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M. Aouchiche, P. Hansen,
A. Hertz, C. Sellal

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GERAD HEC Montréal
3000, chemin de la Côte-Sainte-Catherine
Montréal (Québec) Canada H3T 2A7

Tél. : 514 340-6053
Téléc. : 514 340-5665
info@gerad.ca
www.gerad.ca

Bounds on differences between some graph theoretic invariants

Mustapha Aouchiche[a]
Pierre Hansen[a]
Alain Hertz[b]
Cherif Sellal[b]

[a] *GERAD & HEC Montréal, Montréal (Québec) Canada, H3T 2A7*

[b] *GERAD & Polytechnique Montréal, Montréal (Québec) Canada, H3C 3A7*

mustapha.aouchiche@gerad.ca
pierre.hansen@gerad.ca
alain.hertz@gerad.ca
cherif.sellal@gerad.ca

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Abstract: In the present paper, we are interested in bounding differences between graph invariants as well as in characterizing the corresponding extremal graphs. This kind of results belongs to the more general form known as AGX Form 1 which is extensively studied using the AutoGraphiX system at GERAD, Montreal. The graph invariants involved in the present work are the proximity, the remoteness, the eccentricity, the average distance, the frequencies of the maximum and minimum degrees, the domination number, the stability number and the chromatic number.

Key Words: Proximity, remoteness, graph invariants, extremal graphs, AutoGraphiX.

1 Introduction

Since GRAPH [14, 15], a system defined about two decades ago, several other systems for automated, or computer assisted, discovery of conjectures in graph theory have been developed. They include newGRAPH, due to Stevanović [33], Graffiti, due to Fajtlowicz [19], Graffiti.pc, due to Delavina [20], GraPHedron due to Mélot [28] and AutoGraphix (AGX for short), due to Caporossi and Hansen [4, 11].

The AGX system was systematically tested in the thesis of Aouchiche [1]. Pairwise comparisons between 20 invariants were studied, and all results and/or conjectures were of the following form (called AGX Form 1):

$$\ell_n \le i_1(G) \oplus i_2(G) \le u_n$$

where $i_1(G)$ and $i_2(G)$ are invariants, $\oplus$ is one of the four operations $+, -, \times, /$, and ℓ_n and u_n are lower and upper bounding functions of the order n of G which are *best possible*, i.e., such that for each value of n (except possibly very small ones where border effects appear) there is a graph G for which the bound is tight. These pairwise comparisons gave rise to 1520 cases, more than half of which were easily proved automatically by AGX, and about 360 were proved by hand, either by the GERAD Montreal group, or by graph theorists of various countries (mainly Serbia and China).

Several papers were devoted to prove results of the AGX Form 1, a list of which can be found in [3, 5]. In the present paper, we explore forward the AGX Form 1, and focus our attention on the difference between pairs of invariants in terms of their order. Our results involve the following invariants which are defined in the next section: the proximity, the remoteness, the eccentricity, the average distance, the frequencies of the maximum and minimum degrees, the domination number, the stability number and the chromatic number. They were all first conjectured using the AGX system.

While the average distance is widely studied, see e.g. [9,16,21–23,29,32], the eccentricity, introduced in [16], seems to be less studied then the average distance (see [18,26,27,31]). Also, despite their recent introduction [1, 7], the proximity and the remoteness attracted the attention of several graph theorists [6, 25, 27, 30, 34]. Five conjectures were listed in [7], four of them were settled in [27, 30, 34], and the last one (that bounds the difference between the average eccentricity and the remoteness) is still open. Particular cases of this open conjecture are solved by Sedlar [30]. Further results of the AGX Form 1 involving the proximity and the remoteness can be found in [6, 8, 27, 34].

2 Definitions and notations

Let $G = (V, E)$ be a finite undirected graph, where V is the vertex set, and E the edge set of G. The cardinality of V is also called the *order* of G. Two vertices u and v are said to be *adjacent* if $\{u, v\}$ (also denoted by uv or vu) belongs to E. For any subset U of V, the subgraph of G *induced* by U is the graph $H = (U, E(U))$, where $E(U)$ consists of those edges of G with both ends in U. We denote by $n_\Delta(G)$ the number of vertices of maximum degree in G, while $n_\delta(G)$ is the number of vertices of minimum degree in G.

Given two vertices u and v of G, a *path* of length ℓ between u and v is a sequence $(u_0 = u, u_1, \ldots, u_\ell = v)$ of distinct vertices such that $u_i u_{i+1}$ is an edge of G for all $i \in \{0, 1, \ldots, \ell - 1\}$. A *cycle* C is a sequence $(u_0, u_1, \ldots, u_{\ell-1})$ of distinct vertices such that $u_i u_{i+1}$ is an edge of G for all $i \in \{0, 1, \ldots \ell - 1\}$ (where the addition is modulo ℓ). We denote by P_n the path of order n, and by C_n the cycle of order n. A graph G is connected if for any pair of vertices u and v of G, there is a path between u and v. If G is not connected, its vertex set can be partitioned into *connected components*, i.e., maximal induced subgraphs that are connected. A graph G is a *tree* if it is connected and has no cycle.

A set of vertices in a graph G is *stable* if it induces a subgraph with no edges. The *stability number* of G, also called *independence number*, and denoted by $\alpha(G)$, is the maximum cardinality of a stable set in G. A k-*coloring* of G is a partition of its vertex set into k stable sets. The *chromatic number* of G, denoted by $\chi(G)$, is the smallest integer k such that G admits a k-coloring. A set of vertices in G is *dominating* if all vertices of G are adjacent to at least one vertex of this set, or belongs to it. The *domination number* of G, denoted by $\beta(G)$ is the minimum cardinality of a dominating set in G.

The distance between two vertices u and v in G, denoted $d_G(u,v)$, is the number of edges on a shortest path between u and v. For a vertex v of a graph G, $\sigma_G(v)$ denotes the *transmission* of v in G, i.e.,

$$\sigma_G(v) = \sum_{w\in V} d_G(v,w)$$

and $\epsilon_G(v)$ denotes the *eccentricity* of v in G, i.e.,

$$\epsilon_G(v) = \max_{w\in V} d_G(v,w).$$

The *diameter* of G, denoted by $D(G)$, is the maximum eccentricity of any vertex in G, i.e., $D(G) = \max_{v\in V}\epsilon_G(v)$.

We denote by $K_{a,b}$ the complete bipartite graph having a vertices in one part, and b in the other one, and by $K_{a,b}-e$ the graph obtained from $K_{a,b}$ by removing an edge. The *comet*, denoted by $CO_{n,k}$, is the graph obtained by linking a vertex of degree 1 of a star on $k+1$ vertices to one of the endpoints of the path P_{n-k-1} on $n-k-1$ vertices. Also, we denote by $KI_{n,k}$ the *kite* which is obtained by linking a vertex of a clique on k vertices to one of the endpoints of a path P_{n-k} on $n-k$ vertices. A *double comet* (*double kite*) is the graph obtained by considering two disjoint comets (kites) G_1 and G_2 and linking a vertex of maximum eccentricity in G_1 with a vertex of maximum eccentricity in G_2. A double comet (double kite) with n vertices and diameter not larger than $n-3$ is *balanced* if the two vertices of maximum degree have a degree that differs by at most one unit. We denote by $DC_{n,\ell}$ ($DK_{n,\ell}$) the balanced double comet (balanced double kite) with n vertices and diameter ℓ. For illustration, the graphs $CO_{7,4}$, $KI_{7,4}$, $DC_{9,5}$ and $DK_{9,5}$ are shown in Figure 1.

Given a graph $G=(V,E)$, we are mainly interested in the four following invariants, respectively called the *eccentricity*, the *proximity*, the *remoteness*, and the *average distance* of a connected graph G:

$$\epsilon(G) = \frac{\sum\limits_{v\in V}\epsilon_G(v)}{n} \qquad \pi(G) = \frac{\min\limits_{v\in V}\sigma_G(v)}{n-1} \qquad \rho(G) = \frac{\max\limits_{v\in V}\sigma_G(v)}{n-1} \qquad \mu(G) = \frac{\sum\limits_{v\in V}\sigma_G(v)}{n(n-1)}.$$

In the next section, we give bounds on the differences of the form $\pi(G)-i(G)$, where $i(G)$ is an invariant among $n_\delta(G)$, $n_\Delta(G)$ and $\beta(G)$. In Section 4, we prove an upper bound on $\rho(G)-n_\Delta(G)$, while an upper bound on $\epsilon(G)-\mu(G)$ is given in Section 5 for the class of trees. Finally, in Sections 6 and 7, we prove upper and lower bounds on $\chi(G)-n_\Delta(G)$ and $\alpha(G)-n_\delta(G)$, respectively.

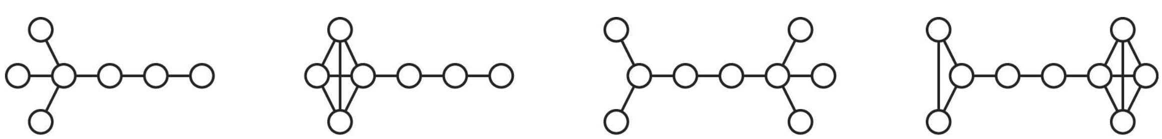
3 Comparing proximity to other invariants

Let G be a connected graph of order n. The following result was proved in [7].

Proposition 3.1

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

Moreover, the lower bound is reached if and only if G contains a dominating vertex, while the upper bound is reached if and only if G is the path P_n or the cycle C_n on n vertices.



$CO_{7,4}$ $KI_{7,4}$ $DC_{9,5}$ $DK_{9,5}$

Figure 1: A comet, a kite, a double comet and a double kite

We now give the second possible largest value of the proximity of a graph G of order n.

Lemma 3.1 *Let G be a connected graph of order n. If G is not isomorphic to the cycle C_n or to the path P_n on n vertices, then*

$$\pi(G) \le \begin{cases} \frac{n^2-4}{4(n-1)} & \text{if } n \text{ is even} \\ \frac{n^2-5}{4(n-1)} & \text{if } n \text{ is odd.} \end{cases}$$

Moreover, the bound is reached if G is isomorphic to $CO_{n,3}$ or $KI_{n,3}$ (and possibly also by other graphs).

Proof. Since G is not isomorphic to C_n or P_n, it follows from Property 3.1 that $\pi(G)$ is strictly smaller than $\pi(C_n) = \pi(P_n)$. It then follows from the definition of the proximity that $\pi(G)$ is at most equal to $\pi(C_n) - \frac{1}{n-1}$. Hence,

$$\pi(G) \le \begin{cases} \frac{n^2}{4(n-1)} - \frac{1}{n-1} = \frac{n^2-4}{4(n-1)} & \text{if } n \text{ is even} \\ \frac{n+1}{4} + \frac{1}{n-1} = \frac{n^2-5}{4(n-1)} & \text{if } n \text{ is odd.} \end{cases}$$

It is easy to verify that this bound is attained for G equal to $CO_{n,3}$ or $KI_{n,3}$. □

Theorem 3.2 *Let G be a connected graph of order $n \ge 4$. Then*

$$\begin{aligned} 1-n &\le \min\{\pi(G) - n_\delta(G), \pi(G) - n_\Delta(G)\} \\ &\le \max\{\pi(G) - n_\delta(G), \pi(G) - n_\Delta(G)\} \le \begin{cases} \frac{n^2-4n}{4(n-1)} & \text{if } n \text{ is even} \\ \frac{n^2-4n-1}{4(n-1)} & \text{if } n \text{ is odd.} \end{cases} \end{aligned}$$

Moreover, the lower bound is reached if and only if G is a clique, while the upper bound is reached if G is isomorphic to $CO_{n,3}$ or $KI_{n,3}$ (and possibly also by other graphs).

Proof. Notice first that $\pi(G)$ reaches its minimum value 1 when G has a dominating vertex, while $n_\Delta(G)$ and $n_\delta(G)$ reach their maximum value n only for regular graphs. Hence, both $\pi(G) - n_\Delta(G)$ and $\pi(G) - n_\delta(G)$ are at least equal to $1-n$ and this lower bounds is attained only for cliques.

For the upper bound, let us first show that it is not reached when G is isomorphic to C_n or P_n. Since $n_\Delta(C_n) = n_\delta(C_n) = n > n_\Delta(P_n) = n-2 \ge n_\delta(P_n) = 2$, it is sufficient to show that $\pi(P_n) - n_\delta(P_n)$ is strictly smaller that the proposed upper bound.

$$\begin{aligned} \pi(P_n) - n_\delta(P_n) &= \begin{cases} \frac{n^2}{4(n-1)} - 2 & \text{if } n \text{ is even} \\ \frac{n+1}{4} - 2 & \text{if } n \text{ is odd} \end{cases} \\ &= \begin{cases} \frac{n^2-8n+8}{4(n-1)} & \text{if } n \text{ is even} \\ \frac{n^2-8n+7}{4(n-1)} & \text{if } n \text{ is odd} \end{cases} \\ &< \begin{cases} \frac{n^2-4n}{4(n-1)} & \text{if } n \text{ is even} \\ \frac{n^2-4n-1}{4(n-1)} & \text{if } n \text{ is odd.} \end{cases} \end{aligned}$$

If G is not isomorphic to C_n or P_n, then it follows from Lemma 3.1 and the inequalities $n_\Delta(G) \ge 1$ and $n_\delta(G) \ge 1$ that

$$\max\{\pi(G) - n_\delta(G), \pi(G) - n_\Delta(G)\} \le \begin{cases} \frac{n^2-4}{4(n-1)} - 1 & \text{if } n \text{ is even} \\ \frac{n^2-5}{4(n-1)} - 1 & \text{if } n \text{ is odd.} \end{cases} = \begin{cases} \frac{n^2-4n}{4(n-1)} & \text{if } n \text{ is even} \\ \frac{n^2-4n-1}{4(n-1)} & \text{if } n \text{ is odd.} \end{cases}$$

It is easy to verify that this bound is attained for G equal to $CO_{n,3}$ or $KI_{n,3}$. □

Theorem 3.3 *Let G be a connected graph of order $n \geq 2$ and with a given diameter $D(G) = \ell$. Then*

$$\pi(G) \leq \begin{cases} \frac{2\ell n-\ell^2}{4(n-1)} & \text{if } \ell \text{ is even} \\ \frac{2\ell n-\ell^2+1}{4(n-1)} & \text{if } \ell \text{ is odd and } n \text{ is even} \\ \frac{2\ell n-\ell^2-1}{4(n-1)} & \text{if both } \ell \text{ and } n \text{ are odd.} \end{cases}$$

Moreover, the upper bound is reached by balanced double comets $DC_{n,\ell}$ and balanced double kites $DK_{n,\ell}$.

Proof. Consider an induced path $P = (v_0, v_1, \cdots, v_\ell)$ of length ℓ in G. Let $a = \lceil \frac{\ell-1}{2} \rceil$ and $b = \lceil \frac{\ell}{2} \rceil$. We obviously have $\pi(G) \leq \min\{\frac{\sigma_G(v_a)}{n-1}, \frac{\sigma_G(v_b)}{n-1}\}$. The sum of the distances from v_a or from v_b to the other vertices of P is $\frac{1}{2}\lfloor \frac{\ell}{2} \rfloor(\lfloor \frac{\ell}{2} \rfloor + 1) + \frac{1}{2}\lceil \frac{\ell}{2} \rceil(\lceil \frac{\ell}{2} \rceil + 1)$. Also, $\min\{\frac{\sigma_G(v_a)}{n-1}, \frac{\sigma_G(v_b)}{n-1}\}$ is maximised by linking half of the $n-\ell-1$ other vertices of G to v_1 and the other half to $v_{\ell-1}$. More precisely, without loss of generality, we may assume that $\lceil \frac{n-\ell-1}{2} \rceil$ vertices of G not in P are linked to v_1 and are at distance $\lceil \frac{\ell-1}{2} \rceil$ of v_a, while $\lfloor \frac{n-\ell-1}{2} \rfloor$ vertices of G not in P are linked to $v_{\ell-1}$ and are at distance $\lceil \frac{\ell}{2} \rceil$ of v_a. In summary,

$$(n-1)\pi(G) \leq \sigma_G(v_a) \leq \frac{1}{2}\lfloor \tfrac{\ell}{2} \rfloor(\lfloor \tfrac{\ell}{2} \rfloor + 1) + \frac{1}{2}\lceil \tfrac{\ell}{2} \rceil(\lceil \tfrac{\ell}{2} \rceil + 1) + \lceil \tfrac{n-\ell-1}{2} \rceil \lceil \tfrac{\ell-1}{2} \rceil + \lfloor \tfrac{n-\ell-1}{2} \rfloor \lceil \tfrac{\ell}{2} \rceil.$$

If ℓ is even, we therefore get

$$(n-1)\pi(G) \leq \tfrac{\ell}{2}(\tfrac{\ell}{2} + 1) + (n-\ell-1)\tfrac{\ell}{2} = \tfrac{2n\ell-\ell^2}{4}.$$

If ℓ is odd, while n is even, then

$$\begin{aligned}(n-1)\pi(G) &\leq \tfrac{1}{2}\tfrac{\ell-1}{2}(\tfrac{\ell-1}{2} + 1) + \tfrac{1}{2}\tfrac{\ell+1}{2}(\tfrac{\ell+1}{2} + 1) + \tfrac{n-\ell-1}{2}\tfrac{\ell-1}{2} + \tfrac{n-\ell-1}{2}\tfrac{\ell+1}{2} \\ &= \tfrac{2\ell n-\ell^2+1}{4}.\end{aligned}$$

Finally, if both ℓ and n are odd, then

$$\begin{aligned}(n-1)\pi(G) &\leq \tfrac{1}{2}\tfrac{\ell-1}{2}(\tfrac{\ell-1}{2} + 1) + \tfrac{1}{2}\tfrac{\ell+1}{2}(\tfrac{\ell+1}{2} + 1) + \tfrac{n-\ell}{2}\tfrac{\ell-1}{2} + \tfrac{n-\ell-2}{2}\tfrac{\ell+1}{2} \\ &= \tfrac{2\ell n-\ell^2-1}{4}.\end{aligned}$$

□

Theorem 3.4 *Let G be a connected graph of order $n \geq 2$. Then*

$$\pi(G) - \beta(G) \leq \frac{n^2 - 8n + z}{36(n-1)} \text{ with } z = \begin{cases} -9 & \text{if } n = 9 \text{ or } 17 \pmod{18} \\ 0 & \text{if } n = 0 \text{ or } 8 \pmod{18} \\ 3 & \text{if } n = 11 \text{ or } 15 \pmod{18} \\ 7 & \text{if } n = 1, 7 \text{ or } 13 \pmod{18} \\ 12 & \text{if } n = 2 \text{ or } 6 \pmod{18} \\ 15 & \text{if } n = 3 \text{ or } 5 \pmod{18} \\ 16 & \text{if } n = 4, 10 \text{ or } 16 \pmod{18} \\ 24 & \text{if } n = 12 \text{ or } 14 \pmod{18} \end{cases}$$

Moreover, if $2 \leq n \leq 9$, then the bound is attained by all graphs G with a dominating vertex, while if $n \geq 10$, then the bound is reached by balanced double comets $DC_{n,\ell}$ and balanced double kites $DK_{n,\ell}$ with diameter $\ell = 2 + 3\lfloor \frac{n}{9} \rfloor$.

Proof. Since the statement of the theorem is clearly true for $n = 2$, we can assume $n \geq 3$. Also, notice that if $D(G) = 1$ (i.e., G is a clique), then $\pi(G) - \beta(G) = 0$, while if G is a star (i.e., $G = K_{1,n-1}$), then $D(G) = 2$ and $\pi(G) - \beta(G)$ also equals 0. Hence, the upper bound on the difference $\pi(G) - \beta(G)$ is always attained for at least one graph which is not a clique. From now on, we therefore assume $D(G) \geq 2$.

It was proved in [24] that $\beta(G) \geq \lceil \frac{D(G)+1}{3} \rceil$ and we know from Theorem 3.3 that $\pi(G) \leq \frac{2D(G)n - D(G)^2 + x}{4(n-1)}$, with $x = 0, 1$ or -1, depending on the parity of n and $D(G)$. Hence,

$$\pi(G) - \beta(G) \leq \frac{2D(G)n - D(G)^2 + x}{4(n-1)} - \lceil \frac{D(G)+1}{3} \rceil.$$

Let $F(\ell)$ and $f(\ell, n)$ be defined as follows:

$$F(\ell) = \frac{2\ell n - \ell^2}{4(n-1)} - \lceil \frac{\ell+1}{3} \rceil$$

$$f(\ell, n) = \frac{x}{4(n-1)} \text{ with } x = \begin{cases} 0 & \text{if } \ell \text{ is even} \\ 1 & \text{if } \ell \text{ is odd and } n \text{ is even} \\ -1 & \text{if both } \ell \text{ and } n \text{ are odd.} \end{cases}$$

We then have $\pi(G) - \beta(G) \leq F(D(G)) + f(D(G), n)$. Moreover,

- if $\ell = 0(mod\ 3)$, then $F(\ell+2) + f(\ell+2, n) = F(\ell) + f(\ell, n) + \frac{n-\ell-1}{n-1}$;
- if $\ell = 1(mod\ 3)$ then $F(\ell-2) + f(\ell-2, n) = F(\ell) + f(\ell, n) + \frac{\ell-2}{n-1}$.

This implies that given any n, the integer ℓ for which $F(\ell) + f(\ell, n)$ reaches its maximal value is equal to $2 + 3a$ for some integer $a \geq 0$, which implies $\lceil \frac{\ell+1}{3} \rceil = \frac{\ell+1}{3}$. We now show that this optimum value is reached for $a = \lfloor \frac{n}{9} \rfloor$.

So assume $\ell = 2 + 3\lfloor \frac{n}{9} \rfloor$. Then

$$F(\ell+3) = F(\ell) + \frac{2n - 6l - 5}{4(n-1)} = F(\ell) + \frac{2n - 18\lfloor \frac{n}{9} \rfloor - 17}{4(n-1)} \leq F(\ell) - \frac{1}{4(n-1)}$$

and

$$F(\ell-3) = F(\ell) - \frac{2n - 6l + 13}{4(n-1)} = F(\ell) - \frac{2n - 18\lfloor \frac{n}{9} \rfloor + 1}{4(n-1)} \leq F(\ell) - \frac{1}{4(n-1)}.$$

Since considering $F(\ell)$ as a continuous function, it is quadratic concave, this proves that the maximum value of $F(\ell)$ with ℓ integer is reached when $\ell = 2 + 3\lfloor \frac{n}{9} \rfloor$.

Consider now any integer $\ell' = 2 + 3a'$ with $a' \neq \lfloor \frac{n}{9} \rfloor$. It follows from the defintion of f that $f(\ell', n) \leq f(\ell, n) + \frac{1}{4(n-1)}$. Also, we have shown that $F(\ell') \leq \max\{F(\ell-3), F(\ell+3)\}$. Hence,

$$F(\ell') + f(\ell', n) \leq \left(F(\ell) - \frac{1}{4(n-1)}\right) + \left(f(\ell, n) + \frac{1}{4(n-1)}\right) = F(\ell) + f(\ell, n).$$

This means that the upper bound on $\pi(G) - \beta(G)$ is reached for graphs G of order n with diameter $D(G) = 2 + 3\lfloor \frac{n}{9} \rfloor$. We now analyze the value of $F(D(G)) + f(D(G), n)$ according to the value of $n \mod 18$.

If $n = 0(mod\ 18)$, then $D(G) = 2 + 3\frac{n}{9} = \frac{n+6}{3}$. Hence, both n and $D(G)$ are even, which means that $f(D(G), n) = 0$ and

$$F(D(G)) + f(D(G), n) = \frac{2\frac{n+6}{3}n - \frac{(n+6)^2}{9}}{4(n-1)} - \frac{n+9}{9} = \frac{n^2 - 8n}{36(n-1)}.$$

If $n = 1(mod\ 18)$, then $D(G) = 2 + 3\frac{n-1}{9} = \frac{n+5}{3}$. Hence n is odd while $D(G)$ is even, which means that $f(D(G), n)$ is again equal to 0. We therefore have

$$F(D(G)) + f(D(G), n) = \frac{2\frac{n+5}{3}n - \frac{(n+5)^2}{9}}{4(n-1)} - \frac{n+8}{9} = \frac{n^2 - 8n + 7}{36(n-1)}.$$

Similar computations can be done for the other values of $n \mod 18$, and we get the result in the statement of the theorem. It is easy to check that the upper bound equals 0 for $2 \leq n \leq 9$, which means that it is reached by all graphs having a dominating vertex. For $n \geq 10$, it follows from Theorem 3.3 and the above proof that the upper bound is reached by balanced double comets $DC_{n,\ell}$ and balanced double kites $DK_{n,\ell}$ with diameter $\ell = 2 + 3\lfloor \frac{n}{9} \rfloor$. □

4 The remoteness and the maximum degree frequency

Let G be a connected graph of order n. The following result was proved in [7].

Proposition 4.1

$$1 \leq \rho(G) \leq \frac{n}{2}$$

Moreover, the lower bound is reached if and only if G is a clique, while the upper bound is reached if and only if G is the path P_n on n vertices.

We now give the second possible largest value of the remoteness of a graph G of order n

Lemma 4.1 *Let G be a connected graph of order n. If G is not the path P_n, then*

$$\rho(G) \leq \frac{n^2 - n - 2}{2(n-1)}$$

Moreover, the bound is reached if G is isomorphic to $CO_{n,3}$ or $KI_{n,3}$ (and possibly also by other graphs).

Proof. Since G is not isomorphic to P_n, it follows from Property 4.1 that $\rho(G)$ is strictly smaller than $\rho(P_n) = \frac{n}{2}$. It then follows from the definition of the proximity that $\rho(G)$ is at most equal to $\frac{n}{2} - \frac{1}{n-1} = \frac{n^2-n-2}{2(n-1)}$. It is easy to verify that this bound is attained for G equal to $CO_{n,3}$ or $KI_{n,3}$. □

Theorem 4.2 *Let G be a connected graph of order $n \geq 4$. Then*

$$1 - n \leq \rho(G) - n_\Delta(G) \leq \frac{n^2 - 3n}{2(n-1)}$$

Moreover, the lower bound is reached if and only if G is a clique, while the upper bound is reached if G is isomorphic to $CO_{n,3}$ or $KI_{n,3}$ (and possibly also by other graphs).

Proof. Notice first that $\rho(G)$ reaches its minimum value 1 when G is a clique, while $n_\Delta(G)$ reaches its maximum value n for regular graphs. We therefore have $\rho(G) - n_\Delta(G) \geq 1 - n$, and this lower bound is attained only for cliques.

For the upper bound, let us first show that it is not reached when G is isomorphic to P_n. This follows from the fact that $\rho(P_n) - n_\Delta(P_n) = \frac{n}{2} - (n-2) \leq 0 < \frac{n^2-3n}{2(n-1)}$.

If G is not isomorphic to P_n, then Lemma 4.1 and the inequaly $n_\Delta(G) \geq 1$ give

$$\rho(G) - n_\Delta(G) \leq \frac{n^2 - n - 2}{2(n-1)} - 1 = \frac{n^2 - 3n}{2(n-1)}.$$

It is easy to verify that this bound is attained for G equal to $CO_{n,3}$ or $KI_{n,3}$. □

5 Average eccentricity and average distance

Lemma 5.1 *Let T be a tree of order n and let $P = (v_0, v_1, \cdots, v_{D(T)})$ be a path of length $D(T)$ in T. If there is $j \leq \frac{D(T)}{2}$ such that the degree of v_k is at most 2 for $k \geq j+1$, then $\epsilon(T) - \mu(T) \leq \epsilon(P_n) - \mu(P_n)$.*

Proof. Let $\ell = D(T)$ and suppose T is not the path P_n. Let w be a leaf in T different from v_0 and v_ℓ, and let T' be the graph obtained from T by deleting the edge incident to w and adding an edge between w and v_ℓ. Note that it follows from the assumptions that $d_T(v_\ell, w) \geq \frac{\ell}{2} + 1$. It is now sufficient to prove that $\epsilon(T) - \mu(T) \leq \epsilon(T') - \mu(T')$ since we can then repeat this transformation until we obtain the path P_n.

Clearly, T' has diameter $\ell+1$ and $\epsilon(v)$ is increased by 1 unit for at least $n - \frac{\ell+1}{2}$ vertices v in T. Hence,

$$\epsilon(T') \geq \epsilon(T) + \frac{2n-\ell-1}{2n}. \tag{1}$$

To measure the difference between $\mu(T')$ and $\mu(T)$, first notice that

$$\begin{aligned}
\mu(T) &= \frac{1}{n(n-1)} \sum_{v \in V} \sigma_T(v) = \frac{1}{n(n-1)}(\sigma_T(w) + \sum_{v \neq w} \sigma_T(v)) \\
&= \frac{1}{n(n-1)}(\sigma_T(w) + \sum_{v \neq w} \left(d_T(v,w) + \sum_{u \neq v,w} d_T(v,u) \right) \\
&= \frac{1}{n(n-1)}(2\sigma_T(w) + \sum_{v \neq w} \sum_{u \neq v,w} d_T(v,u))
\end{aligned}$$

Similarly, we get

$$\mu(T') = \frac{1}{n(n-1)}(2\sigma_{T'}(w) + \sum_{v \neq w} \sum_{u \neq v,w} d_{T'}(v,u)).$$

Since $\sum_{v \neq w} \sum_{u \neq v,w} d_T(v,u)) = \sum_{v \neq w} \sum_{u \neq v,w} d_{T'}(v,u)$, we have

$$\mu(T') = \mu(T) + \frac{2(\sigma_{T'}(w) - \sigma_T(w))}{n(n-1)}. \tag{2}$$

By construction, we have $\sigma_{T'}(w) = \sigma_T(v_\ell) - d_T(v_\ell, w) + n - 1$, and since $d_T(v_\ell, w) \geq \frac{\ell}{2} + 1$, we have:

$$\begin{aligned}
2(\sigma_{T'}(w) - \sigma_T(w)) &\leq 2(\sigma_T(v_\ell) - \tfrac{\ell}{2} + n - 2 - \sigma_T(w)) \\
&= 2n - 4 - \ell + 2(\sigma_T(v_\ell) - \sigma_T(w)). \qquad (3)
\end{aligned}$$

In T, v_ℓ is at distance at most ℓ from the vertices outside P, and at distance $\ell - i$ from v_i $(i = 1, \cdots, \ell-1)$. Hence,

$$\sigma_T(v_\ell) \leq \frac{\ell(\ell-1)}{2} + \ell(n-\ell) = n\ell - \frac{\ell^2}{2} - \frac{\ell}{2}. \tag{4}$$

If w is adjacent to a vertex in P, then it is at distance at least two from the vertices outside P and the sum of the distances from w to the vertices in P is minimized when w is adjacent to $v_{\lfloor \frac{\ell}{2} \rfloor}$. In such a case, we therefore have

$$\begin{aligned}
\sigma_T(w) &\geq \frac{(\lfloor \frac{\ell}{2} \rfloor + 1)(\lfloor \frac{\ell}{2} \rfloor + 2) + (\lceil \frac{\ell}{2} \rceil + 1)(\lceil \frac{\ell}{2} \rceil + 2)}{2} - 1 + 2(n - \ell - 2) \\
&\geq (\frac{\ell}{2} + 1)(\frac{\ell}{2} + 2) - 1 + 2(n - \ell - 2) \\
&= 2n + \frac{\ell^2}{4} - \frac{\ell}{2} - 3. \qquad (5)
\end{aligned}$$

This is the best possible lower bound on $\sigma_T(w)$ because if w is not adjacent to a vertex in P, then the bound increases by ℓ units since the distance from w to the $\ell+1$ vertices in P increases by one unit for each of them, while the distance from w to its neighbour outside P decreases from 2 to 1.

Putting together (2) to (5), we get

$$\begin{aligned}
\mu(T') - \mu(T) &= \frac{2(\sigma_{T'}(w) - \sigma_T(w))}{n(n-1)} \\
&\leq \frac{2n - 4 - \ell + 2(\sigma_T(v_\ell) - \sigma_T(w))}{n(n-1)}
\end{aligned}$$

$$\begin{aligned} &\leq \frac{2n-4-\ell+2\Big((n\ell-\frac{\ell^2}{2}-\frac{\ell}{2})-(2n+\frac{\ell^2}{4}-\frac{\ell}{2}-3)\Big)}{n(n-1)} \\ &= \frac{-4n-2\ell+4-3\ell^2+4n\ell}{2n(n-1)}. \end{aligned} \tag{6}$$

We therefore get from (1) and (6)

$$\begin{aligned} (\epsilon(T')-\mu(T'))-(\epsilon(T)-\mu(T)) &\geq \frac{2n-\ell-1}{2n}-\frac{-4n-2\ell+4-3\ell^2+4n\ell}{2n(n-1)} \\ &= \frac{2n^2-5\ell n+n+3\ell^2+3\ell-3}{2n(n-1)}. \end{aligned}$$

It remains to show that $F(\ell)=2n^2-5\ell n+n+3\ell^2+3\ell-3\geq 0$. Since F is a quadratic convex function, it reaches its minimum value when its derivative equals 0, which means that $-5n+6\ell+3=0$, i.e., $\ell=\frac{5n-3}{6}$. It can be checked that $F(\frac{5n-3}{6})=\frac{31}{3}n^2-9n-4>0$ for all $n\geq 2$. □

Theorem 5.1 *Let T be a tree of order n. Then*

$$\epsilon(T)-\mu(T)\leq\frac{5n-10}{12}-\frac{n \bmod 2}{4n}.$$

Moreover, the bound is reached if and only if T is the path P_n.

Proof. We follow a similar proof as the one used in [30] for determining an upper bound on $\epsilon(T)-\rho(T)$.

Let T be a tree which maximizes the difference $\epsilon(T)-\mu(T)$. Assume, by contradiction, that T is not the path P_n. Let $P=(v_0,v_1,\cdots,v_{D(T)})$ be a longest path in T. Let G_i be the connected component of $T\setminus P$ rooted in v_i, and let V_i be the vertex set of G_i. We know from Lemma 5.1 that there are two vertices v_j and v_k on P of degree at least 3 such that $j\leq\frac{D(T)}{2}<k$. Let us choose such a pair of vertices on P with minimum value $k-j$. Let w_j be a neighbor of v_j outside P, and let w_k be a neighbor of v_k outside P. Let T' be the tree obtained from T as follows:

- for every $w\neq w_j,v_{j+1}$ adjacent to v_j, remove the edge v_jw and add the edge w_jw;
- for every $w\neq w_k,v_{k-1}$ adjacent to v_k, remove the edge v_kw and add the edge w_kw.

Note that the diameter of T' is two units larger than the diameter of T. Now, let

$$\begin{aligned} V'_j &= \{v\in V_j : d_T(v,w_j)<d_T(v,v_j)\}, \\ V'_k &= \{v\in V_k : d_T(v,w_k)<d(v,v_k)\}. \end{aligned}$$

Consider the following partition of the vertices of T

$$\begin{aligned} X_1 &= V_0\cup\ldots\cup V_{j-1}\cup(V_j\setminus(V'_j\cup\{v_j\}), \\ X_2 &= V'_j, \\ X_3 &= \{v_j\}\cup V_{j+1}\cup\ldots\cup V_{k-1}\cup\{v_k\}, \\ X_4 &= V'_k, \\ X_5 &= (V_k\setminus(V'_k\cup\{v_k\})\cup V_{j+1}\cup\ldots\cup V_{D(T)}. \end{aligned}$$

Let $x_i=|X_i|$. We clearly have $\epsilon_{T'}(v)=\epsilon_T(v)+1$ for every vertex in $X_2\cup X_3\cup X_4$, while $\epsilon_{T'}(v)=\epsilon_T(v)+2$ for every vertex in $X_1\cup X_5$. Hence

$$\epsilon(T')=\epsilon(T)+\frac{\phi}{n}$$

where $\phi = 2x_1 + x_2 + x_3 + x_4 + 2x_5$. Let us now analyze how the average distance varies when transforming T to T'. If $v \in X_1$, then

$$d_{T'}(v,u) - d_T(v,u) = \begin{cases} 0 & \text{if } u \in X_1 \\ -1 & \text{if } u \in X_2 \\ 1 & \text{if } u \in X_3 \cup X_4 \\ 2 & \text{if } u \in X_5. \end{cases}$$

Hence, $\sigma_{T'}(v) = \sigma_T(v) + \tau_1$ for all $v \in X_1$, where $\tau_1 = -x_2 + x_3 + x_4 + 2x_5$.

If $v \in X_2$, then

$$d_{T'}(v,u) - d_T(v,u) = \begin{cases} -1 & \text{if } u \in X_1 \\ 0 & \text{if } u \in X_2 \cup X_3 \cup X_4 \\ 1 & \text{if } u \in X_5. \end{cases}$$

Hence, $\sigma_{T'}(v) = \sigma_T(v) + \tau_2$ for all $v \in X_2$, where $\tau_2 = -x_1 + x_5$.

If $v \in X_3$, then

$$d_{T'}(v,u) - d_T(v,u) = \begin{cases} 1 & \text{if } u \in X_1 \cup X_5 \\ 0 & \text{if } u \in X_2 \cup X_3 \cup X_4. \end{cases}$$

Hence, $\sigma_{T'}(v) = \sigma_T(v) + \tau_3$ for all $v \in X_3$, where $\tau_2 = x_1 + x_5$.

By symmetry, we also have $\sigma_{T'}(v) = \sigma_T(v) - \tau_4$ for all $v \in X_4$ and $\sigma_{T'}(v) = \sigma_T(v) - \tau_5$ for all $v \in X_5$, where $\tau_4 = x_1 - x_5$ and $\tau_5 = 2x_1 + x_2 + x_3 - x_4$.

We thus have

$$n(n-1)\mu(T') = \sum_{i=1}^{5} \sum_{v \in X_i} \sigma_{T'}(v) = \sum_{i=1}^{5} \sum_{v \in X_i} (\sigma_T(v) + \tau_i) = n(n-1)\mu(T) + \sum_{i=1}^{5} x_i \tau_i.$$

Notice that $(n-1)\phi - n\tau_1 = (2n-2)x_1 + (2n-1)x_2 - x_3 - x_4 - 2x_5 > 0$ because x_3, x_4, x_5 are at most equal to $n-4$, while x_1 and x_2 are at least equal to 1. Similarly $(n-1)\phi - n\tau_i > 0$ for $i = 2, 3, 4, 5$. Hence

$$(\epsilon(T') - \mu(T')) - (\epsilon(T) - \mu(T)) = \frac{\phi}{n} - \frac{\sum_{i=1}^{5} x_i \tau_i}{n(n-1)} > \frac{\phi}{n} - \frac{\sum_{i=1}^{5} x_i \phi}{n^2} = 0$$

which contradicts that fact that T maximizes the difference $\epsilon(T) - \mu(T)$.

Hence the path P_n maximizes $\epsilon(T) - \mu(T)$ among all trees T and it is not difficult to check that $\epsilon(P_n) - \mu(P_n) = \frac{5n-10}{12} - \frac{n \mod 2}{4n}$. □

6 The chromatic number and the maximum degree frequency

Theorem 6.1 *Let G be a connected graph of order $n \geq 3$. Then.*

$$\begin{cases} 2-n & \text{if } n \text{ is even,} \\ 3-n & \text{if } n \text{ is odd} \end{cases} \leq \chi(G) - n_\Delta(G) \leq n-2.$$

Moreover, the lower bound is reached, for example, by the cycle C_n as well as by the regular bipartite graphs. The upper bound is reached if and only if G is a kite $KI_{n,n-1}$.

Proof. Since $\chi(G) \geq 2$ and $n_\Delta(G) \leq n$, we clearly have $\chi(G) - n_\Delta(G) \geq 2 - n$. This lower bound is clearly only reached by bipartite regular graphs, which means that n must be even. Hence, if n is odd, then $\chi(G) - n_\Delta(G) \geq 3 - n$. The bound is then reached, for example by the cycle C_n.

We now prove the upper bound $n-2$ is valid and can only be reached if $G = KI_{n,n-1}$. If $\chi(G) = n$, then G is a clique and $n_\Delta(G) = n$, which means that $\chi(G) - n_\Delta(G) = 0 < n-2$. Also, if $\chi(G) \neq n-1$ or $n_\Delta(G) \neq 1$, then $\chi(G) - n_\Delta(G) < n-2$. So assume $\chi(G) = n-1$ and $n_\Delta(G) = 1$. We then know that G

is not the cycle C_n. Since G is not a clique, Brook's theorem [10] implies $n-1=\chi(G)\le\Delta(G)$. Hence, G contains a dominating vertex v.

Let G' be the induced subgraph obtained by removing v from G. Clearly, $\chi(G')=n-2$. Hence, G' is not the cycle C_{n-1} since we would have $\chi(G')=2<n-2$ if $n=5$, and $\chi(G')=3<n-2$ if $n>5$. Also, since $n_\Delta(G)=1$, we necessarily have $\Delta(G')\le n-3$, which implies that G' is not a clique. If G' is connected, then we can again apply Brook's theorem, and we get $\chi(G')\le\Delta(G')\le n-3$, a contradiction. So assume G' is not connected.

Let $H_1,...,H_r$ denote the connected components of G'. We then have

$$n-1=\chi(G)=\max_i\ \chi(H_i)+1.$$

Hence, there is a connected component H_i such that $\chi(H_i)=n-2$. But since every H_i contains at most $n-2$ vertices, we deduce that G' contains only two connected components, one being a clique or order $n-2$, and the other one an isolated vertex. But this implies that $G=KI_{n,n-1}$. □

7 The stability number and the minimum degree frequency

Theorem 7.1 *Let G be a connected graph of order $n\ge5$. Then*

$$1-n\le\alpha(G)-n_\delta(G)\le n-3.$$

Moreover, the lower bound is reached if and only if G is a clique, while the upper bound is reached, for example, by $K_{2,n-2}-e$.

Proof. Since $\alpha(G)\ge1$ and $n_\delta(G)\le n$, we clearly have $\alpha(G)-n_\delta(G)\ge1-n$, and this bound is only reached if G is a clique. Let us now prove that the upper bound is valid. Since G is connected, we have $\alpha(G)\le n-1$, and this bound is attained only for $G=S_n$. In such a case, $\alpha(S_n)-n_\delta(S_n)=0<n-3$. So assume $\alpha(G)\le n-2$. We then have $\alpha(G)-n_\delta(G)\le n-3$. The bound is reached for, example, by $G=K_{2,n-2}-e$. □

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