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Eigenvalues, Diameter, and Mean Distance in Graphs*

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Abstract. It is well-known that the second smallest eigenvalue λ_2 of the difference Laplacian matrix of a graph G is related to the expansion properties of G. A more detailed analysis of this relation is given. Upper and lower bounds on the diameter and the mean distance in G in terms of λ_2 are derived.

1. Introduction

This paper is a part of a larger project where the influence of the Laplacian eigenvalues of a graph on the structure of the graph is studied. At the beginning of this project we shall explore the second smallest eigenvalue λ_2 of the difference Laplacian matrix of a graph. (Notice that the smallest eigenvalue λ_1 is always equal to 0.) The first attempt in this direction was made by Fiedler [5] who defines the value of λ_2 as the *algebraic connectivity* of the graph. Besides this, λ_2 was related to the expanding properties of the graph [1, 2, 12] and to the isoperimetric numbers [10]. There are some other recent papers which study this quantity [6, 7, 9]; cf. also [4, §9.3] for few older references. More details can be found in a survey paper [11].

In the present paper we give upper and lower bounds on the diameter and the mean distance of a graph in terms of its second smallest eigenvalue λ_2. In each of the bounds, the dependence on λ_2 is reciprocial. Cf. theorems 2.3, 2.6, 3.4, 3.5, 4.2, and 4.3 for details.

We assume the knowledge of the standard terminology of graph theory. Graphs are finite, undirected, loops and multiple edges are allowed. Each loop counts one to the degree of the corresponding vertex.

The *difference Laplacian matrix* of a graph G of order n is an $n \times n$ matrix $Q = [q_{uv}]$ which is indexed by vertices of G. Its diagonal entry q_{vv} $(v \in V(G))$ is equal to the degree of the vertex v of G minus the number of loops at this vertex, and for $u \neq v$, q_{uv} is the negative value of the number of edges between vertices u and v in G. Thus $Q = diag(deg(v)) - A$ where A is the usual adjacency matrix of G. Notice

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that loops have no influence on the Laplacian matrix. It should be noted that the matrix $Q(G)$ has its rows and columns indexed by $V(G)$ and that no ordering on $V(G)$ is assumed. Also, $Q(G)$ acts on the vector space $l^2(V(G)) \approx \mathbf{R}^n$, $n = |V(G)|$, which consists of all complex vectors $(x_v)_{v \in V(G)}$ with entries indexed by $V(G)$. For our purpose only real vectors will be needed, and it will always be assumed that the entries x_v are real.

The Laplacian Q is a positive semidefinite matrix with the smallest eigenvalue $\lambda_1 = 0$ (a corresponding eigenvector has all coordinates equal to 1). The second eigenvalue $\lambda_2 = \lambda_2(G)$, which is of our main interest, is non-negative and $\lambda_2 = 0$ if and only if G is disconnected (see, e.g., [5] for more details).

2. Growth and the Diameter vs. the Second Smallest Eigenvalue – Upper Bounds

From now on we shall fix and use the following notation. G is a given graph of order n, $\lambda_2 = \lambda_2(G)$ its second smallest Laplacian eigenvalue, $\lambda_\infty = \lambda_\infty(G)$ its largest Laplacian eigenvalue, and $\Delta = \Delta(G)$ its maximal vertex degree. Moreover, an arbitrary vertex $w \in V(G)$ is chosen, and for $k = 0, 1, 2, \ldots$ let $B_k = B_k(w)$ be the set of vertices of G which are at distance at most k from w. Denote by $b_k = |B_k|$, and let e_k be the number of edges with one end in B_k and the other end in $B_{k+1} \backslash B_k$.

First we will derive results relating λ_2 with the growth of G. By the growth we mean the increase of numbers b_k when k increases. Our first result shows that the graph G has exponential growth, i.e., $b_k \geq \alpha^k$, where α is a constant bounded below as a function of λ_2.

2.1. Lemma. $b_k - b_{k-1} > \dfrac{2\lambda_2}{n(\Delta + \lambda_2)}[b_k(n - b_k) + b_{k-1}(n - b_{k-1})]$.

Proof. Fiedler [13] derived a useful expression for λ_2:

$$\lambda_2 = \min \frac{2n \sum_{uv \in E} (x_u - x_v)^2}{\sum_{u \in V} \sum_{v \in V} (x_u - x_v)^2} \tag{2.1}$$

where the minimum is taken over all non-constant vectors $x = (x_v)_{v \in V} \in l^2(V)$. If we choose x as

$$x_v = \begin{cases} 1, & v \in B_{k-1} \\ 0, & v \in B_k \backslash B_{k-1} \\ -1, & v \notin B_k \end{cases}$$

then (2.1) implies

$$n(e_{k-1} + e_k) \geq \lambda_2[b_{k-1}n_k + (n - b_k)n_k + 4b_{k-1}(n - b_k)]$$

where $n_k = b_k - b_{k-1}$. Since $e_{k-1} + e_j \leq \Delta n_k$, a routine calculation shows that

$$\frac{\Delta}{\lambda_2} nn_k \geq 2b_k(n - b_k) + 2b_{k-1}(n - b_{k-1}) - n_k(n - n_k) >$$

$$> 2[b_k(n - b_k) + b_{k-1}(n - b_{k-1})] - nn_k$$

which was to be shown. □

By replacing, in Lemma 2.1, the values b_k with a function $y(k)$, $k \in \mathbf{R}^+$, and b_{k-1} with $y(k - dk)$ we get a differential inequality for y. This suggests that the solution

$$y(t) = \frac{n}{1 + (n-1)e^{-\beta t}}, \qquad \beta = \frac{4\lambda_2}{\Delta + \lambda_2} \tag{2.2}$$

of the boundary problem

$$y' = \frac{\beta}{n} y(n - y), \qquad y(0) = 1 \tag{2.3}$$

may be dominated, in the integer points $k > 1$, by the numbers b_k. This is settled by our next lemma.

2.2. Lemma. Let G be a connected graph and let $y(t)$ be the solution (2.2) of (2.3). If $k > 1$ and $b_k \leq \frac{n}{2}$ then $b_k > y(k)$.

Proof. Since $b_0 = y(0)$, it follows from Lemma 2.1 that it is sufficient to prove that

$$y(k) - y(k-1) < \frac{\beta}{2n}[y(k)(n - y(k)) + y(k-1)(n - y(k-1))] \tag{2.4}$$

Let β be as in (2.2), $c := e^{-\beta}$, and $x := (n-1)e^{-\beta(k-1)}$. It is straight from (2.2) that (2.4) is equivalent to

$$\frac{2(1-c)}{\beta} < \frac{c(1+x)}{1+cx} + \frac{1+cx}{1+x}$$

which can be put, by a routine calculation, in the equivalent form:

$$\beta(c-1)\left[\frac{1}{1+cx} + \frac{x}{1+x}\right] < 2\beta - 2(1-c) \tag{2.5}$$

Notice that $(1 + cx)^{-1} \leq \frac{1}{2}$ and $x(1 + x)^{-1} \leq (1 + c)^{-1}$ where we have used the fact that $y(k) \leq \frac{n}{2}$. We will mention at the end of the proof how to justify this inequality.

It follows now that to prove (2.5), it suffices to show that

$$\beta(1-c)\left[\frac{1}{2} + \frac{1}{1+c}\right] < 2\beta - 2(1-c)$$

which reduces to

$$4(c^2 + 2\beta c - 1) + \beta(1-c)^2 > 0.$$

A numerical calculation shows that this is true for all $\beta \in (0,2]$. Since $\lambda_2 \leq \Delta$ for all graphs except the complete graphs [10] (for which the whole theorem is trivial), $\beta \leq 2$, and we are done.

It remains to show that $y(k) \leq \frac{n}{2}$. In order to do this, we first show that $y(k-1+t) < b_k$ for all $t \in (0,1)$. The proof goes as above, using $y(k-1+t)$ instead of $y(k)$ in (2.4). Along these lines, c is replaced by $e^{-\beta i}$, and the condition $y(k-1+t) \leq \frac{n}{2}$ is recovered by searching for the smallest t where $y(k-1+t) = \frac{n}{2} \geq b_k$. □

2.3. Theorem. *The eigenvalue λ_2 imposes an upper bound on the diameter of G:*

$$diam(G) \leq 2\left\lceil \frac{\Delta + \lambda_2}{4\lambda_2} ln(n-1) \right\rceil. \tag{2.6}$$

Proof. The theorem is immediate if we show that $b_k = b_k(w) > \frac{n}{2}$ (w is arbitrary) for $k \geq \frac{1}{\beta} ln(n-1)$. If $b_k \leq \frac{n}{2}$ then by Lemma 2.2

$$b_k > y(k) \geq y\left(\frac{1}{\beta} ln(n-1)\right) = \frac{n}{2},$$

a contradiction. □

Notice that in (2.6) the natural logarithms are used.

2.4. Lemma. Let $r > 1$ be an integer and let $B, C \subset V$ be subsets of vertices of G which are at distance at least $r+1$. Then

$$(r-1)^2 < \frac{\lambda_\infty}{4\lambda_2} \cdot \frac{(n - |B| - |C|)(|B| + |C|)}{|B|\,|C|}. \tag{2.7}$$

Proof. We give the proof for the case $B = B_k$, $C = V \backslash B_{k+r}$ since we will take the advantage of the previously introduced notation. The general proof is the same.

Let us define $x \in l^2(V)$ as

$$x_v = \begin{cases} t, & \text{if } v \in B \\ t + r - 1, & \text{if } v \in C \\ t + i - 1, & \text{if } v \in B_{k+i} \backslash B_{k+i-1}, \quad 1 \leq i \leq r \end{cases}$$

where the constant t is chosen in such a way that

$$\sum_{v \in V} x_v = 0. \tag{2.8}$$

Since $r > 1$, $x \neq 0$. Let $b := |B|$, $c := |C|$. Then $\|x\|^2 = (x,x) > bt^2 + c(t + r - 1)^2 =: f(t)$. The function $f(t)$ has its minimum at $t = -c(r-1)/(b+c)$, hence

$$\|x\|^2 > b\left(\frac{c(r-1)}{b+c}\right)^2 + c\left(\frac{c(r-1)}{b+c} + r - 1\right)^2 = (r-1)^2 \frac{bc}{b+c}. \tag{2.9}$$

An eigenvector of the smallest eigenvalue $\lambda_1 = 0$ is $1 = (1, 1, \dots, 1)^t$. Therefore by the well-known Courant-Fischer principle and (2.8)

$$\lambda_2 = \min_{\substack{z \neq 0 \\ z \perp 1}} \frac{(Qz, z)}{(z, z)} \leq \frac{(Qx, x)}{(x, x)}. \tag{2.10}$$

Since $(Qx, x) = \sum_{uv \in E} (x_u - x_v)^2 = e_{k+1} + \cdots + e_{k+r-1}$, the obtained inequalities (2.10) and (2.9) will imply (2.7) if we show that

$$e_{k+1} + \cdots + e_{k+r-1} \leq \frac{\lambda_\infty}{4}(n - b - c). \tag{2.11}$$

Let H be the induced subgraph of G with vertex set $B_{k+r} \backslash B_k$. By the Cauchy Interlacing Inequalities it follows that

$$\lambda_\infty(H) \leq \lambda_\infty(G). \tag{2.12}$$

Next, define a vector $z \in l^2(V(H))$ by setting

$$z_v = \begin{cases} 1, & \text{if } v \in B_{i+1} \backslash B_i \text{ for some even } i \\ -1, & \text{otherwise} \end{cases}.$$

Now, by (2.12)

$$\lambda_\infty(G) \geq \lambda_\infty(H) \geq \frac{(Q(H)z, z)}{(z, z)} = \frac{1}{n - b - c} \sum_{uv \in E(H)} (z_u - z_v)^2 = \frac{4}{n - b - c} \sum_{i=1}^{r-1} e_{k+i}$$

which implies (2.11) and ends the proof. □

A simple corollary to Lemma 2.4 is a result which establishes the exponential growth of the balls B_k.

2.5. Lemma. Let $r > 1$ be an integar, $\alpha > 1$ a real number, and let B, C be subsets of $V(G)$, which are at distance at least $r + 1$. If $n - |C| \leq \alpha |B| \leq \frac{n}{2}$ then

$$r < \sqrt{\frac{\lambda_\infty}{\lambda_2}} \sqrt{\frac{\alpha^2 - 1}{4\alpha}} + 1. \tag{2.13}$$

Proof. Let $b = |B|$, $c = |C|$. It is clear that $b + c \geq n - \alpha b + b \geq \frac{n}{2}$ and hence

$$(n - (b + c))(b + c) \leq (n - \alpha b + b)(\alpha b - b). \tag{2.14}$$

By (2.7), (2.14) and the assumptions of the Lemma we have:

$$\frac{4\lambda_2}{\lambda_\infty}(r - 1)^2 < \frac{(n - (b + c))(b + c)}{bc} \leq \frac{(n - \alpha b + b)(\alpha - 1)}{c} \leq$$

$$\leq (\alpha - 1)\frac{n - \alpha b + b}{n - \alpha b} = (\alpha - 1)\left(1 + \frac{1}{\alpha} \frac{\alpha b}{n - \alpha b}\right) \leq \frac{\alpha^2 - 1}{\alpha}$$

which settles the inequality (2.13). □

The key corollary to (2.13) is that if $r \geq \sqrt{\frac{\lambda_\infty}{\lambda_2}}\sqrt{\frac{\alpha^2-1}{4\alpha}} + 1$ then either $|B_{k+r}| > \frac{n}{2}$, or $|B_{k+r}| > \alpha|B_k|$. It means that the graph expands pretty fast. More precisely, in $r \cdot \left\lceil log_\alpha\left(\frac{n}{2}\right)\right\rceil$ steps we reach more than half of its vertices. The main result of this section follows:

2.6. Theorem. *For any* $\alpha > 1$

$$diam(G) \leq 2 \cdot \left\lceil \sqrt{\frac{\lambda_\infty}{\lambda_2}}\sqrt{\frac{\alpha^2-1}{4\alpha}} + 1 \right\rceil \left\lceil log_\alpha \frac{n}{2} \right\rceil. \tag{2.15}$$

Now, the question is which α to take in (2.15) to get the best possible upper bound. For each particular choice of values of n, λ_2, and λ_∞ one can find by numerical methods good approximations to the optimal value of α.

For several values of the quotient $\frac{\lambda_\infty}{\lambda_2}$, good estimates for the best possible α were found by help of a computer. The results are assembled in Table 1. The values in the first column present $q = \lambda_\infty/\lambda_2$, next to it the best α is given, and finally $r = 1 + \lceil\sqrt{q}\sqrt{(\alpha^2-1)/(4\alpha)}\rceil$. As an upper bound one may take any row in which $q \geq \lambda_\infty/\lambda_2$. For example, if $\lambda_\infty/\lambda_2 = 36.3$ then we see from the row of $q = 45$ that $r = 10$, $\alpha = 7.336$, and hence

$$diam(G) \leq 20 \cdot \left\lceil \frac{log(n/2)}{log(7.336)} \right\rceil.$$

For large values of λ_∞/λ_2 a very good approximation to the optimum is the value of α which minimizes $f(\alpha) = \sqrt{\frac{\alpha^2-1}{\alpha}}/ln\,\alpha$. The solution is approximately equal to $\alpha = 6.7869766$.

Table 1.

q	α	r	q	α	r
1.0	16.062	3	16.0	9.109	7
1.1	14.613	3	22.0	9.019	8
1.2	13.407	3	30.0	8.648	9
1.4	11.515	3	45.0	7.336	10
1.6	22.544	4	80.0	7.336	13
1.8	20.049	4	100.0	9.109	16
2.0	18.055	4	200.0	8.123	21
2.4	15.066	4	400.0	6.904	27
3.0	12.082	4	700.0	7.538	37
3.4	10.681	4	1000.0	7.528	44
4.0	16.062	5	2000.0	7.102	60
5.0	12.877	5	4000.0	6.710	82
7.0	9.250	5	8000.0	6.987	118
10.0	10.099	6	10,000.0	6.803	130

2.7. Corollary. For any graph G

$$diam(G) \le 2\left\lceil 1.28837452\sqrt{\frac{\lambda_\infty}{\lambda_2}}+1\right\rceil\left\lceil\frac{log\frac{n}{2}}{log\,6.7869766}\right\rceil.$$

2.8. Remarks. The bounds (2.6) and (2.15) are incomparable in general. However, in most cases (2.15) is much stronger than the bound of Theorem 2.3. Theorem 2.6 also improves an eigenvalue bound on the diameter obtained by Alon and Milman [2]:

$$diam(G) \le 2\left\lceil\sqrt{\frac{2\Delta}{\lambda_2}}log_2 n\right\rceil.$$

One should note that $\lambda_\infty \le 2\Delta$ (cf. [5]). Another eigenvalue bound was found by Chung [3]. Her result applies for k-regular graphs only and uses "the second largest eigenvalue by absolute value" of the adjacency matrix of a graph. More precisely, if $\lambda(G) = min\{\lambda_2, 2k - \lambda_\infty\}$, then:

$$diam(G) \le \left\lceil\frac{log(n-1)}{log\left(\frac{k}{|k-\lambda(G)|}\right)}\right\rceil. \tag{2.16}$$

Notice that $\lambda(G) = 0$ for bipartite graphs, so (2.16) is trivial. But in cases when $\lambda_2 \ge 2k - \lambda_\infty$, (2.16) compares favorably with our bounds.

3. The Mean Distance

The results of Section 2 give rise to an upper bound on the mean distance of a graph. We will be using the notation of the previous section. A vertex $w \in V(G)$ is fixed, and let $n_k := b_k - b_{k-1} (k \ge 0)$ and

$$S(w) := \sum_k kn_k.$$

The *mean distance* $\bar{\rho}(G)$ of G is equal to the average of all distances between distinct vertices of G. In other words

$$\bar{\rho}(G) := \frac{1}{n(n-1)}\sum_{u\in V(G)} S(u).$$

3.1. Lemma. $S(w) = \sum_{k\ge 0}(n - b_k)$.

Proof. $\sum_k (n-b_k) = \sum_k\sum_{i>k} n_i = n_1 + 2n_2 + 3n_3 + \cdots = S(w)$. □

For t a positive number, define a sequence $\beta_{i,t}$ $(i = 0, 1, 2, \ldots)$ by $\beta_{0,t} := t$ and

$$\beta_{i,t} := -\omega + \sqrt{\omega^2 + \beta_{i-1,t}\left(n + \frac{n(\Delta+\lambda_2)}{2\lambda_2} - \beta_{i-1,t}\right)}, \qquad i > 0$$

where $\omega = \dfrac{n(\Delta - \lambda_2)}{4\lambda_2}$. The following properties of this sequence are easy to verify:

3.2. Lemma. As far as each of the values $\beta_{j,t}$ below is between 0 and n we have:
(a) $\beta_{i,t}$ is increasing as a function of i. More precisely,

$$\beta_{i,t} - \beta_{i-1,t} = \frac{2\lambda_2}{n(\Delta + \lambda_2)}[\beta_{i,t}(n - \beta_{i,t}) + \beta_{i-1,t}(n - \beta_{i-1,t})].$$

(b) $\beta_{i+1,t} = \beta_{i,\beta_{1,t}}$.
(c) $\beta_{i,t}$ is continuous and increasing as a function of t.
(d) There is a unique $t > 0$ and unique integer L such that

$$\beta_{0,t} \leq 1, \qquad \beta_{1,t} > 1, \qquad \beta_{L,t} = \frac{n}{2}.$$

To see the motivation for introducing the numbers $\beta_{i,t}$ compare Lemma 3.2(a) with Lemma 2.1. Note that $b_k \geq \beta_{k,1}$. Let t and L be as in Lemma 3.2(d). For $k = 0, 1, \ldots, L$, let $s_k := \beta_{L-k,t}$.

3.3. Lemma. Let K be the largest integer for which $b_K < \frac{n}{2}$. Then for each $k \geq 0$, $n - b_{K+k+1} \leq s_k$.

Proof. By induction. For $k = 0$ this is trivial by definitions of $\beta_{L,t}$ and K. For $k > 0$, the assumption $s_k < n - b_{K+k+1}$ implies by Lemma 3.2(a) and Lemma 2.1 that $s_{k-1} < n - b_{K+k}$. This leads to a contradiction. □

3.4. Theorem. $\bar{\rho}(G) \leq \frac{n}{n-1}\left(\left\lceil \frac{\Delta + \lambda_2}{4\lambda_2} ln(n-1) \right\rceil + \frac{1}{2}\right)$.

Proof. Let L and K be as above. By definition of L and Lemma 2.2, $L \leq \left\lceil \frac{\Delta + \lambda_2}{4\lambda_2} ln(n-1) \right\rceil$ and $L \geq K + 1$. Then by Lemmas 3.1, 3.2, and 3.3,

$$\begin{aligned} S(w) &= \sum_{k \geq 0} (n - b_k) = (K+1)n - \sum_{k=0}^{K} b_k + \sum_{k > K} (n - b_k) \leq \\ &\leq (K+1)n - \sum_{k=0}^{K} \beta_{k,1} + \sum_{i=0}^{L-1} s_i \leq \\ &\leq Ln - \sum_{k=0}^{L-1} \beta_{k,1} + \sum_{k=1}^{L} \beta_{k,t} \leq \left(L + \frac{1}{2}\right)n \leq n \cdot \left(\left\lceil \frac{\Delta + \lambda_2}{4\lambda_2} ln(n-1) \right\rceil + \frac{1}{2}\right). \end{aligned}$$

Now the inequality we are trying to prove becomes obvious since w was an arbitrary vertex of G. □

Another bound on $\bar{\rho}(G)$ parallels the diameter bound of Theorem 2.6.

3.5. Theorem. *For any* $\alpha > 1$

$$\bar{\rho}(G) < \frac{n}{n-1}\left\lceil 1 + \sqrt{\frac{\lambda_\infty}{\lambda_2}}\sqrt{\frac{\alpha^2 - 1}{4\alpha}} \right\rceil \left(\frac{1}{2} + \left\lceil log_\alpha \frac{n}{2} \right\rceil\right).$$

Proof. The idea is similar to the proof of Theorem 3.4. First, let β_k be lower bounds for b_k. According to Lemma 2.5 we choose $\beta_k = \alpha_0\alpha^{i-1}$, if $ir \leq k < (i+1)r$, where $r = \left\lceil 1 + \sqrt{\frac{\lambda_\infty}{\lambda_2}}\sqrt{\frac{\alpha^2-1}{4\alpha}} \right\rceil$ and $1 < \alpha_0 \leq \alpha$ is chosen in such a way that $\alpha_0\alpha^{L-1} = \frac{n}{2}$ for some integer L. Clearly

$$L = \left\lceil \frac{\log(n/2)}{\log \alpha} \right\rceil.$$

Take K such that $b_K \leq \frac{n}{2}$ and $b_{K+1} > \frac{n}{2}$. Note that $rL \geq K + 1$. Next verify that $n - b_{K+k+1} \leq \alpha\beta_{rL-k-1}$. The consequence of the above stated inequalities is that:

$$\begin{aligned} S(w) &= \sum_{k \geq 0} (n - b_k) \leq \sum_{k=0}^{rL-1} (n - \beta_k) + \sum_{k \geq K+1} (n - b_k) \\ &\leq rLn - \sum_{k=0}^{rL-1} \beta_k + \sum_{i=0}^{rL-1} \alpha\beta_i = rLn + (\alpha - 1)\sum_{k=0}^{rL-1} \beta_i \\ &= rLn + (\alpha - 1)r\frac{\alpha_0}{\alpha}\sum_{i=0}^{L-1} \alpha^i < rLn + r\frac{n}{2} = r\cdot n\left(L + \frac{1}{2}\right). \end{aligned}$$

This proves the theorem since w is an arbitrary vertex. □

In Theorem 3.5 we have the freedom to choose such an α which minimizes the upper bound. As for the Corollary 2.7 a good value for α, when $\frac{\lambda_\infty}{\lambda_2}$ and n are both large, is $\alpha = 6.7869766$. Cf. Section 2.

4. Lower Bounds

In this section we will prove that λ_2 provides also lower bounds on the diameter and the mean distance of a graph. We start with a lemma:

4.1. Lemma. For each pair u, v of distinct vertices of G choose a shortest path P_{uv} from u to v. Then any edge $e \in E(G)$ belongs to at most $\frac{n^2}{4}$ of the paths P_{uv}.

Proof. Let $e \in E(G)$. Define a graph Γ_e as follows. It has vertex set $V(G)$, and vertices u and v are adjacent in Γ_e iff e lies on P_{uv}. We have to show that $|E(\Gamma_e)| \leq \frac{n^2}{4}$.

First we observe that Γ_e has no triangles. Assume that there is a triangle uvw in Γ_e. Orient the paths P_{uv}, P_{uw}, P_{vw} from u to v, u to w, and from v to w, respectively. If x and y are the endpoints of e, two of these paths use e in the same direction, say from x to y. We may assume w.l.o.g. that these two paths are P_{uw} and P_{vw}. This implies that $dist(u,y) > dist(u,x)$ and $dist(v,y) > dist(v,x)$. But then $dist(u,v) \leq dist(u,x) + dist(v,x) < dist(u,x) + dist(y,v)$ and similarly $dist(u,v) < dist(u,y) + dist(v,x)$ which shows that a shortest path from u to v cannot use the edge $e = xy$.

That a graph Γ of order n with no triangle has at most $\frac{n^2}{4}$ edges can be shown by induction on n. For $n = 0$ and $n = 1$ this is clear. If $n \geq 2$, take any two adjacent vertices, say v, u. Then $deg_\Gamma(v) + deg_\Gamma(u) \leq n$ since v and u have no common neighbors. By induction hypothesis

$$|E(\Gamma)| = |E(\Gamma - u - v)| + deg(v) + deg(u) - 1 \leq \frac{(n-2)^2}{4} + n - 1 = \frac{n^2}{4}. \quad \square$$

The lower bound (4.1) on the diameter of G in the following theorem is due to Brendan McKay [8].

4.2. Theorem. *For a graph G of order n, its second Laplacian eigenvalue λ_2 imposes upper bounds on the diameter and the mean distance of G,*

$$diam(G) \geq \frac{4}{n\lambda_2} \tag{4.1}$$

and

$$(n-1)\bar{\rho}(G) \geq \frac{2}{\lambda_2} + \frac{n-2}{2}. \tag{4.2}$$

Proof. For each pair $u, v \in V$ choose a shortest path P_{uv} from u to v. Let $x \in l^2(V)$ be an eigenvector for λ_2. It can be shown easily that

$$2n \sum_{uv \in E} (x_u - x_v)^2 = \lambda_2 \cdot \sum_{u \in V} \sum_{v \in V} (x_u - x_v)^2 \tag{4.3}$$

just by using the facts that $\sum_{v \in V} x_v = 0$ (orthogonality to the eigenvector of λ_1) and that $\sum_{uv \in E} (x_u - x_v)^2 = \lambda_2 \sum_{v \in V} x_v^2$. Each term on the right hand side of (4.3) can be estimated:

$$(x_u - x_v)^2 = [(x_u - x_{v_1}) + (x_{v_1} - x_{v_2}) + \cdots + (x_{v_{k-1}} - x_v)]^2 \leq k \sum_{e \in E(P_{uv})} \delta^2(e) \tag{4.4}$$

where $P_{uv} = uv_1v_2 \ldots v_{k-1}v$ (so $k = dist(u,v)$) and $\delta^2(e) = (x_a - x_b)^2$, $e = ab$. Let χ_{uv}: $E(G) \to \{0,1\}$ be the characteristic function of P_{uv}, i.e.

$$\chi_{uv}(e) = \begin{cases} 1, & \text{if } e \in P_{uv} \\ 0, & \text{otherwise.} \end{cases}$$

Now by (4.4)

$$\sum_{v \in V} \sum_{u \in V} (x_u - x_v)^2 \leq \sum_{v \in V} \sum_{u \in V} dist(u,v) \sum_{e \in E} \delta^2(e)\chi_{uv}(e)$$
$$= \sum_{e \in E} \delta^2(e) \sum_{v \in V} \sum_{u \in V} dist(u,v)\chi_{uv}(e). \tag{4.5}$$

To show (4.1) we use in (4.5) the fact that $dist(u,v) \leq diam(G)$ and Lemma 4.1 which says that

$$\sum_{v\in V}\sum_{u\in V}\chi_{uv}(e) \le 2\cdot\frac{n^2}{4} = \frac{n^2}{2}$$

If we combine the obtained result with (4.3) we get

$$2n\sum_{uv\in E}(x_u - x_v)^2 = 2n\sum_{e\in E}\delta^2(e) \le \lambda_2\cdot diam(G)\cdot\frac{n^2}{2}\sum_{e\in E}\delta^2(e)$$

which forces (4.1) to be true.

To prove (4.2), however, we continue (4.5) as follows

$$\begin{aligned}\sum_{v\in V}\sum_{u\in V} dist(u,v)\chi_{uv}(e) &\le \sum_{v\in V}\sum_{u\in V} dist(u,v) - \sum_{v\in V}\sum_{u\in V\setminus\{v\}}(1-\chi_{uv}(e))\\ &\le n(n-1)\bar{\rho}(G) - 2\binom{n}{2} + 2\frac{n^2}{4} = n(n-1)\bar{\rho}(G) - \frac{n(n-2)}{2}.\end{aligned} \tag{4.6}$$

From (4.3), (4.5), and (4.6) we conclude:

$$2n\sum_{e\in E}\delta^2(e) \le \lambda_2\cdot\sum_{e\in E}\delta^2(e)\cdot\left[n(n-1)\bar{\rho}(G) - \frac{1}{2}n(n-2)\right]$$

which is equivalent to (4.2). □

The bounds of Theorem 4.2 can make much sense only in the case when λ_2 is small. We expect that they can be improved to give non-trivial bounds also in cases when λ_2 is large. However, the following examples show that (4.1) is, in a sense, best possible.

Let $P_{k,t}$ be the tree of diameter $t + 2$ which is obtained from the path P_{t+1} by joining to each of its two end vertices, k new vertices. One can show that

$$\frac{4}{n\lambda_2(P_{k,t})} > \gamma(k,t) := \frac{12k^2t + 8kt^2 + t^3}{3(2k+t+1)^2}$$

where $n = 2k + t + 1$ is the number of vertices of $P_{k,t}$. Since

$$\lim_{k/t\to\infty}\gamma(k,t) = t,$$

the graphs $P_{k,t}$ satisfy, for any $\varepsilon > 0$,

$$diam(P_{k,t}) > \frac{4}{n\lambda_2} > diam(P_{k,t}) - 2 - \varepsilon$$

as soon as $\frac{k}{t}$ is large enough.

At the end we present a result which is also due to McKay [8].

4.3. Theorem. *Let T be a tree of order n and $\lambda_2, \lambda_3, \ldots, \lambda_n$ the non-zero eigenvalues of its difference Laplacian matrix. Then*

$$(n-1)\bar{\rho}(T) = 2\sum_{i=2}^{n}\frac{1}{\lambda_i}. \tag{4.7}$$

Proof. Let Q be the Laplacian matrix of G, and

$$\mu(x) = x^n + c_{n-1}x^{n-1} + \cdots + c_2x^2 + c_1x$$

its characteristic polynomial. Notice that $\lambda_1 = 0$ is a zero of $\mu(x)$. By the Vieta's formulas

$$\sum_{i=2}^{n} \frac{1}{\lambda_i} = \left|\frac{c_2}{c_1}\right| \tag{4.8}$$

and by the matrix-tree-theorem and its generalizations (see, e.g., [4, Theorem 1.4] for details) $\frac{1}{n}|c_1| = 1$ (= the number of spanning trees of T) and

$$|c_2| = \sum_{\substack{s,t \in V \\ s \neq t}} \kappa(T_{s,t})$$

where $\kappa(H)$ denotes the number of spanning trees of H, and $T_{s,t}$ is the (unicyclic) graph obtained from T by identifying vertices s and t. Clearly, $\kappa(T_{s,t}) = dist(s, t)$, so $|c_2| = \frac{1}{2}n(n-1)\bar{\rho}(T)$. By (4.8), the formula (4.7) is settled. □

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