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ON THE LARGEST EIGENVALUE OF UNICYCLIC GRAPHS

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Abstract. We first establish some relations between the graph structure and its largest eigenvalue. Applying these results to unicyclic graphs (with a fixed number of points), we explain some facts about the λ_1-ordering of these graphs. Most of these facts were suggested by the experiments conducted on the expert system "GRAPH", which has been developed and implemented at the Faculty of Electrical Engineering, University of Belgrade.

1. Introduction. In this paper we will consider only finite, undirected graphs, without loops or multiple lines. Our basic terminology follows [5]; for everything about graph spectra, not given here, see [2]. In the spectral graph theory, there are some attempts which are concerned with the ordering of the graphs (within a fixed number of points) according to some spectral invariants. For example, in [2], the λ-ordering, i.e. the lexicographic ordering with respect to a nonincreasing sequence of eigenvalues, is usually assumed. Very natural is the m-ordering, i.e. the lexicographic ordering with respect to spectral moments (see [3], and also [4] in the context of unicyclic graphs). Of course, due to the existence of cospectral graphs none of these orderings is fine enough. Nevertheless, for some special kind of graphs, even λ_1-ordering, i.e. an ordering according to the largest eigenvalue, is of interest. In this paper we will provide some results about the λ_1-ordering of graphs, focusing our attention only to unicyclic graphs. The analogous results for trees can be easily reproduced; for some accounts, see [8].

In the sequel lines, we give some useful results together with the necessary notation.

$G-v$ $(G-e)$ denotes the subgraph of G with a point v (line e) removed. In general, if H is a subgraph of G, $G-V(H)$ is the graph remaining when the points of H are removed from G. The next three lemmas are taken from [10].

LEMMA A. *Let v be a point of a graph G, and let $C(v)$ be the collection of all cycles containing v. Then $P(G,\lambda)$, the characteristic polynomial of G, satisfies*

(a) $$P(G,\lambda)=\lambda P(G-v,\lambda)-\sum_{u\sim v}P(G-v-u,\lambda)-2\sum_{Z\in C(v)}P(G-V(Z),\lambda).$$

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Note that for an empty graph, i.e. for $H = K_0$, we define $P(H,\lambda) = 1$. In particular, if v is of degree one, then (a) becomes

$$\text{(a}'\text{)} \qquad P(G,\lambda) = \lambda P(G-v,\lambda) - P(G-v-u,\lambda).$$

Remark. If $\lambda > \lambda_1(G-v)$, then from (a) we easily get

$$\text{(a}''\text{)} \qquad P(G,\lambda) - \lambda P(G-v,\lambda) < 0.$$

LEMMA B. *Let $e = uv$ be a line of G, and let $C(e)$ be the collection of all cycles containing e. Then $P(G\lambda)$ satisfies*

$$\text{(b)} \qquad P(G,\lambda) = P(G-e,\lambda) - P(G-v-u,\lambda) - 2\sum_{Z\in C(e)} P(G-V(Z),\lambda)$$

LEMMA C. *Let G and H be the rooted graphs with roots r and s, respectively. Then the characteristic polynomial of the coalescence $G\cdot H$ (roots are identified) satisfies*

$$\text{(c)} \quad P(G\cdot H,\lambda) = P(G-r,\lambda)P(H,\lambda) + P(G,\lambda)P(H-s,\lambda) - \lambda P(G-r,\lambda)P(H-s,\lambda).$$

If H is a spanning subgraph of G, we shall write $H \leq G$; in particular, if it is a proper spanning subgraph, we then write $H < G$. We now have (see [7], for example).

LEMMA D. *Let G be a connected graph. If $H < G$ (H is not necessarily connected, then, for every $\lambda \geq \lambda_1(G)$,*

$$\text{(d)} \qquad P(H,\lambda) > P(G,\lambda)$$

holds.

Remark. If G is not necessarily connected, then (d) holds for every $\lambda > \lambda_1(G)$.

The next lemma follows from the maximum characterization of the largest eigenvalue for symmetric matrices, see [9], and also [1]. If uv is a line of G, while w is a point nonadjacent to u, then we shall denote by G' the graph obtained from G by switching the line uv from v to w, i.e. $G' = G - uv + uw$.

LEMMA E. *Suppose G and G' are both connected graphs. If $x > 0$ is an eigenvector corresponding to the largest eigenvalue of G, then, whenever $x(v) \leq x(w)$, $\lambda_1(G') \geq \lambda_1(G)$ holds; in particular, if $x(v) < x(w)$, we have $\lambda_1(G') > \lambda_1(G)$.*

2. Main results. In order to examine the λ_1-ordering of unicyclic graph, we first exhibit some rules which relate the graph structure and its largest eigenvalue.

THEOREM 1 [7]. *Let C he any connected graph with at least two points. If A and B are the graphs as in Fig. 1, then $P(A,\lambda) > P(B,\lambda)$ for $\lambda > \min(\lambda_1(A), \lambda_1(B))$; in particular, $\lambda_1(A) < \lambda_1(B)$.*

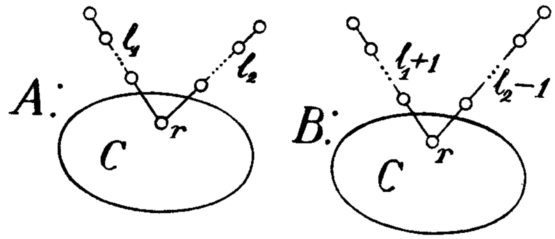

Fig. 1

THEOREM 2. *Let C be any connected graph with at least two points. If A and B are the graphs as in Fig. 2, then $P(A,\lambda) > P(B,\lambda)$ for $\lambda > \max(\lambda_1(A), \lambda_1(B))$; in particular, $\lambda_1(A) < \lambda_1(B)$.*

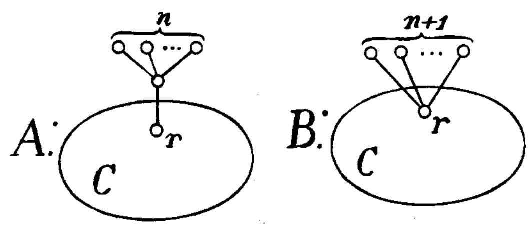

Fig. 2

Proof. Let $G = C$ be a rooted graph with a root r. Next, let s and t be the points of $H = K_{1,n}$ whose degrees are n and 1, respectively. With this in mind, $A(B)$ is obtained from G and H by identifying the roots r and s (r and t). From (c) we get

$$P(A,\lambda) - P(B,\lambda) = (P(G,\lambda) - \lambda P(G-r,\lambda))(P(H-s,\lambda) - P(H-t,\lambda)).$$

Let $\mu = \max(\lambda_1(G), \lambda_1(H))$. By (a$''$), if $\lambda > \mu$, we have $P(G,\lambda) - \lambda P(G-r,\lambda) < 0$. Also, for $\lambda > \mu$, since $H - s < H - t$, from (d) we get $P(H-t,\lambda) < P(H-s,\lambda)$. Thus if $\lambda > \mu$, we have $P(A,\lambda) > P(B,\lambda)$, and consequently $\lambda_1(A) < \lambda_1(B)$. $\square$

Let $C(T_1, T_2, \ldots, T_g)$ be an arbitrary unicyclic graph, where T_i is a rooted tree appended to the i-th point of a cycle (points on the cycle are naturally ordered around the cycle, g denotes its length). Applying the above two theorems, we easily get that $C(T_1, T_2, \ldots, T_g)$ is less than $C(S_1, S_2, \ldots, S_g)$ with respect to λ_1-ordering; here S_i is a star on $n_i = |V(T_i)|$ points whose central point is a root. For brevity. we shall denote $C(S_1, S_2, \ldots, S_g)$ by $C(n_1, n_2, \ldots, n_g)$.

Let $C_{n,g} = \{C(n_1, n_2, \ldots, n_g) \mid n_1 + n_2 + \cdots + n_g = n - g\}$.

Theorem 3. *If G belongs to $C_{n,g}$ and $G \neq C(n-g,0,\dots,0)$ then*

$$\lambda_1(G) < \lambda_1(C(n-g,0,\dots,0)).$$

Proof. Suppose $G_m \in C_{n,g}$ is a graph whose largest eigenvalue attains the maximum value among all graphs from $C_{n,g}$. Also, suppose that $G_m = C(m_1, m_2, \dots, m_g)$, where $m_i \neq 0$ if $i = i_1, i_2, \dots, i_k$ ($k \geq 2$). Now, if $x(i_s) \neq x(i_t)$ for some s and t ($1 \leq s < t \leq k$) then, by Lemma E, we get a contradiction to the choice of G_m. Indeed, if say $x(i_s) < x(i_t)$, we can switch a pendant line at i_s, from i_s to i_t. So assume $x(i_s) = x(i_2) = \cdots = x(i_k) = a$. Let now p be an endpoint in G_m. Since $\lambda_1(G_m)x(P) = a$, it follows that $x(p)$ does not depend on the particular p we choose. If again we switch a pendant line at i_s, from i_s to i_t, then by Lemma E. $\lambda_1(G'_m) \geq \lambda_1(G_m)$, but due to the choice of G_m, the equality must hold. This means that x is an eigenvector of G'_m which corresponds to the largest eigenvalue. Consequently, observing the point i_t with graphs G_m and G'_m, we get

$$\lambda a = x(i_{t-1}) + x(i_{t+1}) + m_t x(p), \qquad \lambda a = x(i_{t-1}) + x(i_{t+1}) + (m_t+1)x(p)$$

where, for short $\lambda = \lambda_1(G_m) = \lambda_1(G'_m)$, while the indices in above are reduced modulo g. The latter implies $x(p) = 0$, which is an obvious contradiction. $\square$

On the basis of results mentioned so far, we have that among all unicyclic graphs on n points and girth g, $C(n-g,0,\dots,0)$ is the greatest with respect to λ_1-ordering; for some accounts on the smallest graphs, see [4] and [7].

We now proceed to see what happens if we reduce the girth.

Theorem 4. *Let C be any connected graph with at least three points. If A and B are the graphs obtained from C as shown in Fig. 3 then $P(B,\lambda) < P(A,\lambda)$ for $\lambda > \max(\lambda_1(A), \lambda_1(B))$; in particular $\lambda_1(A) < \lambda_1(B)$.*

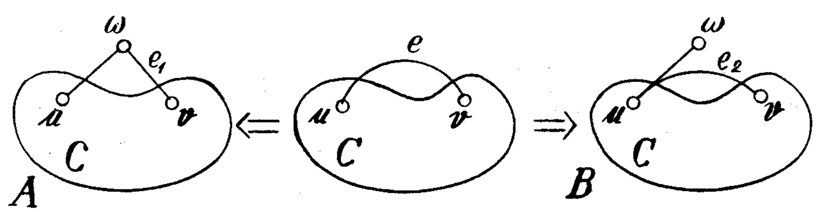

Fig. 3

Proof. Let $e_1 = wv$ and $e_2 = uv$ (see Fig. 3). We first notice that $A - e_1 = B - e_2$. Next, let Z be any cycle of $C + e$ containing $e = uv$. By Z_1 (Z_2) we denote the corresponding cycle A (B) containing e_1 (e_2). It is easy to see that $A - V(Z_1)$ and $B - V(Z_2)$ differ only in an isolated point appearing with the latter graph. So, by (b), we have

$$\Delta = P(A,\lambda) - P(B,\lambda) = P(B-u-v,\lambda) - P(A-w-v,\lambda) + 2Q(\lambda),$$

where

$$Q(\lambda) = (\lambda - 1)\sum_i P(H_i, \lambda),$$

H_i' is being some spanning subgraphs of C. Now let $\mu = \max(\lambda_1(A), \lambda_1(B))$. By (d), since $B - u - v < A - w - v$, we have $P(B - u - v, \lambda) > P(A - w - v, \lambda)$ for $\lambda > \mu$. Also, if $\lambda > \mu$, $P(H_i\lambda) > 0$ for each i. So, we get $\Delta > O$ for $\lambda > \mu$, and consequently $\lambda_1(A) < \lambda_1(B)$. □

Remark. The latter inequality on eigenvalues is contained in [6]. It is also worth mentioning that it not a direct consequence of Lemma E.

The next theorem is a direct generalization of the previous one.

THEOREM 5. *Let A_n (B_n) be the graph obtained from A (B) of Fig. 3 by adding to the point w just n pendant lines (see Fig. 4). Then $P(B_n, \lambda) < P(A_n, \lambda)$ for $\lambda > \max(\lambda(A_0), \lambda_1(B_0))$; in particular, $\lambda_1(A_n) < \lambda_1(B_n)$.*

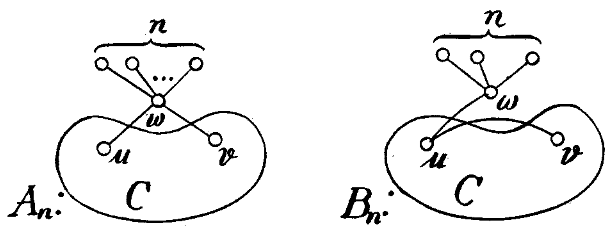

Fig. 4

Proof. By induction on n. Let $e(f)$ be any pendant line of $A_n(B_n)$ at w. Applying (b) on A_n (B_n) with respect to e (f), we get

$$\Delta_n = P(A_n, \lambda) - P(B_n, \lambda) = \lambda\Delta_{n-1} - \lambda^{n-1}(P(M, \lambda) - P(N, \lambda)),$$

where $M = A_0 - w$, $N = B_0 - w$ are fixed graphs not depending on n. By Theorem 4, if $\lambda > \mu$ $(\mu = \max(\lambda_1(A_0)\lambda_1(B_0)))$, then $\Delta_0 > 0$. Furthermore, since $N < M$, we have $P(N, \lambda) - P(M, \lambda) > 0$, if $\lambda > \max(\lambda_1(M), \lambda_1(N))$ (and also $\lambda > \mu$). Thus, $\Delta_n > 0$ for each n. This proves the first part of the theorem. As before, we now get $\lambda_1(A_n) < \lambda_1(B_n)$. □

Applying the two theorems above to any graph from $C_{n,g'}$ and also Theorem 2 if necessary, we can get the unicyclic graph in $C_{n,g-1}$ which is greater with respect to λ_1-ordering. Indeed, we have that $C(n_1, n_2, \dots, n_{g-1} + n_g + 1)$ is greater than $C(n_1, n_2, \dots, n_g)$ in the same sense. So we can reduce the girth g to three. For the graphs in $C_{n,3}$ we shall now prove some additional results; for the graphs in $C_{n,g}$ $(g \geq 4)$, the analogous results are rather complicated.

THEOREM 6. *Let A, B and C be the graphs as in Fig. 5. Then we have: $P(A, \lambda) > P(B, \lambda)$ if $\lambda > \max(\lambda_1(A), \lambda_1(B))$, and also $P(B, \lambda) > P(C, \lambda)$ if $\lambda > \max(\lambda_1(B), \lambda_1(C))$; in particular, $\lambda_1(A) < \lambda_1(B) < \lambda_1(C)$.*

Proof. We first prove the inequalities concerning B and C. To this end, we may use an induction on $n = n_2$. For convenience, we will now assume $B = B_n$ and $C = C_n$. Also, let v' (u') be the points of degree one adjacent to v (u) in B_n (C_n). Applying (a$'$) at points v' (u') we get

$$\Delta_n = P(B_n, \lambda) - P(C_n, \lambda) = \lambda \Delta_{n-1} - \lambda^{n-1}(P(B_0 - v, \lambda) - P(C_0 - u, \lambda)).$$

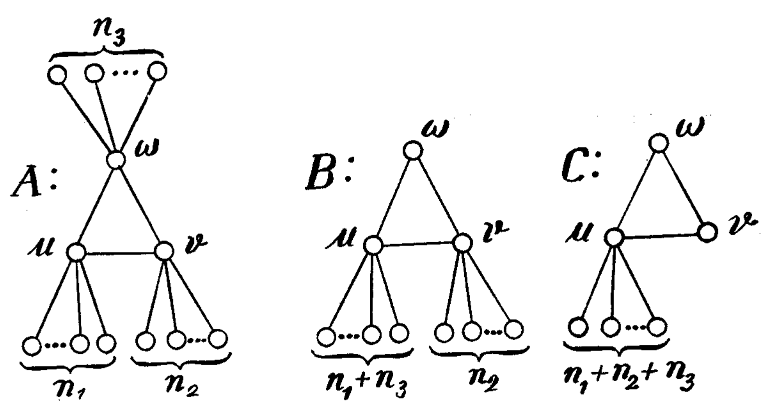

Fig. 5

Since $C_0 - u < B_0 - 1$, by (d), $P(B_0 - v, \lambda) - P(C_0 - u, \lambda) < 0$ for any $\lambda > \max(\lambda_1(B), \lambda_1(C))$. So, by induction, since $\Delta_0 = 0$ we get $\Delta_n > 0$ for any n. As before, we get $\lambda_1(B) < \lambda_1(C)$.

Analogously, again by induction on $n = n_2$, we prove the desired results for A and B. It is interesting to mention that this part of the proof is in some steps based on the results from the former part. □

A better evidence in λ_1-ordering of graphs in $C_{n,3}$ can be deduced from Lemma E and the next theorem.

THEOREM 7. *Let u, v, w be the points of the triangle of a graph $G = C(n_u, n_v, n_w)$ from $C_{n,3}$. If $n_u \geq n_v \geq n_w$, then $x(u) \geq x(v) \geq x(w)$, where x is an eigenvector corresponding to the largest eigenvalue of G.*

Proof. Let $\lambda = \lambda_1(G)$. Then, by simple calculations, we get

$$x(u) = \lambda/(\lambda^2 + \lambda - n_u), \quad x(v) = \lambda/(\lambda^2 + \lambda - n_v), \quad x(w) = \lambda/(\lambda^2 + \lambda - n_w)$$

where x is suitably normalized. This completes the proof. □

Remark. From the above results, if G is an arbitrary unicyclic graph on n points different from C_n and $K_{1,n} + x$, then

$$\lambda_1(C_n) < \lambda_1(G) < \lambda_1(K_{1,n} + x).$$

The left inequality is well known (see [2], for example); the right one can be found in [1]. It is interesting to mention that the same conclusions holds if, instead of λ_1-ordering, we assume m-ordering (see [4]).

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