Les Cahiers du GERAD ISSN: 0711–2440

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G–2014–68

September 2014

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Abstract: Proximity π and remoteness ρ are respectively the minimum and the maximum, over the vertices of a connected graph, of the average distance from a vertex to others. The distance spectral radius ∂_1 of a connected graph is the largest eigenvalue of its distance matrix. In the present paper, we are interested in a comparison between the proximity and the remoteness of a simple connected graph on the one hand and its distance eigenvalues on the other hand. We prove, among other results, lower and upper bound on the distance spectral radius using proximity and remotemess, and lower bounds on $\partial_1 - \pi$ and on $\partial_1 - \rho$. In addition, several conjectures, obtained with the help of the system AutoGraphiX, are formulated.

Key Words: Distance matrix, eigenvalues, proximity, remoteness, conjectures.

Résumé : La proximité π et l'éloignement ρ sont respectivement le minimum et le maximum, pour les sommets d'un graphe connexe, de la distance moyenne d'un sommet vers les autres. Le rayon spectral des distances ∂_1 d'un graphe connexe est la plus grande valeur propre de sa matrice des distances. Dans le présent article, nous nous intéressons à une comparaison entre la proximité et l'éloignement d'un graphe connexe d'une part et ses valeurs propres des distances d'autre part. Nous prouvons, entre autres résultats, des bornes inférieure et supérieure sur le rayon spectral des distances, en fonction de la proximité et de l'éloignement, et des bornes inférieures sur $\partial_1 - \pi$ et sur $\partial_1 - \rho$. De plus, nous proposons plusieurs conjectures obtenues avec l'aide d'AutoGraphiX.

Mots clés : Matrice des distances, valeurs propres, proximité, éloignement, conjectures.

1 Introduction

Let $G = (V, E)$ denote a simple and connected graph, with vertex set V and edge set E, containing $n = |V|$ vertices and $m = |E|$ edges. All the graphs considered in the present paper are finite, simple and connected. 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 $\overline{\ell}$. 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 ecc. That is

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

The *proximity* π of G is the minimum average distance from a vertex of G to all others. Similarly, the *remoteness* ρ of G is the maximum average distance from a vertex to all others. The two last concepts were introduced in [1, 4]. They are close to the concept of transmission $t(v)$ of a vertex v, which is the sum of the distances from v to all others. That is, if we denote $\tilde{t}(v)$ the average distance from a vertex v to all other vertices in G, we have

$$\pi = \min_{v\in V} \tilde{t}(v) = \min_{v\in V} \frac{t(v)}{n-1} \qquad \text{and} \qquad \rho = \max_{v\in V} \tilde{t}(v) = \max_{v\in V} \frac{t(v)}{n-1}.$$

The transmission of a vertex is also known as the *distance* of a vertex [16] and the minimum distance (transmission) of a vertex is studied in [31]. A notion very close to the average distance from a vertex is the *vertex deviation* introduced by Zelinka [42] as

$$m_1(v) = \frac{1}{n}\sum_{u\in V} d(u, v) = \frac{t(v)}{n}.$$

The vector composed of the vertex transmissions in a graph was first introduced by Harary [22] in 1959, under the name *status* of a graph, as a measure of the "weights" of individuals in social networks. The same vector was called *the distance degree sequence* by Bloom, Kennedy and Quintas [10]. It was used to tackle the problem of graph isomorphism. Randić [32] conjectured that two graphs are isomorphic if and only if they have the same distance degree sequence. The conjecture was refuted by several authors such as Slater [37], Buckley and Harary [11], and Entringer, Jackson and Snyder [16]. The transmission of a graph was also introduced by Sabidussi [34] in 1966 as a measure of *centrality* in social networks. The notion of centrality is widely used in different branches of sciences (see for example [27] and the references therein) such as transportation–network theory, communication network theory, electrical circuits theory, psychology, sociology, geography, game theory and computer science. Notions closely related to that of the distance from a vertex are those of *a center* and *a centroid* already introduced by Jordan [26] in 1869. For mathematical properties of these two concepts see the survey [38], as well as the references therein. In 1964, Hakimi [21] used for the first time the sum of distances in solving facility location problems. In fact, Hakimi [21] considered two problems, subsequently considered in many works: the first problem was to determine a vertex $u \in V$ so as to minimize $max_{v\in V}\{d(u, v) : u \in V\}$, *i.e.*, the center of a graph; and the second problem is to determine a vertex $u \in V$ so as to minimize the sum of distances from u, *i.e.*, the centroid. Interpretations of these problems can be found, for instance, in [18]. In view of the interest of the transmission vector in different domains of sciences, it is natural to study the properties of its extremal values themselves, and among the set of graph parameters. A direct study of the minimum and the maximum values of the transmission is not adequate since they do not have the same order of magnitude as the majority of the distance graph parameters. Proximity and remoteness appear to be more convenient than minimum and maximum transmissions in comparisons with other metric invariants, such as the diameter, radius, average eccentricity and average distance, as they have the same order of magnitude when viewed as functions of the order n of G. Indeed, it follows from the definitions that

$$\pi \le r \le ecc \le D, \qquad \pi \le \overline{\ell} \le \rho \le D,$$

where $\overline{\ell}$ denotes the average distance, *i.e.*,

$$\overline{\ell} = \frac{1}{n(n-1)} \sum_{(u,v)\in V\times V} d(u,v) = \frac{1}{n(n-1)} \sum_{v\in V} t(v).$$

Since their introduction in [1, 4] and the first studies of their properties [7, 8], proximity and remoteness attracted the attention of several authors. In [35], Sedlar *et al.* proved a series of AutoGraphiX (a software devoted to conjecture–making in graph theory, see [1, 2, 12, 13]) conjectures in two of which remoteness ρ is involved. Those results are gathered in the next theorem. First, recall the following defintions. The (*vertex*) *connectivity* ν of a connected graph G is the minimum number of vertices whose removal disconnects G or reduces it to a single vertex. The *algebraic connectivity* a of a graph G is the second smallest eigenvalue of its Laplacian $L = Diag - A$, where $Diag$ is the diagonal square matrix indexed by the vertices of G whose diagonal entries are the degrees in G, and A is the adjacency matrix of G.

Theorem 1.1 ([35]) *Let G be a connected graph on $n \geq 2$ vertices with vertex connectivity ν, algebraic connectivity a and remoteness ρ. Then*

$$\nu \cdot \rho \leq n - 1$$

with equality if and only if G is the complete graph K_n; and

$$a \cdot \rho \leq n$$

with equality if and only if G is the complete graph K_n. Moreover, if G is not complete, then

$$a \cdot \rho \leq n - 1 - \frac{1}{n-1}$$

with equality if and only if $G \cong K_n - M$, where M is any non empty set of disjoint edges.

Ma, Wu and Zhang [29] proved an AutoGraphiX conjecture that consists of an upper bound on $ecc - \pi$ together with the corresponding extremal graphs.

Theorem 1.2 ([29]) *For a connected graph G on $n \geq 3$ vertices,*

$$ecc - \pi \leq \begin{cases} \frac{(3n+1)(n-1)}{4n} - \frac{n+1}{4} & \text{if } n \text{ is odd,} \\ \frac{n-1}{2} - \frac{n}{4(n-1)} & \text{if } n \text{ is even,} \end{cases}$$

with equality if and only if G is the path P_n.

Sedlar [36] studied three AutoGraphiX conjectures involving proximity and remoteness. She solved the conjecture stated in the following theorem.

Theorem 1.3 ([36]) *Among all connected graphs G on $n \geq 3$ vertices with average distance $\overline{\ell}$ and proximity π, the difference $\overline{\ell} - \pi$ is maximum for a graph G composed of three paths of almost equal lengths with a common end point.*

Sedlar [36] also proved partial results related to another conjecture: while the conjecture is stated for all connected graphs, the results are proved for trees only.

Theorem 1.4 ([36]) *Among all trees on $n \geq 3$ vertices, the difference $ecc - \pi$ is maximum for the path P_n.*

A *Soltés* or *path-complete* graph [39] is the graph obtained from a clique and a path by adding at least one edge between an endpoint of the path and the clique. The Soltés graphs are known to maximize the average distance $\overline{\ell}$ when the number of vertices and of edges are fixed [39].

Finally, Wu and Zhang [41] proved the following two theorems, first conjectured in [8].

Theorem 1.5 ([41]) *Among all connected graphs G on $n \geq 3$ vertices with average distance $\overline{\ell}$ and remoteness ρ, the Soltés graphs with diameter $\lfloor (n+1)/2 \rfloor$ maximize the difference $\rho - \overline{\ell}$.*

Theorem 1.6 ([41]) *Let G be a connected graph on $n \geq 3$ vertices with remoteness ρ and radius r. Then*

$$\rho - r \geq \begin{cases} \frac{3-n}{4} & \text{if } n \text{ is odd} \\ \frac{n^2}{4n-4} - \frac{n}{2} & \text{if } n \text{ is even.} \end{cases}$$

The inequality is best possible as shown by the cycle C_n if n is even and by the graph composed of the cycle C_n together with two crossed edges on four successive vertices of the cycle.

Note that Sedlar [36] proved the above theorem for the class of trees on an odd number of vertices.

Recently, Hua and Das [24] proved two AutoGraphiX conjectures involving proximity and remoteness in graphs, and refuted two other conjectures. Further results involving the girth of a graph in addition to proximity and remoteness are proved in [5].

The distance eigenvalues of a connected graph, denoted by $\partial_1, \partial_2, \ldots, \partial_n$, are those of its distance matrix, and are indexed such that $\partial_1 \geq \partial_2 \geq \ldots \geq \partial_n$. The interest in the spectral properties of the distance matrix of a graph began during the 70's with the appearance of the paper [20] by Graham and Pollack. In that paper the authors established a relationship between the number of negative eigenvalues of the distance matrix and the addressing problem in data communication systems. In the same paper [20], it was proved that the determinant of the distance matrix of a tree is function of the number vertices only.

Theorem 1.7 ([20]) *If T is a tree on $n \geq 2$ vertices with distance matrix $\mathcal{D}$, then*

$$det(\mathcal{D}) = (-1)^{n-1}(n-1)2^{n-2}.$$

This impressive result made distance matrix spectral properties a research subject of great interest. The generalization of the above theorem for general graphs is that the determinant of the distance matrix depends only on the *blocks* of the graph. This generalization was first conjectured by Hosoya, Murakami and Gotoh [23] and then proved by Graham, Hoffman and Hosoya [19]. Therefore, the interest extended to the study of the eigenvalues of the distance matrix. In [30], Merris studied the distance spectrum of a tree with a given number of vertices. In order to estimate the distance eigenvalues of a tree on n vertices and $m = n - 1$ edges, he associated the matrix $K = K(T) = Q^TQ = 2I_m + A(T^*)$ to the tree T, where Q is the incidence matrix of T (arbitrarily oriented), I_m is the unit $m \times m$–matrix, and $A(T^*)$ denotes the adjacency matrix of the line graph T^* of T. Note the similarity between the matrix K and the Laplacian of T defined by $L(T) = QQ^T = Diag(T) - A(T)$. The main result proved in [30] is the following:

Theorem 1.8 ([30]) *Let T be a tree. Then the eigenvalues of $-2K^{-1}$ interlace the distance eigenvalues of T.*

A *pendent vertex* (also written *pendant vertex*) of T is a vertex of degree 1. A *pendent neighbor* is a vertex adjacent to a pendent vertex. Suppose T has n_1 pendent vertices and n'_1 pendent neighbors. A series of corollaries for Theorem 1.8 were proved and they are gathered below.

Corollary 1.9 ([30]) *Let T be a tree with n_1 pendent vertices and n'_1 pendent neighbors.*

- *Let ∂ be a distance eigenvalue of T of multiplicity k. Then $k \leq n_1$.*
- *Among the distance eigenvalues of T, $\partial = -2$ occurs with multiplicity at least $n_1 - n'_1 - 1$.*
- *If D denotes the diameter of T, then*

$$\begin{aligned}
(i) &\qquad \partial_n \leq \frac{-1}{1 - \cos\left(\frac{\pi}{D+1}\right)}; \\
(ii) &\qquad \partial_{\lfloor \frac{D}{2} \rfloor} > -1; \\
(iii) &\qquad \partial_{n'_1} > -1 \qquad \textit{(provided } n > 2n'_1\textit{);} \\
(iv) &\qquad \partial_{n-n'_1+2} < -2; \\
(v) &\qquad \partial_{n_1} \geq -2; \\
(vi) &\qquad \partial_{n-n_1+2} \leq -2.
\end{aligned}$$

The second point of the above corollary was improved by Collins [14].

Theorem 1.10 ([14]) *Let T be a tree with n_1 pendent vertices and n'_1 pendent neighbors. Then, among the distance eigenvalues of T, $\partial = -2$ occurs with multiplicity at least $n_1 - n'_1$.*

The problem of bounding the largest distance eigenvalue is, in some way, a recent research subject. Actually, first bounds on ∂_1 go back to the paper [33] by Ruzieh and Powers in 1990. The next theorem is among the results proved in that paper.

Theorem 1.11 ([33]) *If G is a graph of order n, then $n-1 \leq \partial_1(G) \leq \partial_1(P_n)$. Moreover, the lower bound is reached if and only if G is the complete graph K_n, and the upper is reached if and only if G is the path P_n.*

Ruzieh and Powers [33] also computed the spectrum as well as the eigenspaces of the distance matrix of the path P_n.

Since then, many researchers were interested in bounding the largest distance eigenvalue of a graph, and many results related to the distance spectra of graphs are established in the graph theory literature. For more details about these results see the surveys [6] and [40] as well as the references therein.

Recently, graphs with at least three distance eigenvalues less than -1 were studied in [28]. Among other results in [28], it is shown that $\partial_{n-1} \leq -1$ for all $n \geq 4$ and $\partial_{n-2} \leq -1$ for all $n \geq 7$, also all graphs with $\partial_{n-1} = -1$ were characterized.

In the present paper, we are interested in a comparison between the proximity π and the remoteness ρ of simple connected graph on the one hand and its distance eigenvalues on the other hand. In the next section, we prove some results first conjectured using the AutoGraphiX system.

2 Results

In this section, we compare, for a given connected graph with a fixed number of vertices n, the proximity π and the remoteness ρ, on the one hand, and the distance eigenvalues ∂_1, ∂_2 and ∂_n, on the other hand.

Our first result is a series of inqualities ordering π, ℓ, $\partial_1/(n-1)$ and ρ. Before the statement of these results, recall the following definition. We say that G is a k–transmission regular graph if $t(v) = k$ for every $v \in V$. Note that there exist graphs which are transmission regular but not (degree) regular. Indeed, the graph on 9 vertices illustrated in Figure 1 is 14–transmission regular but not degree regular, and it is the smallest graph wiht this property. For more examples of transmission regular but not degree regular graphs see [9, 3].

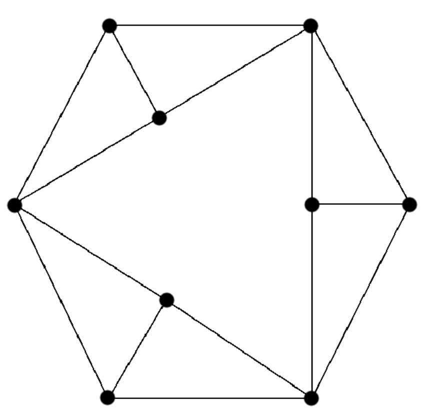

Figure 1: The smallest transmission regular but not degree regular graph.

Theorem 2.1 *Let G be a graph on $n \geq 4$ vertices with largest distance eigenvalue ∂_1, proximity π and remoteness ρ. Then*

$$\pi \leq \overline{\ell} \leq \frac{\partial_1}{n-1} \leq \rho$$

with equalities if and only if G is a transmission regular graph.

Proof. Since the distance matrix is irreducible, then from matrix theory (see, e.g., [17, p. 63]), we have

$$\min_{v\in V} \ t(v) \quad \leq \quad \frac{1}{n}\sum_{v\in V} t(v) \quad \leq \quad \partial_1 \quad \leq \quad \max_{v\in V} \ t(v).$$

Introducing π, ρ and $\overline{\ell}$, we have

$$(n-1)\cdot\pi \quad \leq \quad (n-1)\overline{\ell} \quad \leq \quad \partial_1 \quad \leq \quad (n-1)\cdot\rho$$

and the inequalities follow.

Equalities hold if and only if $t(v) = (n-1)\pi = (n-1)\rho$ for every vertex v in G, *i.e.*, if G is a transmission regular graph. □

The above theorem is very easy to prove, so its interest is more in the corollaries that we can derive than in its proof. The first of these corollaries is a lower bound on the difference between the distance spectral radius and the proximity, $\partial_1 - \pi$, of a graph on a give number of vertices n.

Corollary 2.2 *Let G be a graph on $n \geq 2$ vertices with largest distance eigenvalue ∂_1 and proximity π. Then*

$$\partial_1 - \pi \geq n-2$$

with equalities if and only if G is the complete graph K_n.

Proof. Using the inequality of Theorem 2.1, we have

$$\partial_1 - \pi \geq (n-1)\pi - \pi = (n-2)\pi \geq n-2.$$

Equality holds if and only if $\pi = 1$ and the graph is transmission regular. The only transmission regular graph with $\pi = 1$ is the complete graph K_n. □

The second corollary is a lower bound on the sum of the remoteness and the second largest distance eigenvalue, $\rho + \partial_2$, of a graph with given number of vertices n.

Corollary 2.3 *Let G be a graph on $n \geq 4$ vertices with second largest distance eigenvalue ∂_2 and remoteness ρ. Then*

$$\rho + \partial_2 \geq 0$$

with equality if and only if G is the complete graph K_n.

Proof. If $\partial_2 \geq 0$, the inequality is trivial. Thus, assume that $\partial_2 \leq 0$.

Since all diagonal entries of $\mathcal{D}$ are zeros, we have $\partial_1 + \partial_2 + \cdots + \partial_n = 0$. Therefore

$$-\partial_2 \leq \frac{\partial_1}{n-1}.$$

Now, using Theorem 2.1, we have

$$-\partial_2 \leq \frac{\partial_1}{n-1} \leq \rho.$$

Equality holds if and only if $\partial_2 = \partial_3 = \cdots = \partial_n = -\partial_1/(n-1)$, *i.e.*, the distance matrix $\mathcal{D}$ has exactly two distinct eigenvalues. The only graph with this property is the complete graph K_n (see [25]). □

The bound in the above corollary is best possible among the bounds of the form $\rho+\partial_k \geq 0$, with a fixed integer k, over the class of all connected graphs. Indeed, if we consider the complete bipartite graphs $K_{\lfloor n/2\rfloor,\lceil n/2\rceil}$, on $n \geq 3$, we get

$$\rho(K_{\lfloor n/2\rfloor,\lceil n/2\rceil}) + \partial_3(K_{\lfloor n/2\rfloor,\lceil n/2\rceil}) = \begin{cases} -\frac{1}{2} & \text{if } n \text{ is odd,} \\ -\frac{1}{2} - \frac{1}{2(n-1)} & \text{if } n \text{ is even,} \end{cases}$$

which is negative for $n \geq 3$. However, all the graphs with $\rho + \partial_k < 0$, obtained after computer experiments with AutoGraphiX, have diameter $D = 2$. Therefore we suggest the following conjecture.

Conjecture 2.4 *Let G be a graph on $n \geq 4$ vertices with diameter $D \geq 3$, remoteness ρ and distance eigenvalues $\partial_1 \geq \partial_2 \geq \cdots \partial_n$. Then*

$$\rho + \partial_3 > 0.$$

If true, the bound in the above corollary is best possible among the bounds of the form $\rho + \partial_k \geq 0$, with a fixed integer k, over the class of all connected graphs with diameter $D \geq 3$. Indeed, if we consider the graph $K^*_{\lfloor n/2\rfloor,\lceil n/2\rceil}$, with diameter $D = 3$, obtained from the complete bipartite graph $K_{\lfloor n/2\rfloor,\lceil n/2\rceil}$, on $n \geq 3$ by deleting an edge, we get

$$\rho(K^*_{\lfloor n/2\rfloor,\lceil n/2\rceil}) + \partial_4(K^*_{\lfloor n/2\rfloor,\lceil n/2\rceil}) = \begin{cases} -\frac{1}{2} + \frac{2}{n-1} & \text{if } n \text{ is odd,} \\ -\frac{1}{2} + \frac{3}{2(n-1)} & \text{if } n \text{ is even,} \end{cases}$$

which is negative for $n \geq 6$. However, if we express k as a function of the diameter, we can strengthen Corollary 2.12, over the class of trees. Indeed, using Theorem 1.8, particularly the inequality $\partial_{\lfloor \frac{D}{2} \rfloor} > -1$, we straightaway get the following result.

Proposition 2.5 *Let T be a tree on $n \geq 4$ vertices with proximity π, diameter D and distance spectrum $\partial_1 \geq \partial_2 \geq \cdots \geq \partial_n$. Then*

$$\rho + \partial_{\lfloor \frac{D}{2} \rfloor} > 0.$$

Note that the inequality in the above propostion can potentially be improved. Experiments using the AutoGraphiX system led to the following conjecture.

Conjecture 2.6 *Let G be a graph on $n \geq 4$ vertices with diameter D, remoteness ρ and distance spectrum $\partial_1 \geq \partial_2 \geq \cdots \geq \partial_n$. Then*

$$\pi + \partial_{\lfloor \frac{7D}{8} \rfloor} > 0.$$

Note that there exist graphs with $\pi + \partial_{\lfloor \frac{7D}{8} \rfloor + 1} < 0$, such as the paths P_8 and P_9.

Returning to the corollaries of Theorem 2.1, we give the following upper bound on the sum of the proximity and the smallest distance eigenvalue, $\pi + \partial_n$, of a graph with a given number of vertices n.

Corollary 2.7 *Let G be a graph on $n \geq 4$ vertices with second largest distance eigenvalue ∂_2 and proximity π. Then*

$$\pi + \partial_n \leq 0$$

with equality if and only if G is the complete graph K_n.

Proof. The least distance eigenvalue ∂_n is at most the average of the negative distance eigenvalues. Thus

$$-\partial_n \;\geq\; \frac{1}{p^-}\sum_{\partial_i > 0} \partial_i \;\geq\; \frac{\partial_1}{p^-} \;\geq\; \frac{\partial_1}{n-1} \;\geq\; \pi$$

where p^- denotes the number of negative eigenvalues of the distance matrix $\mathcal{D}$.

Equality holds if and only if $\partial_2 = \partial_3 = \cdots = \partial_n = -\partial_1/(n-1)$, *i.e.*, the distance matrix $\mathcal{D}$ has exactly two distinct eigenvalues. The only graph with this property is the complete graph K_n (see [25]). □

Theorem 2.8 *Let G be a graph on $n \geq 4$ vertices with largest distance eigenvalue ∂_1 and remoteness ρ. Then*

$$\partial_1 - \rho \geq n - 2$$

with equalities if and only if G is the complete graph K_n.

Proof. Assume, without loss of generality, that the vertices of G are indexed such that $t(v_1) = \max\{t(v),\ v \in V\} = (n-1)\rho$. Let $\mathbb{1}$ denote the all 1's vector. Then

$$\begin{aligned}
\mathbb{1}^T \mathcal{D} \mathbb{1} &= \sum_{1 \leq i,j \leq n} d(v_i, v_j) = 2t_1 + \sum_{2 \leq i,j \leq n} d(v_i, v_j) \\
&= 2(n-1)\rho + \sum_{2 \leq i,j \leq n} d(v_i, v_j) \\
&\geq 2(n-1)\rho + (n-1)(n-2) = n\rho + n(n-2) + (n-2)(\rho - 1) \\
&\geq n\rho + n(n-2).
\end{aligned}$$

Now, applying Rayleigh quotient, we have

$$\partial_1 = \max_{x \neq 0} \frac{x^T \mathcal{D} x}{x^T x} \geq \frac{\mathbb{1}^T \mathcal{D} \mathbb{1}}{\mathbb{1}^T \mathbb{1}} \geq \rho + n - 2.$$

Therefore, the inequality follows.

From the previous inequalities, equality holds if and only if $\rho = 1$, *i.e.*, if and only if G is the complete graph K_n. $\square$

Proposition 2.9 *Let G be a graph on $n \geq 4$ vertices with least distance eigenvalue ∂_n and remoteness ρ. Then*

$$\partial_n + \rho \leq 0$$

with equallity if and only if G is K_n.

Proof. It is easy to see that $\rho \leq D$, where D denotes the diameter, with equality if and only if $D = 1$, *i.e.*, G is the complete graph K_n. Thus, it sufices to prove that $\partial_n + D \leq 0$.

The least eigenvalue is the minimum of the Rayleigh quotient, *i.e.*,

$$\partial_n = \min_{X \neq 0} \frac{X^T \mathcal{D} X}{X^T X}.$$

If we consider the vector X with $X_i = 1$ and $X_j = -1$ for two vertices i and j such that $d(i,j) = D$, and $X_k = 0$ for $k \neq i, j$, then the quotient equals $-D$ and the inequality follows. $\square$

Note that Corollary 2.7 can also be obtained as an immediate consequence of the above propostion, since $\pi \leq \rho$.

The inequality in Proposition 2.9 is best possible among inequalities of the form $\rho + \partial_k \leq 0$ since there exist graphs with $\rho + \partial_{n-1} > 0$. For instance, the distance characteristic polynomial of the graph $K_n - e$, obtained from the complete graph K_n by deleting an edge, is

$$P_{\mathcal{D}}(t) = \left(t - \frac{n-1+\sqrt{(n-1)^2+8}}{2}\right)\left(t - \frac{n-1-\sqrt{(n-1)^2+8}}{2}\right)(t+2)(t+1)^{n-3}.$$

Thus, for $K_n - e$, we have $\rho + \partial_{n-1} = \frac{1}{n-1} > 0$.

To prove our next result, we use the interlacing theorem, which we recall here.

Theorem 2.10 ([15, p. 19]) *Let M be a Hermitian matrix with eigenvalues $\lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_n(M)$ and N one of its principal submatices; let $\lambda_1(N) \geq \lambda_2(N) \geq \cdots \geq \lambda_k(N)$ be the eigenvalues of N. Then the inequalities $\lambda_i(M) \geq \lambda_i(N) \geq \lambda_{i+n-k}(M)$ hold for $i = 1, \ldots, k$.*

Theorem 2.11 *Let G be a graph on $n \geq 4$ vertices with second largest distance eigenvalue ∂_2. Then*

$$\partial_2 \geq -1$$

with equality if and only if G is the complete graph K_n.

Proof. If the graph is complete, then $\partial_1 = -1$, and equality holds.

Now, assume that G is not complete. Let P be an induced path on 3 vertices in G. It ie easy to see that the distance spectrum of P is $(1+\sqrt{3}, 1-\sqrt{3}, -2)$. Applying the interlacing theorem with M and N as the distance matrices of G and P respectively, we get

$$\partial_2 \geq \partial_2^P = 1 - \sqrt{3} > -1.$$

This completes the proof. □

The following result is an immediate consequence of the above theorem.

Corollary 2.12 *Let G be a graph on $n \geq 4$ vertices with second largest distance eigenvalue ∂_2 and proximity π. Then*

$$\pi + \partial_2 \geq 0$$

with equality if and only if G is the complete graph K_n.

The above corollary is the best result of the form $\pi + \partial_i$, for a fixed $i \in \{1, 2, \ldots n\}$, that we can obtain. Indeed, for the star S_n, we have $\pi + \partial_3 = 1 - 2 = -1$. However, if we express i as a function of the diameter, we can strengthen Corollary 2.12, over the class of trees. Indeed, using Theorem 1.8, particularly the inequality $\partial_{\lfloor \frac{D}{2} \rfloor} > -1$, we straightaway get the following result.

Proposition 2.13 *Let T be a graph on $n \geq 4$ vertices with proximity π, diameter D and distance spectrum $\partial_1 \geq \partial_2 \geq \cdots \geq \partial_n$. Then*

$$\pi + \partial_{\lfloor \frac{D}{2} \rfloor} > 0.$$

Note that over the classe of trees on n vertices, $\pi = 1$ only for the star S_n. Thus, the inequality in the above propostion can potentially be improved. Experiments using the AutoGraphiX system led to the following conjecture.

Conjecture 2.14 *Let G be a graph on $n \geq 4$ vertices with diameter D, proximity π and distance spectrum $\partial_1 \geq \partial_2 \geq \cdots \geq \partial_n$. Then*

$$\pi + \partial_{\lfloor \frac{2D}{3} \rfloor} > 0.$$

If true, the bound in the above conjecture is the best possible since there exist graphs with $\pi + \partial_{\lfloor \frac{2D}{3} \rfloor + 1} < 0$ such as that illustrated in Figure 2. Indeed, for the tree T on $n = 22$ vertices, we have $D = 6$, $\pi \simeq 1.285714$ and $\partial_5 \simeq -1.286208$, therefore $\pi + \partial_5 \simeq -0.000494$. Note that the tree in Figure 2 belongs to a family of trees called double-tailed comets known to maximize the proximity over the class of trees with a given order and diameter (see [8]).

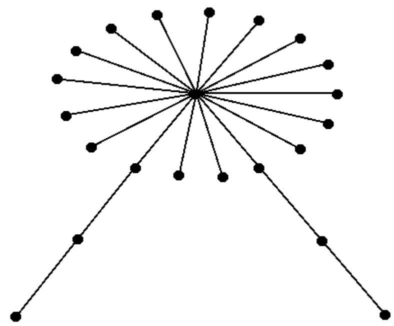

Figure 2: A tree T with $\pi + \partial_{\lfloor \frac{2D}{3} \rfloor + 1} < 0$

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