac{2(n_2 - n_1)}{n-1} + \frac{(n_3 - n_1)(n_2 - n_3)}{(n-1)^2} \\ &< 4 + \frac{2(n-4)}{n-1} + \frac{(n-4)^2}{(n-1)^2} = 7 - \frac{12}{n-1} + \frac{9}{(n-1)^2}. \end{aligned}$$

Easy computations show that this bound is less than the desired one for all $n \ge 8$.

If $d_G(v, v') = 2$, computations similar to those of the case $d_G(v, v') = 1$ show that the inequality is strict for all $n \ge 8$.

To be done, it remains to prove that the inequality is true for $n = 7$ in the case $D = \overline{D}$ and $e_G(v) = e_{\overline{G}}(v') = 3$. We consider all possible values of n_1, n_2 and n_3 ($n_1, n_2, n_3 \ge 1$ and $n_1 + n_2 + n_3 = 6$), and for each possibility, the corresponding bound on $\rho \cdot \overline{\rho}$ computed from the bounds (4) and (5). These values, gathered in Table 1, are compared to the value obtained from the theorem, which is 5. □

Remark. Note that the bound provided in Theorem 5 is not valid for $n = 4, 5, 6$ (if $n \le 3$, then G and $\overline{G}$ cannot be connected simultaneously). For the path P_4 (resp. the comets $Co_{5,3}$ and $Co_{6,4}$), $\rho \cdot \overline{\rho} = 4$ (resp. $9/2$ and $24/5$) while the corresponding value provided by Theorem 5 is $10/3$ (resp. $63/16$ and $112/25$).

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